`qlanth`

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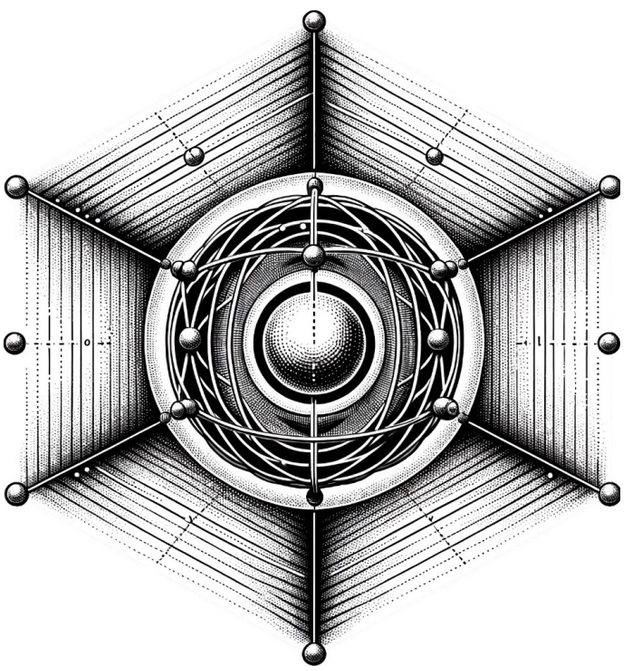

Juan David Lizarazo Ferro,
Christopher Dodson
& Rashid Zia

Brown University,
Department of Physics

Providence, Rhode Island
2024 AD

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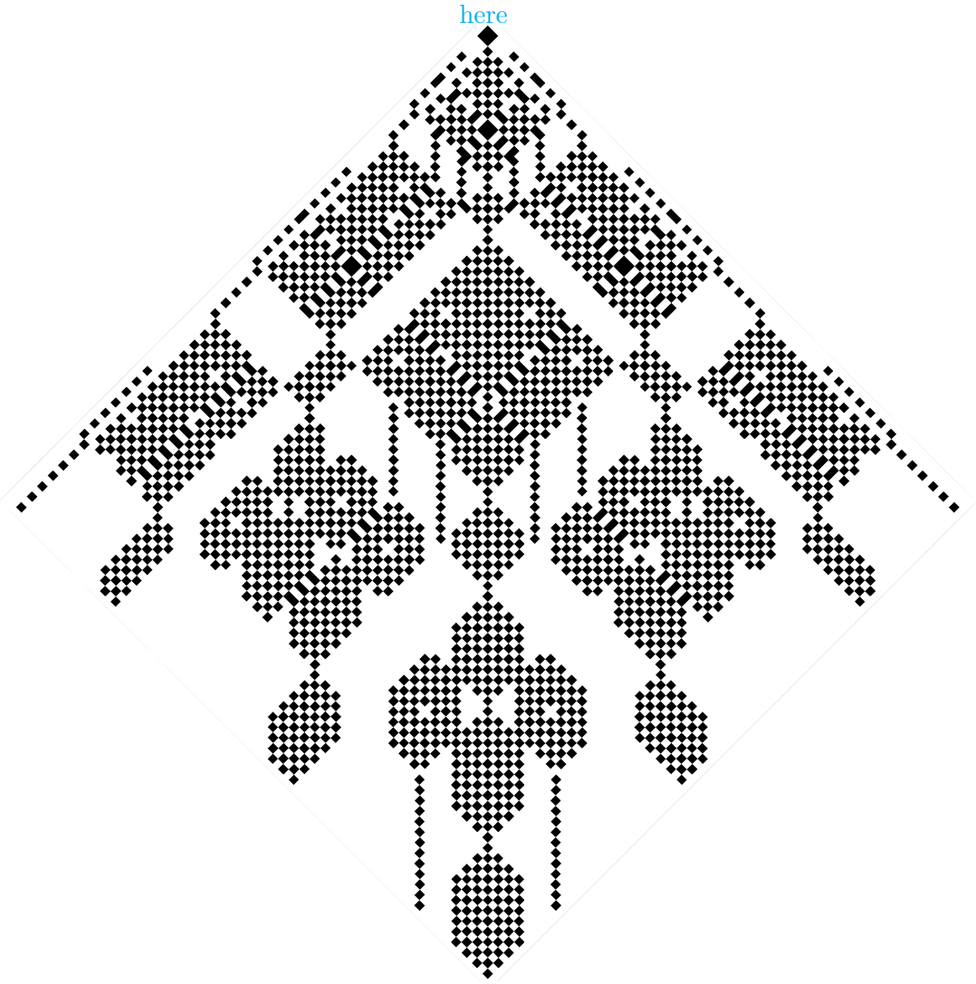

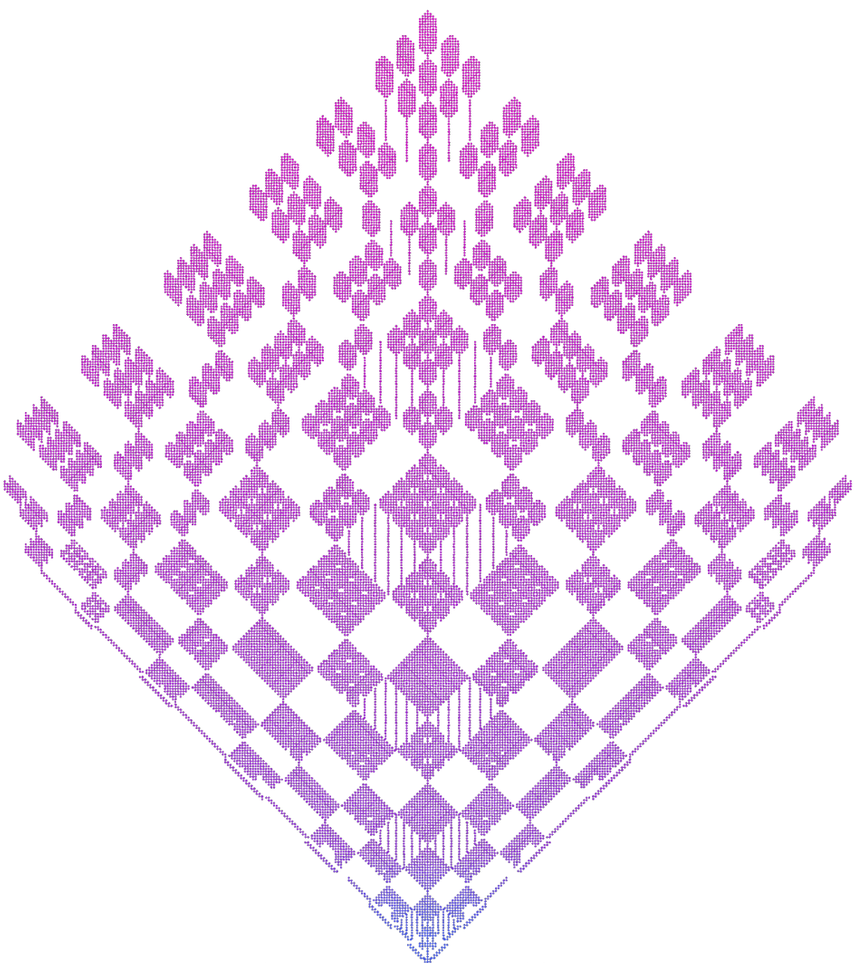

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qlanth is a tool that can be used to estimate the electronic structure of lanthanide ions in crystals. For this purpose it uses a single configuration description and a corresponding effective Hamiltonian. This Hamiltonian aims to describe the observed properties of ions embedded in solids in a picture that imagines them as free-ions modified by the influence of the lattice in which they find themselves in.

This picture of lanthanide ions is one that developed and mostly matured in the second half of the last century by the efforts of John Slater,[1] Giulio Racah,[2] Brian Judd,[3] Gerhard Dieke,[4] Hannah Crosswhite,[5] Robert Cowan,[6] Michael Reid,[7] William Carnall,[8] Clyde Morrison,[9] Richard Leavitt,[10] Brian Wybourne,[11] Richard Trees,[12] and Katherine Rajnak[13] among others. The goal of this tool is to provide a modern implementation of the methods that resulted from their work. This code is written in Wolfram language.

Separate to their specific use in this code, **qlanth** also includes data that might be of use to those interested in the single-configuration description of lanthanide ions. These data include the coefficients of fractional parentage (as calculated by Velkov and parsed here), and reduced matrix elements for all the operators in the effective Hamiltonian. These are provided as standard *Mathematica* associations that should be simple to use elsewhere. One feature of **qlanth** is that symbolic expressions are maintined up to the very last moment where numerical approximations are inevitable. As such, the symbolic expressions that result for the matrix representation of the Hamiltonian, result in linear combinations of the model parameters with symbolic coefficients.

The included *Mathematica* notebook `qlanth.nb` lists most of the functions included in **qlanth** and should be considered complementary to this document. The `/examples` folder includes notebooks containing the result of this description for most of the trivalent lanthanide ions in lanthanum fluoride. LaF_3 is remarkable in that it was one of the systems in which a systematic study [Car+89] of all of the trivalent lanthanide ions were studied.

This code was originally authored by Christopher Dodson and Rashid Zia for their research into magnetic dipole transitions in lanthanide ions [DZ12]. Here it has been rewritten and expanded by David Lizarazo. It has also benefited from conversations with Tharnier Puel at the University of Iowa.

This document has 17 sections. Section 1 gives an overview the semi-empirical Hamiltonian. Section 2 explains the details of the basis in which the semi-empirical Hamiltonian is evaluated, together with the method of fractional parentage, additional quantum numbers, Kramer's degeneracy, and the JJ' block structure of the semi-empirical Hamiltonian. Section 3 gives a detailed explanation of each of the interactions include in the semi-empirical Hamiltonian. Section 4 gives explains the implicit assumptions in the orientation of the coordinate system. Section 5 gives an overview of the attendant experimental setups and considerations about uncertainty. Section 6 is about the calculation of magnetic and forced electric dipole transitions. Section 7 explain certain constraints often used for the parameters in the semi-empirical Hamiltonian.

Section 8 explains the details of fitting the Hamiltonian to experimental data.Section 9 lists included auxiliary *Mathematica* notebooks. Section 11 explains the details of an abbreviated Python extension to **qlanth**. Section 12 explains some of the included experimental data. Section 13 contains a few assorted details on running **qlanth**. Section 14 has a brief comment on units. Section 15 and Section 16 include a summary of notation and definitions used throughout this document. Finally, Section 17 contains a printout of the code included in **qlanth**.

Besides being a fully functional code that works out of the box, **qlanth** is unique in that it also includes computational routines that can generate from scratch (or close to scratch) the necessary reduced matrix elements which in other codes are simply loaded from other vintages. Great care was taken to comment every loop, variable, procedure, and data provenance. To highlight this, the code relevant to the different functions has been interspersed in the parts where they are mentioned.

[1] [Sla29] [2] [Rac42a; Rac42b; Rac43; Rac49] [3] [Jud62; Jud63b; Jud63a; Jud66; Jud67; JCC68; CCJ68; Jud82; Jud83; JS84; JC84; Jud85; Jud86; Jud88; Jud89; JL93; Jud96; Jud05] [4] [DC63; PDC67; Die68] [5] [CCJ68; Cro71; Cro+76; Cro+77; DC63; JCC68; JC84] [6] [Cow81] [7] [Rei81] [8] [CFW65; Car+89; Car92; CFR68d; CFR68e; CFR68c; CFR68b; CFR68a; Car+70; Car+76; GW+91] [9] [MWK76; ML79; MW94; Mor80; MT87; MKW77b; MKW77a; ML82; Mor+83] [10] [Lea87; Lea82; LM80; ML79; ML82] [11] [CFW65; CW63; RW63; RW64b; RW64a; Wyb64a; Wyb64b; Wyb65; Wyb70; WS07] [12] [Tre52; Tre51; Tre58] [13] [RW63; RW64b; RW64a; Raj65]

Contents

1 The semi-empirical Hamiltonian

Electrons in a multi-electron ion are subject to a number of interactions. They are attracted to the nucleus about which they orbit. Being bundled together with other electrons, they experience repulsion from all of them. Having spin, they are also subject to various magnetic interactions. The spin of each electron interacts with the magnetic field generated by its own orbital angular momentum and of other electrons. And between pairs of electrons, the spin of one can influence the others spin through the interaction of their respective magnetic dipoles.

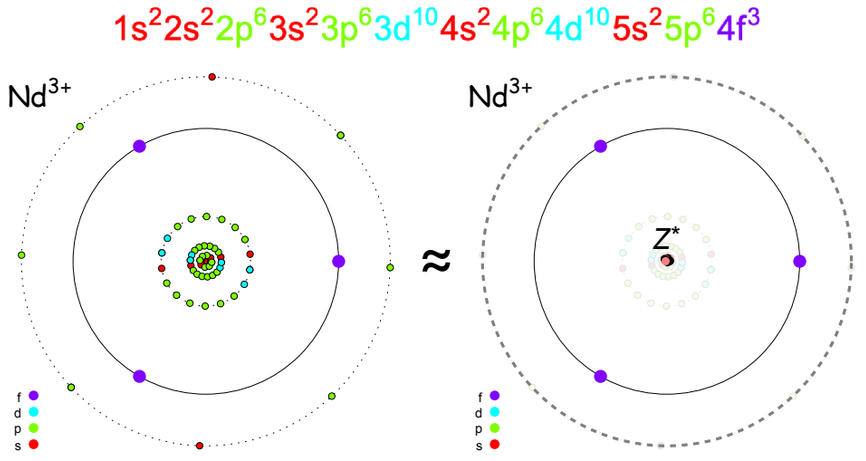

Figure 1: The trivalent neodymium ion shielded by $5s^2$ and $5p^6$ closed shells.

To describe the effect of the charges in the lattice surrounding the ion, the crystal field is introduced. In the simplest of embodiments, the crystal field is simply seen as the electrostatic field due to surrounding charges. This model is of limited applicability if taken too literally; however, if only symmetry considerations are assumed, the model is seen to have greater validity but a somewhat less clear physical origin.

The Hilbert space of a multi-electron ion is a vast stage. In principle, a basis for it should have a countable infinity of bound states and an uncountable infinity of unbound states. This is clearly too much to handle, but thankfully, this large stage can be put in some order thanks to the exclusion principle. The exclusion principle (together with that graceful tendency of things to drift downwards the energetic wells) provides the shell structure. This shell structure, in turn, makes it possible that an atom with many electrons, can be described effectively as an aggregate of an inert core, and a fewer active valence electrons.

Take for instance a triply ionized (or trivalent) neodymium atom, as depicted in Fig-1. In principle, this gives us the daunting task of dealing with the enormous Hilbert space of 57 electrons. However, 54 of them arrange themselves in a xenon core, so that we are only left to deal with only three. Three are still a challenging task, but much less so than 57. Furthermore, the exclusion principle also guides us in what type of orbital we could possibly place these three electrons, in the case of the lanthanide ions, this being the 4f orbitals. But not really, there are many more unoccupied orbitals outside of the xenon core, two of these electrons, if they are willing to pay the energetic price, they could find themselves in a 5d or a 6s orbital.

Here we shall assume a single-configuration description. Meaning that all the valence electrons in the ions that we study will all be considered to be located in f-orbitals, or what is the same, that they are described by $\underline{f}^n$ wavefunctions. Table 2 shows the (ground) configuration for the trivalent lanthanide ions. This is, however, a harsh approximation, but thankfully one can make some corrections to it. The effects that arise in the single configuration description because of omitting all the other possible orbitals where the

58	59	60	61	62	63	64	65	66	67	68	69	70
Ce^{3+}	Pr^{3+}	Nd^{3+}	Pm^{3+}	Sm^{3+}	Eu^{3+}	Gd^{3+}	Tb^{3+}	Dy^{3+}	Ho^{3+}	Er^{3+}	Tm^{3+}	Yb^{3+}
[Xe] f^1	[Xe] f^2	[Xe] f^3	[Xe] f^4	[Xe] f^5	[Xe] f^6	[Xe] f^7	[Xe] f^8	[Xe] f^9	[Xe] f^{10}	[Xe] f^{11}	[Xe] f^{12}	[Xe] f^{13}
Cerium	Praseodymium	Neodymium	Promethium	Samarium	Europium	Gadolinium	Terbium	Dysprosium	Holmium	Erbium	Thulium	Ytterbium

Figure 2: The trivalent lanthanide row and their ground configurations.

electrons might find themselves, this is what is called *configuration-interaction*.

These effects can be brought within the simplified description through perturbation theory. The task not the usual one of correcting for the energies/eigenvectors given an added perturbation, but rather to consider the effects of using a truncated Hilbert space due to a known interaction. For a detailed analysis of this, see Rudzikas' book [Rud07] on theoretical atomic spectroscopy or this article [Lin74] by Lindgren. What results from this analysis are operators that now act solely within the single configuration but with a coefficient that depends on overlap integrals between different configurations. It is from *configuration-interaction* that the parameters $\alpha, \beta, \gamma, P^{(k)}, T^{(k)}$ enter into the description.

$$\hat{\mathcal{H}} = \underbrace{\hat{\mathcal{H}}_{\text{k}}}_{\text{kinetic}} + \underbrace{\hat{\mathcal{H}}_{\text{e:sn}}}_{\text{e:shielded nuc}} + \overbrace{\underbrace{\hat{\mathcal{H}}_{\text{s:o}}}_{\text{spin-orbit}} + \underbrace{\hat{\mathcal{H}}_{\text{s:s}}}_{\substack{\text{spin:spin} \\ \text{and spin:other-orbit}}} + \underbrace{\hat{\mathcal{H}}_{\text{s:oo}\oplus\text{ecs:o}}}_{\substack{\text{spin:other-orbit} \\ \text{ec-correlated-spin:orbit}}} + \underbrace{\hat{\mathcal{H}}_{\text{Z}}}_{\text{Zeeman}}}^{\text{magnetic interactions}}$$
$$+ \overbrace{\underbrace{\hat{\mathcal{H}}_{\text{e:e}}}_{\text{e:e}} + \underbrace{\hat{\mathcal{H}}_{\mathcal{SO}(3)}}_{\text{Trees effective op}} + \underbrace{\hat{\mathcal{H}}_{\mathcal{G}_2}}_{\text{G}_2\text{ effective op}} + \underbrace{\hat{\mathcal{H}}_{\mathcal{SO}(7)}}_{\mathcal{SO}(7)\text{ effective op}} + \underbrace{\hat{\mathcal{H}}_{\text{Y}}}_{\substack{\text{effective} \\ \text{three-body}}} + \underbrace{\hat{\mathcal{H}}_{\text{cf}}}_{\text{crystal field}}}^{\text{electric interactions}} \tag{1}$$

$$\hat{\mathcal{H}}_{\text{k}} = -\frac{\hbar^2}{2m_e}\sum_{i=1}^{n}\nabla_i^2 \text{ (kinetic energy of } n \text{ valence electrons)} \tag{2}$$

$$\hat{\mathcal{H}}_{\text{e:sn}} = \sum_{i=1}^{n} V_{\text{sn}}(r_i) \text{ (valence-electrons interaction with shielded nuc. charge)} \tag{3}$$

$$\hat{\mathcal{H}}_{\text{s:o}} = \begin{cases} \sum_{i=1}^{n}\xi(r_i)\left(\hat{\underline{s}}_i\cdot\hat{\underline{\ell}}_i\right) & \text{with } \xi(r_i) = \frac{\hbar^2}{2m^2c^2r_i}\frac{\mathrm{d}V_{\text{sn}}(r_i)}{\mathrm{d}r_i} \\ \sum_{i=1}^{n}\zeta\left(\hat{\underline{s}}_i\cdot\hat{\underline{\ell}}_i\right) & \substack{\text{with } \zeta \text{ the radial average of } \xi(r_i) \\ \text{or used as phenomenological parameter}} \end{cases} \tag{4}$$

$$\hat{\mathcal{H}}_{\text{s:s}} = \sum_{k=0,2,4} m^{(k)}\hat{m}_k{}^{ss} \tag{5}$$

$$\hat{\mathcal{H}}_{\text{s:oo}\oplus\text{ecs:o}} = \sum_{k=2,4,6} P^{(k)}\hat{p}_k + \sum_{k=0,2,4} m^{(k)}\hat{m}_k \tag{6}$$

$$\hat{\mathcal{H}}_{\text{Z}} = -\vec{B}\cdot\hat{\mu} = \mu_B\vec{B}\cdot\left(\hat{L} + g_s\hat{S}\right) \text{ (interaction with a magnetic field)} \tag{7}$$

$$\hat{\mathcal{H}}_{\text{e:e}} = \sum_{i>j}^{n,n}\frac{e^2}{\|\vec{r}_i - \vec{r}_j\|} = \sum_{k=0,2,4,6} F^{(k)}\hat{f}_k \text{ (repulsion between valence electrons)} \tag{8}$$

Let $\hat{C}(\mathcal{G}) \coloneqq$ The Casimir operator of group $\mathcal{G}$.

$$\hat{\mathcal{H}}_{\mathcal{SO}(3)} = \alpha\,\hat{C}(\mathcal{SO}(3)) = \alpha\hat{L}^2 \text{ (Trees effective operator)} \tag{9}$$

$$\hat{\mathcal{H}}_{\mathcal{G}_2} = \beta\,\hat{C}(\mathcal{G}_2) \tag{10}$$

$$\hat{\mathcal{H}}_{\mathcal{SO}(7)} = \gamma\,\hat{C}(\mathcal{SO}(7)) \tag{11}$$

$$\hat{\mathcal{H}}_{\text{Y}} = T'^{(2)}\hat{t}_2{}' + T'^{(11)}\hat{t}_{11}{}' + \sum_{\substack{k=2,3,4,6,7,8, \\ 11,12,14,15, \\ 16,17,18,19}} T^{(k)}\hat{t}_k \text{ (effective 3-body int.)} \tag{12}$$

$$\hat{\mathcal{H}}_{\text{cf}} = \sum_{i=1}^{n} V_{\text{CF}}(\hat{r}_i) = \sum_{i=1}^{n}\sum_{k=2,4,6}\sum_{q=-k}^{k}\mathcal{B}_q^{(k)}\mathcal{C}_q^{(k)}(i) \quad \substack{\text{(crystal field interaction} \\ \text{with surroudings)}} \tag{13}$$

One could try to evaluate the coefficients that result in the Hamiltonian. However, within the **semi-empirical** approach, these parameters are left to be fitted against experimental data, or at times approximated through Hartree-Fock analysis. This approach is only *semi* empirical in the sense that the model parameters are fitted from experimental data, but the semi-empirical Hamiltonian that is fitted is based on a clear physical picture inherited from atomic physics.

Putting all of this together leads to the following effective Hamiltonian as show in &qn-1, where "v-electrons" is shorthand for valence electrons. It is important to note that the eigenstates that we'll end up with have shoved under the rug all the radial dependence of the wavefunctions. This dependence having been integrated in the parameters of the effective Hamiltonian. The resulting wavefunctions being solely concerned with the angular

dependence of the wavefunctions, but modulated by the effects of the radial dependence.

Once all the parameters in this semi-empirical Hamiltonian have been fitted to experimental datal what results is a Hamiltonian such as the one for Pr^{3+} in LaF_3 shown in Fig-3. Before we go on to explain in some detail each of the terms included in this Hamiltonian, let us continue to explain the basis used in calculations.

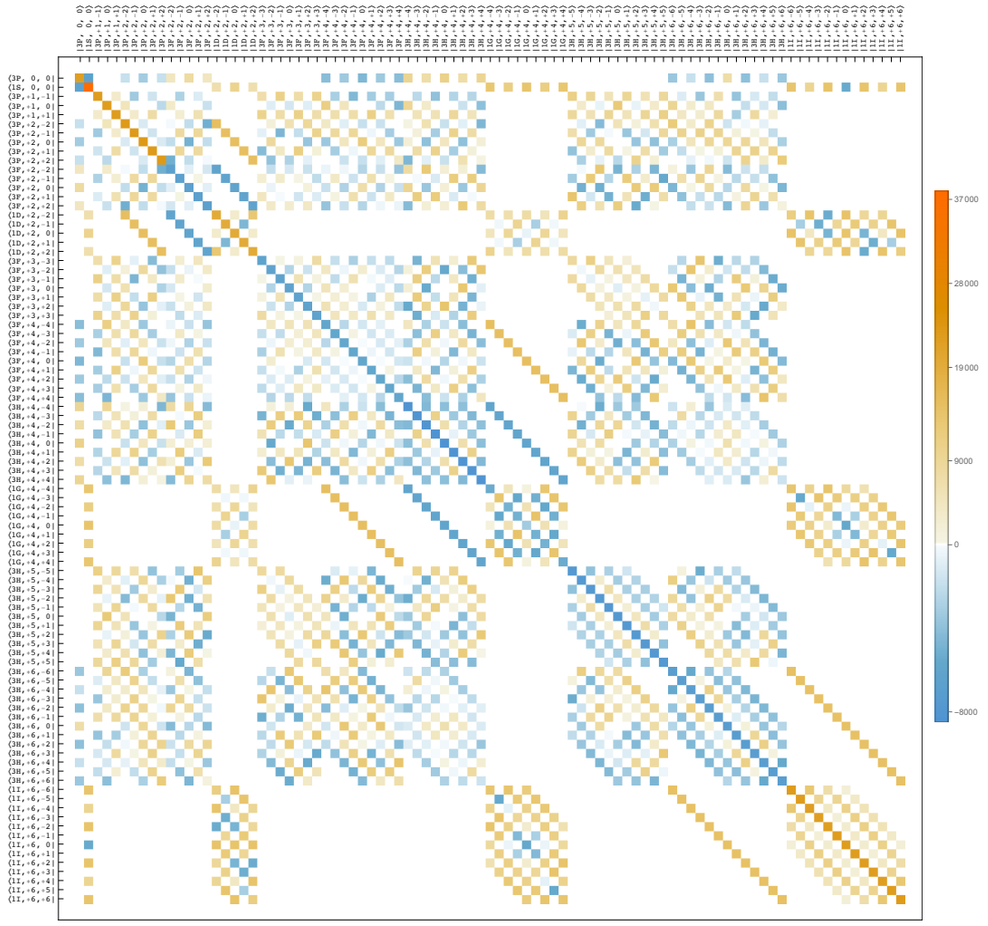

Figure 3: The matrix representation of $\hat{\mathcal{H}}$ for Pr^{3+} in LaF_3 in the $|LSJM_J\rangle$ basis.

2 LS coupling basis

In choosing a coupling scheme (or equivalently, choosing a basis in which to represent the Hamiltonian), there are a myriad options; all of them legitimate in their own right. The art of choosing a useful coupling scheme is that of proposing a basis for the angular part of the wavefunctions that will be close to the actual eigenstates of the system. It being necessary to calculate the matrix elements of the relevant operators, choosing a coupling scheme may also be justified by the easy by which these can be calculated.

qlanth uses LS coupling for its calculations. In LS coupling all the orbital angular momenta are added to form the total orbital angular momentum L, all the spin angular momenta are added to form the total spin angular momentum S, and finally these two angular momenta are then added together to form the total angular momentum J. The exclusion principle is taken into account in limiting the possible LS terms, and demands no further restrictions. Finally this total angular momentum J is complemented with the quantum number[14] M_J describing the projection of J along the z-axis.

It is worthwhile remembering here the spectroscopic hierarchy of descriptive elements: **terms** correspond to $|LS\rangle$ (also noted as $^{2S+1}\mathrm{L}$), **levels** correspond to $|LSJ\rangle$ (also noted as $^{2S+1}\mathrm{L}_J$), and **states** correspond to $|LSJM_J\rangle$ (also noted as $^{2S+1}\mathrm{L}_{J,M_J}$). Fig-4 shows an example of the relationship between a term and its associated levels and states.

In principle the $|LSJM_J\rangle$ description is the primordial one, the $|LSJ\rangle$ resulting from neglecting all parts of the Hamiltonian that have no spherical symmetry, and the $|LS\rangle$

[14] A *good* quantum number is any eigenvalue of an operator that commutes with the Hamiltonian; in other words, they are conserved quantities.

resulting from further neglecting all terms that couple the spin and orbital angular momenta. Note that a *state* is not an *eigen*-state; all of these are assumed to be basis vectors in the type of description attached to them.

Whereas all four quantum numbers $|LSJM_J\rangle$ are required to specify a state, one may, however, use two simpler descriptions as the situation merits. When all the parts of the Hamiltonian without spherical symmetry are excluded, then a description in terms of $|LSJ\rangle$ levels is sufficient, the M_J quantum numbers being redundant and with J being a good quantum number. In a second scenario, when in addition to neglecting all parts without spherical symmetry, one also neglects all parts of the Hamiltonian that couple the spin and orbital degrees of freedom, then the $|LS\rangle$ terms constitute the most parsimonious description, with L and S being separately conserved quantities.

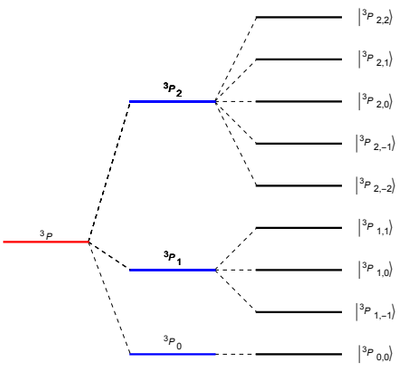

Figure 4: Levels and states associated with the ^3P term in $\underline{\mathrm{f}}^2$.

When a certain level of description has been adopted one can then assume (at one's own peril) that single states, levels, or terms are actual *eigen*-states/levels/terms of the system at hand. This assumption results in simple transition rules between states/levels/terms. One may, however, within each level of description, take an alternate route, the *intermediate coupling* route, of seeing how the different states/levels/terms mix in the eigenstates found by diagonalizing the appropriate Hamiltonian. This results in a more detailed description at the cost of increased complexity.

2.1 $|LSJM_J\rangle$ states

The basis vectors of the $|LSJM_J\rangle$ basis are common eigenvectors of the operators $\hat{L}^2$, $\hat{S}^2$, $\hat{J}^2$, and $\hat{J}_z$. They are formed starting from the allowed LS terms in a given configuration, and are then completed with attendant J and M_J quantum numbers. The LS terms allowed in each configuration $\underline{\mathrm{f}}^n$ are obtained from tables that originate from the original work by Nielson and Koster [NK63]. In **qlanth** these terms are parsed from the file `B1F_-ALL.TXT` which is part of the doctoral research of Dobromir Velkov (under the advisory of Brian Judd) [Vel00] in which he calculated anew the coefficients of fractional parentage.

One of the facts that have to be accounted for in a basis that uses L and S as quantum numbers, is that there might be several linearly independent paths to couple the electron spin and orbital momenta to add up to given total L and total S. For this reason additional labels are necessary to distinguish between these different terms. The simplest way of doing this dates back to the tables of Nielson and Koster [NK63], and consists in assigning consecutive integers to degenerate LS terms, with no further meaning to these integers, except that of discriminating between degenerate terms.

The following are all the LS terms in the $\underline{\mathrm{f}}^n$ configurations. In the notation used, the superscript index before the letter notes the spin multiplicity $2S+1$, the roman letter indicates the value of L in spectroscopic notation ($S\to1, P\to2, D\to3, F\to4, G\to5, H\to6, I\to7, K\to8, L\to9, M\to10, N\to11, O\to12, Q\to3, R\to14, T\to15, U\to16, V\to17$), and the final integer (if present) is the label that discriminates between several degenerate LS and must not be confused with a value of J. This last index we frequently label in the equations contained in this document with the greek letter α (sadly, for historical reasons, we prepend it, rather than append it).

$\underline{\mathrm{f}}^0$ (1 LS term)
^{1}S

$\underline{\mathrm{f}}^1$ (1 LS term)
^{2}F

$\underline{f}^2$
(7 LS terms)

---

^{3}P, ^{3}F, ^{3}H, ^{1}S, ^{1}D, ^{1}G, ^{1}I

$\underline{f}^3$
(17 LS terms)

---

^{4}S, ^{4}D, ^{4}F, ^{4}G, ^{4}I, ^{2}P, ^{2}D1, ^{2}D2, ^{2}F1, ^{2}F2, ^{2}G1, ^{2}G2, ^{2}H1, ^{2}H2, ^{2}I, ^{2}K, ^{2}L

$\underline{f}^4$
(47 LS terms)

---

^{5}S, ^{5}D, ^{5}F, ^{5}G, ^{5}I, ^{3}P1, ^{3}P2, ^{3}P3, ^{3}D1, ^{3}D2, ^{3}F1, ^{3}F2, ^{3}F3, ^{3}F4, ^{3}G1, ^{3}G2, ^{3}G3, ^{3}H1, ^{3}H2, ^{3}H3, ^{3}H4, ^{3}I1, ^{3}I2, ^{3}K1, ^{3}K2, ^{3}L, ^{3}M, ^{1}S1, ^{1}S2, ^{1}D1, ^{1}D2, ^{1}D3, ^{1}D4, ^{1}F, ^{1}G1, ^{1}G2, ^{1}G3, ^{1}G4, ^{1}H1, ^{1}H2, ^{1}I1, ^{1}I2, ^{1}I3, ^{1}K, ^{1}L1, ^{1}L2, ^{1}N

$\underline{f}^5$
(73 LS terms)

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^{6}P, ^{6}F, ^{6}H, ^{4}S, ^{4}P1, ^{4}P2, ^{4}D1, ^{4}D2, ^{4}D3, ^{4}F1, ^{4}F2, ^{4}F3, ^{4}F4, ^{4}G1, ^{4}G2, ^{4}G3, ^{4}G4, ^{4}H1, ^{4}H2, ^{4}H3, ^{4}I1, ^{4}I2, ^{4}I3, ^{4}K1, ^{4}K2, ^{4}L, ^{4}M, ^{2}P1, ^{2}P2, ^{2}P3, ^{2}P4, ^{2}D1, ^{2}D2, ^{2}D3, ^{2}D4, ^{2}D5, ^{2}F1, ^{2}F2, ^{2}F3, ^{2}F4, ^{2}F5, ^{2}F6, ^{2}F7, ^{2}G1, ^{2}G2, ^{2}G3, ^{2}G4, ^{2}G5, ^{2}G6, ^{2}H1, ^{2}H2, ^{2}H3, ^{2}H4, ^{2}H5, ^{2}H6, ^{2}H7, ^{2}I1, ^{2}I2, ^{2}I3, ^{2}I4, ^{2}I5, ^{2}K1, ^{2}K2, ^{2}K3, ^{2}K4, ^{2}K5, ^{2}L1, ^{2}L2, ^{2}L3, ^{2}M1, ^{2}M2, ^{2}N, ^{2}O

$\underline{f}^6$
(119 LS terms)

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^{7}F, ^{5}S, ^{5}P, ^{5}D1, ^{5}D2, ^{5}D3, ^{5}F1, ^{5}F2, ^{5}G1, ^{5}G2, ^{5}G3, ^{5}H1, ^{5}H2, ^{5}I1, ^{5}I2, ^{5}K, ^{5}L, ^{3}P1, ^{3}P2, ^{3}P3, ^{3}P4, ^{3}P5, ^{3}P6, ^{3}D1, ^{3}D2, ^{3}D3, ^{3}D4, ^{3}D5, ^{3}F1, ^{3}F2, ^{3}F3, ^{3}F4, ^{3}F5, ^{3}F6, ^{3}F7, ^{3}F8, ^{3}F9, ^{3}G1, ^{3}G2, ^{3}G3, ^{3}G4, ^{3}G5, ^{3}G6, ^{3}G7, ^{3}H1, ^{3}H2, ^{3}H3, ^{3}H4, ^{3}H5, ^{3}H6, ^{3}H7, ^{3}H8, ^{3}H9, ^{3}I1, ^{3}I2, ^{3}I3, ^{3}I4, ^{3}I5, ^{3}I6, ^{3}K1, ^{3}K2, ^{3}K3, ^{3}K4, ^{3}K5, ^{3}K6, ^{3}L1, ^{3}L2, ^{3}L3, ^{3}M1, ^{3}M2, ^{3}M3, ^{3}N, ^{3}O, ^{1}S1, ^{1}S2, ^{1}S3, ^{1}S4, ^{1}P, ^{1}D1, ^{1}D2, ^{1}D3, ^{1}D4, ^{1}D5, ^{1}D6, ^{1}F1, ^{1}F2, ^{1}F3, ^{1}F4, ^{1}G1, ^{1}G2, ^{1}G3, ^{1}G4, ^{1}G5, ^{1}G6, ^{1}G7, ^{1}G8, ^{1}H1, ^{1}H2, ^{1}H3, ^{1}H4, ^{1}I1, ^{1}I2, ^{1}I3, ^{1}I4, ^{1}I5, ^{1}I6, ^{1}I7, ^{1}K1, ^{1}K2, ^{1}K3, ^{1}L1, ^{1}L2, ^{1}L3, ^{1}L4, ^{1}M1, ^{1}M2, ^{1}N1, ^{1}N2, ^{1}Q

$\underline{f}^7$
(119 LS terms)

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^{8}S, ^{6}P, ^{6}D, ^{6}F, ^{6}G, ^{6}H, ^{6}I, ^{4}S1, ^{4}S2, ^{4}P1, ^{4}P2, ^{4}D1, ^{4}D2, ^{4}D3, ^{4}D4, ^{4}D5, ^{4}D6, ^{4}F1, ^{4}F2, ^{4}F3, ^{4}F4, ^{4}F5, ^{4}G1, ^{4}G2, ^{4}G3, ^{4}G4, ^{4}G5, ^{4}G6, ^{4}G7, ^{4}H1, ^{4}H2, ^{4}H3, ^{4}H4, ^{4}H5, ^{4}I1, ^{4}I2, ^{4}I3, ^{4}I4, ^{4}I5, ^{4}K1, ^{4}K2, ^{4}K3, ^{4}L1, ^{4}L2, ^{4}L3, ^{4}M, ^{4}N, ^{2}S1, ^{2}S2, ^{2}P1, ^{2}P2, ^{2}P3, ^{2}P4, ^{2}P5, ^{2}D1, ^{2}D2, ^{2}D3, ^{2}D4, ^{2}D5, ^{2}D6, ^{2}D7, ^{2}F1, ^{2}F2, ^{2}F3, ^{2}F4, ^{2}F5, ^{2}F6, ^{2}F7, ^{2}F8, ^{2}F9, ^{2}F10, ^{2}G1, ^{2}G2, ^{2}G3, ^{2}G4, ^{2}G5, ^{2}G6, ^{2}G7, ^{2}G8, ^{2}G9, ^{2}G10, ^{2}H1, ^{2}H2, ^{2}H3, ^{2}H4, ^{2}H5, ^{2}H6, ^{2}H7, ^{2}H8, ^{2}H9, ^{2}I1, ^{2}I2, ^{2}I3, ^{2}I4, ^{2}I5, ^{2}I6, ^{2}I7, ^{2}I8, ^{2}I9, ^{2}K1, ^{2}K2, ^{2}K3, ^{2}K4, ^{2}K5, ^{2}K6, ^{2}K7, ^{2}L1, ^{2}L2, ^{2}L3, ^{2}L4, ^{2}L5, ^{2}M1, ^{2}M2, ^{2}M3, ^{2}M4, ^{2}N1, ^{2}N2, ^{2}O, ^{2}Q

$\underline{f}^8$
(119 LS terms)

---

^{7}F, ^{5}S, ^{5}P, ^{5}D1, ^{5}D2, ^{5}D3, ^{5}F1, ^{5}F2, ^{5}G1, ^{5}G2, ^{5}G3, ^{5}H1, ^{5}H2, ^{5}I1, ^{5}I2, ^{5}K, ^{5}L, ^{3}P1, ^{3}P2, ^{3}P3, ^{3}P4, ^{3}P5, ^{3}P6, ^{3}D1, ^{3}D2, ^{3}D3, ^{3}D4, ^{3}D5, ^{3}F1, ^{3}F2, ^{3}F3, ^{3}F4, ^{3}F5, ^{3}F6, ^{3}F7, ^{3}F8, ^{3}F9, ^{3}G1, ^{3}G2, ^{3}G3, ^{3}G4, ^{3}G5, ^{3}G6, ^{3}G7, ^{3}H1, ^{3}H2, ^{3}H3, ^{3}H4, ^{3}H5, ^{3}H6, ^{3}H7, ^{3}H8, ^{3}H9, ^{3}I1, ^{3}I2, ^{3}I3, ^{3}I4, ^{3}I5, ^{3}I6, ^{3}K1, ^{3}K2, ^{3}K3, ^{3}K4, ^{3}K5, ^{3}K6, ^{3}L1, ^{3}L2, ^{3}L3, ^{3}M1, ^{3}M2, ^{3}M3, ^{3}N, ^{3}O, ^{1}S1, ^{1}S2, ^{1}S3, ^{1}S4, ^{1}P, ^{1}D1, ^{1}D2, ^{1}D3, ^{1}D4, ^{1}D5, ^{1}D6, ^{1}F1, ^{1}F2, ^{1}F3, ^{1}F4,

^{1}G1, ^{1}G2, ^{1}G3, ^{1}G4, ^{1}G5, ^{1}G6, ^{1}G7, ^{1}G8, ^{1}H1, ^{1}H2, ^{1}H3, ^{1}H4, ^{1}I1, ^{1}I2, ^{1}I3, ^{1}I4, ^{1}I5, ^{1}I6, ^{1}I7, ^{1}K1, ^{1}K2, ^{1}K3, ^{1}L1, ^{1}L2, ^{1}L3, ^{1}L4, ^{1}M1, ^{1}M2, ^{1}N1, ^{1}N2, ^{1}Q

$\underline{\mathrm{f}}^9$ (73 LS terms)
^{6}P, ^{6}F, ^{6}H, ^{4}S, ^{4}P1, ^{4}P2, ^{4}D1, ^{4}D2, ^{4}D3, ^{4}F1, ^{4}F2, ^{4}F3, ^{4}F4, ^{4}G1, ^{4}G2, ^{4}G3, ^{4}G4, ^{4}H1, ^{4}H2, ^{4}H3, ^{4}I1, ^{4}I2, ^{4}I3, ^{4}K1, ^{4}K2, ^{4}L, ^{4}M, ^{2}P1, ^{2}P2, ^{2}P3, ^{2}P4, ^{2}D1, ^{2}D2, ^{2}D3, ^{2}D4, ^{2}D5, ^{2}F1, ^{2}F2, ^{2}F3, ^{2}F4, ^{2}F5, ^{2}F6, ^{2}F7, ^{2}G1, ^{2}G2, ^{2}G3, ^{2}G4, ^{2}G5, ^{2}G6, ^{2}H1, ^{2}H2, ^{2}H3, ^{2}H4, ^{2}H5, ^{2}H6, ^{2}H7, ^{2}I1, ^{2}I2, ^{2}I3, ^{2}I4, ^{2}I5, ^{2}K1, ^{2}K2, ^{2}K3, ^{2}K4, ^{2}K5, ^{2}L1, ^{2}L2, ^{2}L3, ^{2}M1, ^{2}M2, ^{2}N, ^{2}O

$\underline{\mathrm{f}}^{10}$ (47 LS terms)
^{5}S, ^{5}D, ^{5}F, ^{5}G, ^{5}I, ^{3}P1, ^{3}P2, ^{3}P3, ^{3}D1, ^{3}D2, ^{3}F1, ^{3}F2, ^{3}F3, ^{3}F4, ^{3}G1, ^{3}G2, ^{3}G3, ^{3}H1, ^{3}H2, ^{3}H3, ^{3}H4, ^{3}I1, ^{3}I2, ^{3}K1, ^{3}K2, ^{3}L, ^{3}M, ^{1}S1, ^{1}S2, ^{1}D1, ^{1}D2, ^{1}D3, ^{1}D4, ^{1}F, ^{1}G1, ^{1}G2, ^{1}G3, ^{1}G4, ^{1}H1, ^{1}H2, ^{1}I1, ^{1}I2, ^{1}I3, ^{1}K, ^{1}L1, ^{1}L2, ^{1}N

$\underline{\mathrm{f}}^{11}$ (17 LS terms)
^{4}S, ^{4}D, ^{4}F, ^{4}G, ^{4}I, ^{2}P, ^{2}D1, ^{2}D2, ^{2}F1, ^{2}F2, ^{2}G1, ^{2}G2, ^{2}H1, ^{2}H2, ^{2}I, ^{2}K, ^{2}L

$\underline{\mathrm{f}}^{12}$ (7 LS terms)
^{3}P, ^{3}F, ^{3}H, ^{1}S, ^{1}D, ^{1}G, ^{1}I

$\underline{\mathrm{f}}^{13}$ (1 LS term)
^{2}F

$\underline{\mathrm{f}}^{14}$ (1 LS term)
^{1}S

In **qlanth** these terms may be queried through the function `AllowedNKSLTerms`.

```
AllowedNKSLTerms::usage = "AllowedNKSLTerms[numE] returns a list with
    the allowed terms in the f^numE configuration, the terms are
   given as strings in spectroscopic notation. The integers in the
   last positions are used to distinguish cases with degeneracy.";
AllowedNKSLTerms[numE_] := Map[First, CFPTerms[Min[numE, 14-numE]]];
AllowedNKSLTerms[0]  = {"1S"};
AllowedNKSLTerms[14] = {"1S"};
```

In addition to LS, the $|LSJM_J\rangle$ basis states are also specified by the total angular momentum J (which may go from $|L-S|$ to $|L+S|$). Then for each J, there are $2J+1$ projections on the z-axis. For example, the ordered $|LSJM_J\rangle$ basis for $\underline{\mathrm{f}}^2$ is shown below, where the first element is the LS term given as a string, the second equal to J, and the third one equal to M_J:

$(J=0)$ (2 states)
$\lvert^3\mathrm{P}_{0,0}\rangle$, $\lvert^1\mathrm{S}_{0,0}\rangle$

$(J = 1)$
(3 states)

$|^3\mathrm{P}_{1,-1}\rangle$, $|^3\mathrm{P}_{1,0}\rangle$, $|^3\mathrm{P}_{1,1}\rangle$

$(J = 2)$
(15 states)

$|^3\mathrm{P}_{2,-2}\rangle$, $|^3\mathrm{P}_{2,-1}\rangle$, $|^3\mathrm{P}_{2,0}\rangle$, $|^3\mathrm{P}_{2,1}\rangle$, $|^3\mathrm{P}_{2,2}\rangle$, $|^3\mathrm{F}_{2,-2}\rangle$, $|^3\mathrm{F}_{2,-1}\rangle$, $|^3\mathrm{F}_{2,0}\rangle$, $|^3\mathrm{F}_{2,1}\rangle$, $|^3\mathrm{F}_{2,2}\rangle$, $|^1\mathrm{D}_{2,-2}\rangle$, $|^1\mathrm{D}_{2,-1}\rangle$, $|^1\mathrm{D}_{2,0}\rangle$, $|^1\mathrm{D}_{2,1}\rangle$, $|^1\mathrm{D}_{2,2}\rangle$

$(J = 3)$
(7 states)

$|^3\mathrm{F}_{3,-3}\rangle$, $|^3\mathrm{F}_{3,-2}\rangle$, $|^3\mathrm{F}_{3,-1}\rangle$, $|^3\mathrm{F}_{3,0}\rangle$, $|^3\mathrm{F}_{3,1}\rangle$, $|^3\mathrm{F}_{3,2}\rangle$, $|^3\mathrm{F}_{3,3}\rangle$

$(J = 4)$
(27 states)

$|^3\mathrm{F}_{4,-4}\rangle$, $|^3\mathrm{F}_{4,-3}\rangle$, $|^3\mathrm{F}_{4,-2}\rangle$, $|^3\mathrm{F}_{4,-1}\rangle$, $|^3\mathrm{F}_{4,0}\rangle$, $|^3\mathrm{F}_{4,1}\rangle$, $|^3\mathrm{F}_{4,2}\rangle$, $|^3\mathrm{F}_{4,3}\rangle$, $|^3\mathrm{F}_{4,4}\rangle$, $|^3\mathrm{H}_{4,-4}\rangle$, $|^3\mathrm{H}_{4,-3}\rangle$, $|^3\mathrm{H}_{4,-2}\rangle$, $|^3\mathrm{H}_{4,-1}\rangle$, $|^3\mathrm{H}_{4,0}\rangle$, $|^3\mathrm{H}_{4,1}\rangle$, $|^3\mathrm{H}_{4,2}\rangle$, $|^3\mathrm{H}_{4,3}\rangle$, $|^3\mathrm{H}_{4,4}\rangle$, $|^1\mathrm{G}_{4,-4}\rangle$, $|^1\mathrm{G}_{4,-3}\rangle$, $|^1\mathrm{G}_{4,-2}\rangle$, $|^1\mathrm{G}_{4,-1}\rangle$, $|^1\mathrm{G}_{4,0}\rangle$, $|^1\mathrm{G}_{4,1}\rangle$, $|^1\mathrm{G}_{4,2}\rangle$, $|^1\mathrm{G}_{4,3}\rangle$, $|^1\mathrm{G}_{4,4}\rangle$

$(J = 5)$
(11 states)

$|^3\mathrm{H}_{5,-5}\rangle$, $|^3\mathrm{H}_{5,-4}\rangle$, $|^3\mathrm{H}_{5,-3}\rangle$, $|^3\mathrm{H}_{5,-2}\rangle$, $|^3\mathrm{H}_{5,-1}\rangle$, $|^3\mathrm{H}_{5,0}\rangle$, $|^3\mathrm{H}_{5,1}\rangle$, $|^3\mathrm{H}_{5,2}\rangle$, $|^3\mathrm{H}_{5,3}\rangle$, $|^3\mathrm{H}_{5,4}\rangle$, $|^3\mathrm{H}_{5,5}\rangle$

$(J = 6)$
(26 states)

$|^3\mathrm{H}_{6,-6}\rangle$, $|^3\mathrm{H}_{6,-5}\rangle$, $|^3\mathrm{H}_{6,-4}\rangle$, $|^3\mathrm{H}_{6,-3}\rangle$, $|^3\mathrm{H}_{6,-2}\rangle$, $|^3\mathrm{H}_{6,-1}\rangle$, $|^3\mathrm{H}_{6,0}\rangle$, $|^3\mathrm{H}_{6,1}\rangle$, $|^3\mathrm{H}_{6,2}\rangle$, $|^3\mathrm{H}_{6,3}\rangle$, $|^3\mathrm{H}_{6,4}\rangle$, $|^3\mathrm{H}_{6,5}\rangle$, $|^3\mathrm{H}_{6,6}\rangle$, $|^1\mathrm{I}_{6,-6}\rangle$, $|^1\mathrm{I}_{6,-5}\rangle$, $|^1\mathrm{I}_{6,-4}\rangle$, $|^1\mathrm{I}_{6,-3}\rangle$, $|^1\mathrm{I}_{6,-2}\rangle$, $|^1\mathrm{I}_{6,-1}\rangle$, $|^1\mathrm{I}_{6,0}\rangle$, $|^1\mathrm{I}_{6,1}\rangle$, $|^1\mathrm{I}_{6,2}\rangle$, $|^1\mathrm{I}_{6,3}\rangle$, $|^1\mathrm{I}_{6,4}\rangle$, $|^1\mathrm{I}_{6,5}\rangle$, $|^1\mathrm{I}_{6,6}\rangle$

The order above is an example of the bases ordering used in **qlanth**. Notice how the basis vectors are sorted in order of increasing J, so that for instance not all of the basis states associated with the ^{3}P LS term are contiguous. Within each group for a given J the basis kets are then ordered in decreasing S, then ordered in increasing L, and then according to M_J.

In **qlanth** the ordered basis used for a given $\underline{\mathrm{f}}^n$ is provided by `BasisLSJMJ` which provides a list with $\binom{14}{n}$ elements.

```
BasisLSJMJ::usage = "BasisLSJMJ[numE] returns the ordered basis in L-S-J-MJ with the total orbital angular momentum L and total spin angular momentum S coupled together to form J. The function returns a list with each element representing the quantum numbers for each basis vector. Each element is of the form {SL (string in spectroscopic notation),J, MJ}.
The option ''AsAssociation'' can be set to True to return the basis as an association with the keys corresponding to values of J and the values lists with the corresponding {L, S, J, MJ} list. The default of this option is False.
";
Options[BasisLSJMJ] = {"AsAssociation" -> False};
BasisLSJMJ[numE_, OptionsPattern[]] := Module[
  {energyStatesTable, basis, idx1},
  (
    energyStatesTable = BasisTableGenerator[numE];
```

```
    basis = Table[
      energyStatesTable[{numE, AllowedJ[numE][[idx1]]}],
      {idx1, 1, Length[AllowedJ[numE]]}];
    basis = Flatten[basis, 1];
    If[OptionValue["AsAssociation"],
      (
        Js    = AllowedJ[numE];
        basis = Table[(J -> Select[basis, #[[2]] == J &]), {J, Js}];
        basis = Association[basis];
      )
    ];
    Return[basis]
  )
];
```

2.2 More quantum numbers

Besides using an integer which solves the problem of discriminating between degenerate LS terms by enumerating them, it is also possible to add more useful labels that reflect additional symmetries that the f-electron basis states have in the groups $\mathcal{SO}(7)$ (the Lie group of rotations in seven dimensions) and $\mathcal{G}_2$ (the rank-2 exceptional simple Lie group).

2.2.1 Seniority ν

The seniority number connects different LS terms between configurations, so that a term below can be seen as the *senior* of a term above. To determine the seniority of a given term in configuration $\underline{\mathrm{f}}^n$, one must first find the configuration $\underline{\mathrm{f}}^{\tilde{n}}$ in which this term appeared. For example, $\underline{\mathrm{f}}^5$ contains six degenerate ${}^2G$ terms. The first time this term appeared was in $\underline{\mathrm{f}}^3$, where it had a degeneracy of 2. The 2 degenerate terms in $\underline{\mathrm{f}}^3$ would then both have a seniority of $\boldsymbol{\nu} = 3$ since they first appeared in $\underline{\mathrm{f}}^3$. In consequence two of the six degenerate terms in $\underline{\mathrm{f}}^5$ would have the same degeneracy those two in $\underline{\mathrm{f}}^3$, and are therefore linked to those previous two. The four remaining ones, are considered to be *born* in $\underline{\mathrm{f}}^5$, and therefore have a seniority $\boldsymbol{\nu} = 5$.

These rules seem to be ad-hoc, but they are useful in dealing with the degeneracies in the LS terms as they arrive going up the configurations. It provides a useful way of tracking what happens to each *branch* of the coupling tree as it grows and withers with increasing number of electrons.

There is, however, a deeper meaning to the seniority number. It can be shown that the seniority number (more exactly a quantity related to it) is a sort of spin, a *quasi*-spin, where the spin projections along the 'z-axis' correspond to different number of electrons in $\underline{\mathrm{f}}^n$ configurations [Jud67]. This is a consequence of the exclusion principle. It is also useful to relate matrix elements of operators in one configuration to those in another, through the use of the Wigner-Eckart theorem. This is an interesting and useful theoretical construct, but the method of fractional parentage (which is what is implemented in **qlanth**) is equally adequate, albeit being somewhat less parsimonious than what the quasi-spin view that seniority can provide. As such **qlanth** does not use the seniority numbers that are associated with each LS term[15]. However, in **qlanth** the seniority of a given LS term can be obtained using the function `Seniority`.

```
Seniority::usage = "Seniority[LS] returns the seniority of the given
    term.";
Seniority[LS_] := FindNKLSTerm[LS][[1, 2]];
```

2.2.2 $\mathcal{U}$ and $\mathcal{W}$

Much as L tells us how a rotation acts on an L wavefunction by mixing different M_L components, these other two quantum numbers specify how the wavefunctions transform under the operations of two other two groups. The $\mathcal{W}$ label determines how a wavefunction transforms under a rotation in 7-dimensional space, and $\mathcal{U}$ how they transform under an operator of group $\mathcal{G}_2$. Without going into the group theoretical details, the irreducible representations of $\mathcal{SO}(7)$ can be represented by triples of integer numbers, and those of $\mathcal{G}_2$ as pairs of two integers.

[15] Except for calculating the coefficients of fractional parentage beyond $\underline{\mathrm{f}}^7$, which are useful, but not essential to the calculations of **qlanth**.

In **qlanth** the $\mathcal{W}$ and $\mathcal{U}$ are used in order to determine the matrix elements of the $\hat{\mathcal{C}}(\mathcal{SO}(7))$ and $\hat{\mathcal{C}}(\mathcal{G}_2)$ Casimir operators. These labels can be retrieved, for a given LS string, using the function FindNKLSTerm.

```
FindNKLSTerm::usage = "Given the string LS FindNKLSTerm[SL] returns
    all the terms that are compatible with it. This is only for f^n
    configurations. The provided terms might belong to more than one
    configuration. The function returns a list with elements of the
    form {LS, seniority, W, U}.";
FindNKLSTerm[SL_] := Module[
  {NKterms, n},
  (
    n = 7;
    NKterms = {{}};
    Map[
      If[! StringFreeQ[First[#], SL],
        If[ToExpression[Part[#, 2]] <= n,
          NKterms = Join[NKterms, {#}, 1]
        ]
      ] &,
    fnTermLabels
    ];
    NKterms = DeleteCases[NKterms, {}];
    NKterms
  )
];
```

2.3 $|LSJ\rangle$ levels

When the Hamiltonian only includes spherically symmetric terms (or what is the same, when the crystal field is neglected) then the M_J quantum numbers in the $|LSJM_J\rangle$ basis states are redundant. This permits a simplified description in terms of $|LSJ\rangle$ levels. The following are the different $^{2S+1}\mathrm{L}_J$ levels that span the eigenvectors that result from diagonalizing the Hamiltonian in the level description, these may also be termed *mutiplets*. (In these we have excluded the indices that distinguish between degenerate LS terms)

$\underline{f}^1$ (2 LSJ levels)
$^2\mathrm{F}_{5/2}$, $^2\mathrm{F}_{7/2}$

$\underline{f}^2$ (13 LSJ levels)
$^3\mathrm{P}_0$, $^1\mathrm{S}_0$, $^3\mathrm{P}_1$, $^3\mathrm{P}_2$, $^3\mathrm{F}_2$, $^1\mathrm{D}_2$, $^3\mathrm{F}_3$, $^3\mathrm{F}_4$, $^3\mathrm{H}_4$, $^1\mathrm{G}_4$, $^3\mathrm{H}_5$, $^3\mathrm{H}_6$, $^1\mathrm{I}_6$

$\underline{f}^3$ (41 LSJ levels)
$^4\mathrm{D}_{1/2}$, $^2\mathrm{P}_{1/2}$, $^4\mathrm{S}_{3/2}$, $^4\mathrm{D}_{3/2}$, $^4\mathrm{F}_{3/2}$, $^2\mathrm{P}_{3/2}$, $^2\mathrm{D}_{3/2}$, $^2\mathrm{D}_{3/2}$, $^4\mathrm{D}_{5/2}$, $^4\mathrm{F}_{5/2}$, $^4\mathrm{G}_{5/2}$, $^2\mathrm{D}_{5/2}$, $^2\mathrm{D}_{5/2}$, $^2\mathrm{F}_{5/2}$, $^2\mathrm{F}_{5/2}$, $^4\mathrm{D}_{7/2}$, $^4\mathrm{F}_{7/2}$, $^4\mathrm{G}_{7/2}$, $^2\mathrm{F}_{7/2}$, $^2\mathrm{F}_{7/2}$, $^2\mathrm{G}_{7/2}$, $^2\mathrm{G}_{7/2}$, $^4\mathrm{F}_{9/2}$, $^4\mathrm{G}_{9/2}$, $^4\mathrm{I}_{9/2}$, $^2\mathrm{G}_{9/2}$, $^2\mathrm{G}_{9/2}$, $^2\mathrm{H}_{9/2}$, $^2\mathrm{H}_{9/2}$, $^4\mathrm{G}_{11/2}$, $^4\mathrm{I}_{11/2}$, $^2\mathrm{H}_{11/2}$, $^2\mathrm{H}_{11/2}$, $^2\mathrm{I}_{11/2}$, $^4\mathrm{I}_{13/2}$, $^2\mathrm{I}_{13/2}$, $^2\mathrm{K}_{13/2}$, $^4\mathrm{I}_{15/2}$, $^2\mathrm{K}_{15/2}$, $^2\mathrm{L}_{15/2}$, $^2\mathrm{L}_{17/2}$

$\underline{f}^4$ (107 LSJ levels)
$^5\mathrm{D}_0$, $^3\mathrm{P}_0$, $^3\mathrm{P}_0$, $^3\mathrm{P}_0$, $^1\mathrm{S}_0$, $^1\mathrm{S}_0$, $^5\mathrm{D}_1$, $^5\mathrm{F}_1$, $^3\mathrm{P}_1$, $^3\mathrm{P}_1$, $^3\mathrm{P}_1$, $^3\mathrm{D}_1$, $^3\mathrm{D}_1$, $^5\mathrm{S}_2$, $^5\mathrm{D}_2$, $^5\mathrm{F}_2$, $^5\mathrm{G}_2$, $^3\mathrm{P}_2$, $^3\mathrm{P}_2$, $^3\mathrm{P}_2$, $^3\mathrm{D}_2$, $^3\mathrm{D}_2$, $^3\mathrm{F}_2$, $^3\mathrm{F}_2$, $^3\mathrm{F}_2$, $^3\mathrm{F}_2$, $^1\mathrm{D}_2$, $^1\mathrm{D}_2$, $^1\mathrm{D}_2$, $^1\mathrm{D}_2$, $^5\mathrm{D}_3$, $^5\mathrm{F}_3$, $^5\mathrm{G}_3$, $^3\mathrm{D}_3$, $^3\mathrm{D}_3$, $^3\mathrm{F}_3$, $^3\mathrm{F}_3$, $^3\mathrm{F}_3$, $^3\mathrm{F}_3$, $^3\mathrm{G}_3$, $^3\mathrm{G}_3$, $^3\mathrm{G}_3$, $^1\mathrm{F}_3$, $^5\mathrm{D}_4$, $^5\mathrm{F}_4$, $^5\mathrm{G}_4$, $^5\mathrm{I}_4$, $^3\mathrm{F}_4$, $^3\mathrm{F}_4$, $^3\mathrm{F}_4$, $^3\mathrm{F}_4$, $^3\mathrm{G}_4$, $^3\mathrm{G}_4$, $^3\mathrm{G}_4$, $^3\mathrm{H}_4$, $^3\mathrm{H}_4$, $^3\mathrm{H}_4$, $^3\mathrm{H}_4$, $^1\mathrm{G}_4$, $^1\mathrm{G}_4$, $^1\mathrm{G}_4$, $^1\mathrm{G}_4$, $^5\mathrm{F}_5$, $^5\mathrm{G}_5$, $^5\mathrm{I}_5$, $^3\mathrm{G}_5$, $^3\mathrm{G}_5$, $^3\mathrm{G}_5$, $^3\mathrm{H}_5$, $^3\mathrm{H}_5$, $^3\mathrm{H}_5$, $^3\mathrm{H}_5$, $^3\mathrm{I}_5$, $^3\mathrm{I}_5$, $^1\mathrm{H}_5$, $^1\mathrm{H}_5$, $^5\mathrm{G}_6$, $^5\mathrm{I}_6$, $^3\mathrm{H}_6$, $^3\mathrm{H}_6$, $^3\mathrm{H}_6$, $^3\mathrm{H}_6$, $^3\mathrm{I}_6$, $^3\mathrm{I}_6$, $^3\mathrm{K}_6$, $^3\mathrm{K}_6$, $^1\mathrm{I}_6$, $^1\mathrm{I}_6$, $^1\mathrm{I}_6$, $^5\mathrm{I}_7$, $^3\mathrm{I}_7$, $^3\mathrm{I}_7$, $^3\mathrm{K}_7$, $^3\mathrm{K}_7$, $^3\mathrm{L}_7$, $^1\mathrm{K}_7$, $^5\mathrm{I}_8$, $^3\mathrm{K}_8$, $^3\mathrm{K}_8$, $^3\mathrm{L}_8$, $^3\mathrm{M}_8$, $^1\mathrm{L}_8$, $^1\mathrm{L}_8$, $^3\mathrm{L}_9$, $^3\mathrm{M}_9$, $^3\mathrm{M}_{10}$, $^1\mathrm{N}_{10}$

$\underline{f}^5$ (198 LSJ levels)
$^6\mathrm{F}_{1/2}$, $^4\mathrm{P}_{1/2}$, $^4\mathrm{P}_{1/2}$, $^4\mathrm{D}_{1/2}$, $^4\mathrm{D}_{1/2}$, $^4\mathrm{D}_{1/2}$, $^2\mathrm{P}_{1/2}$, $^2\mathrm{P}_{1/2}$, $^2\mathrm{P}_{1/2}$, $^2\mathrm{P}_{1/2}$, $^6\mathrm{P}_{3/2}$, $^6\mathrm{F}_{3/2}$, $^4\mathrm{S}_{3/2}$, $^4\mathrm{P}_{3/2}$, $^4\mathrm{P}_{3/2}$, $^4\mathrm{D}_{3/2}$, $^4\mathrm{D}_{3/2}$, $^4\mathrm{D}_{3/2}$, $^4\mathrm{F}_{3/2}$, $^4\mathrm{F}_{3/2}$, $^4\mathrm{F}_{3/2}$, $^4\mathrm{F}_{3/2}$, $^2\mathrm{P}_{3/2}$, $^2\mathrm{P}_{3/2}$, $^2\mathrm{P}_{3/2}$, $^2\mathrm{P}_{3/2}$,

$^{2}D_{3/2}$, $^{2}D_{3/2}$, $^{2}D_{3/2}$, $^{2}D_{3/2}$, $^{2}D_{3/2}$, $^{6}P_{5/2}$, $^{6}F_{5/2}$, $^{6}H_{5/2}$, $^{4}P_{5/2}$, $^{4}P_{5/2}$, $^{4}D_{5/2}$, $^{4}D_{5/2}$, $^{4}D_{5/2}$, $^{4}F_{5/2}$, $^{4}F_{5/2}$, $^{4}F_{5/2}$, $^{4}F_{5/2}$, $^{4}G_{5/2}$, $^{4}G_{5/2}$, $^{4}G_{5/2}$, $^{4}G_{5/2}$, $^{2}D_{5/2}$, $^{2}D_{5/2}$, $^{2}D_{5/2}$, $^{2}D_{5/2}$, $^{2}D_{5/2}$, $^{2}F_{5/2}$, $^{2}F_{5/2}$, $^{2}F_{5/2}$, $^{2}F_{5/2}$, $^{2}F_{5/2}$, $^{2}F_{5/2}$, $^{2}F_{5/2}$, $^{2}F_{5/2}$, $^{6}P_{7/2}$, $^{6}F_{7/2}$, $^{6}H_{7/2}$, $^{4}D_{7/2}$, $^{4}D_{7/2}$, $^{4}D_{7/2}$, $^{4}F_{7/2}$, $^{4}F_{7/2}$, $^{4}F_{7/2}$, $^{4}F_{7/2}$, $^{4}G_{7/2}$, $^{4}G_{7/2}$, $^{4}G_{7/2}$, $^{4}G_{7/2}$, $^{4}H_{7/2}$, $^{4}H_{7/2}$, $^{4}H_{7/2}$, $^{2}F_{7/2}$, $^{2}F_{7/2}$, $^{2}F_{7/2}$, $^{2}F_{7/2}$, $^{2}F_{7/2}$, $^{2}F_{7/2}$, $^{2}F_{7/2}$, $^{2}G_{7/2}$, $^{2}G_{7/2}$, $^{2}G_{7/2}$, $^{2}G_{7/2}$, $^{2}G_{7/2}$, $^{2}G_{7/2}$, $^{6}F_{9/2}$, $^{6}H_{9/2}$, $^{4}F_{9/2}$, $^{4}F_{9/2}$, $^{4}F_{9/2}$, $^{4}F_{9/2}$, $^{4}G_{9/2}$, $^{4}G_{9/2}$, $^{4}G_{9/2}$, $^{4}G_{9/2}$, $^{4}H_{9/2}$, $^{4}H_{9/2}$, $^{4}H_{9/2}$, $^{4}I_{9/2}$, $^{4}I_{9/2}$, $^{4}I_{9/2}$, $^{2}G_{9/2}$, $^{2}G_{9/2}$, $^{2}G_{9/2}$, $^{2}G_{9/2}$, $^{2}G_{9/2}$, $^{2}G_{9/2}$, $^{2}H_{9/2}$, $^{2}H_{9/2}$, $^{2}H_{9/2}$, $^{2}H_{9/2}$, $^{2}H_{9/2}$, $^{2}H_{9/2}$, $^{2}H_{9/2}$, $^{6}F_{11/2}$, $^{6}H_{11/2}$, $^{4}G_{11/2}$, $^{4}G_{11/2}$, $^{4}G_{11/2}$, $^{4}G_{11/2}$, $^{4}H_{11/2}$, $^{4}H_{11/2}$, $^{4}H_{11/2}$, $^{4}H_{11/2}$, $^{4}I_{11/2}$, $^{4}I_{11/2}$, $^{4}I_{11/2}$, $^{4}I_{11/2}$, $^{4}K_{11/2}$, $^{4}K_{11/2}$, $^{2}H_{11/2}$, $^{2}H_{11/2}$, $^{2}H_{11/2}$, $^{2}H_{11/2}$, $^{2}H_{11/2}$, $^{2}H_{11/2}$, $^{2}H_{11/2}$, $^{2}I_{11/2}$, $^{2}I_{11/2}$, $^{2}I_{11/2}$, $^{2}I_{11/2}$, $^{2}I_{11/2}$, $^{6}H_{13/2}$, $^{4}H_{13/2}$, $^{4}H_{13/2}$, $^{4}H_{13/2}$, $^{4}I_{13/2}$, $^{4}I_{13/2}$, $^{4}I_{13/2}$, $^{4}K_{13/2}$, $^{4}K_{13/2}$, $^{4}L_{13/2}$, $^{2}I_{13/2}$, $^{2}I_{13/2}$, $^{2}I_{13/2}$, $^{2}I_{13/2}$, $^{2}I_{13/2}$, $^{2}K_{13/2}$, $^{2}K_{13/2}$, $^{2}K_{13/2}$, $^{2}K_{13/2}$, $^{2}K_{13/2}$, $^{6}H_{15/2}$, $^{4}I_{15/2}$, $^{4}I_{15/2}$, $^{4}I_{15/2}$, $^{4}K_{15/2}$, $^{4}K_{15/2}$, $^{4}L_{15/2}$, $^{4}M_{15/2}$, $^{2}K_{15/2}$, $^{2}K_{15/2}$, $^{2}K_{15/2}$, $^{2}K_{15/2}$, $^{2}K_{15/2}$, $^{2}L_{15/2}$, $^{2}L_{15/2}$, $^{2}L_{15/2}$, $^{4}K_{17/2}$, $^{4}K_{17/2}$, $^{4}L_{17/2}$, $^{4}M_{17/2}$, $^{2}L_{17/2}$, $^{2}L_{17/2}$, $^{2}L_{17/2}$, $^{2}M_{17/2}$, $^{2}M_{17/2}$, $^{4}L_{19/2}$, $^{4}M_{19/2}$, $^{2}M_{19/2}$, $^{2}M_{19/2}$, $^{2}N_{19/2}$, $^{4}M_{21/2}$, $^{2}N_{21/2}$, $^{2}O_{21/2}$, $^{2}O_{23/2}$

$\underline{f}^{6}$ (295 LSJ levels)

$^{7}F_{0}$, $^{5}D_{0}$, $^{5}D_{0}$, $^{5}D_{0}$, $^{3}P_{0}$, $^{3}P_{0}$, $^{3}P_{0}$, $^{3}P_{0}$, $^{3}P_{0}$, $^{3}P_{0}$, $^{1}S_{0}$, $^{1}S_{0}$, $^{1}S_{0}$, $^{1}S_{0}$, $^{7}F_{1}$, $^{5}P_{1}$, $^{5}D_{1}$, $^{5}D_{1}$, $^{5}D_{1}$, $^{5}F_{1}$, $^{5}F_{1}$, $^{3}P_{1}$, $^{3}P_{1}$, $^{3}P_{1}$, $^{3}P_{1}$, $^{3}P_{1}$, $^{3}P_{1}$, $^{3}D_{1}$, $^{3}D_{1}$, $^{3}D_{1}$, $^{3}D_{1}$, $^{3}D_{1}$, $^{1}P_{1}$, $^{7}F_{2}$, $^{5}S_{2}$, $^{5}P_{2}$, $^{5}D_{2}$, $^{5}D_{2}$, $^{5}D_{2}$, $^{5}F_{2}$, $^{5}F_{2}$, $^{5}G_{2}$, $^{5}G_{2}$, $^{5}G_{2}$, $^{3}P_{2}$, $^{3}P_{2}$, $^{3}P_{2}$, $^{3}P_{2}$, $^{3}P_{2}$, $^{3}P_{2}$, $^{3}D_{2}$, $^{3}D_{2}$, $^{3}D_{2}$, $^{3}D_{2}$, $^{3}D_{2}$, $^{3}D_{2}$, $^{3}F_{2}$, $^{3}F_{2}$, $^{3}F_{2}$, $^{3}F_{2}$, $^{3}F_{2}$, $^{3}F_{2}$, $^{3}F_{2}$, $^{3}F_{2}$, $^{3}F_{2}$, $^{1}D_{2}$, $^{1}D_{2}$, $^{1}D_{2}$, $^{1}D_{2}$, $^{1}D_{2}$, $^{1}D_{2}$, $^{7}F_{3}$, $^{5}P_{3}$, $^{5}D_{3}$, $^{5}D_{3}$, $^{5}D_{3}$, $^{5}F_{3}$, $^{5}F_{3}$, $^{5}G_{3}$, $^{5}G_{3}$, $^{5}G_{3}$, $^{5}H_{3}$, $^{5}H_{3}$, $^{3}D_{3}$, $^{3}D_{3}$, $^{3}D_{3}$, $^{3}D_{3}$, $^{3}D_{3}$, $^{3}F_{3}$, $^{3}F_{3}$, $^{3}F_{3}$, $^{3}F_{3}$, $^{3}F_{3}$, $^{3}F_{3}$, $^{3}F_{3}$, $^{3}F_{3}$, $^{3}G_{3}$, $^{3}G_{3}$, $^{3}G_{3}$, $^{3}G_{3}$, $^{3}G_{3}$, $^{3}G_{3}$, $^{3}G_{3}$, $^{1}F_{3}$, $^{1}F_{3}$, $^{1}F_{3}$, $^{1}F_{3}$, $^{7}F_{4}$, $^{5}D_{4}$, $^{5}D_{4}$, $^{5}D_{4}$, $^{5}F_{4}$, $^{5}F_{4}$, $^{5}G_{4}$, $^{5}G_{4}$, $^{5}G_{4}$, $^{5}H_{4}$, $^{5}H_{4}$, $^{5}I_{4}$, $^{5}I_{4}$, $^{3}F_{4}$, $^{3}F_{4}$, $^{3}F_{4}$, $^{3}F_{4}$, $^{3}F_{4}$, $^{3}F_{4}$, $^{3}F_{4}$, $^{3}F_{4}$, $^{3}F_{4}$, $^{3}G_{4}$, $^{3}G_{4}$, $^{3}G_{4}$, $^{3}G_{4}$, $^{3}G_{4}$, $^{3}G_{4}$, $^{3}G_{4}$, $^{3}H_{4}$, $^{3}H_{4}$, $^{3}H_{4}$, $^{3}H_{4}$, $^{3}H_{4}$, $^{3}H_{4}$, $^{3}H_{4}$, $^{3}H_{4}$, $^{3}H_{4}$, $^{1}G_{4}$, $^{1}G_{4}$, $^{1}G_{4}$, $^{1}G_{4}$, $^{1}G_{4}$, $^{1}G_{4}$, $^{1}G_{4}$, $^{7}F_{5}$, $^{5}F_{5}$, $^{5}F_{5}$, $^{5}G_{5}$, $^{5}G_{5}$, $^{5}G_{5}$, $^{5}H_{5}$, $^{5}H_{5}$, $^{5}I_{5}$, $^{5}I_{5}$, $^{5}K_{5}$, $^{3}G_{5}$, $^{3}G_{5}$, $^{3}G_{5}$, $^{3}G_{5}$, $^{3}G_{5}$, $^{3}G_{5}$, $^{3}G_{5}$, $^{3}H_{5}$, $^{3}H_{5}$, $^{3}H_{5}$, $^{3}H_{5}$, $^{3}H_{5}$, $^{3}H_{5}$, $^{3}H_{5}$, $^{3}H_{5}$, $^{3}H_{5}$, $^{3}I_{5}$, $^{3}I_{5}$, $^{3}I_{5}$, $^{3}I_{5}$, $^{3}I_{5}$, $^{3}I_{5}$, $^{1}H_{5}$, $^{1}H_{5}$, $^{1}H_{5}$, $^{1}H_{5}$, $^{7}F_{6}$, $^{5}G_{6}$, $^{5}G_{6}$, $^{5}G_{6}$, $^{5}H_{6}$, $^{5}H_{6}$, $^{5}I_{6}$, $^{5}I_{6}$, $^{5}K_{6}$, $^{5}L_{6}$, $^{3}H_{6}$, $^{3}H_{6}$, $^{3}H_{6}$, $^{3}H_{6}$, $^{3}H_{6}$, $^{3}H_{6}$, $^{3}H_{6}$, $^{3}H_{6}$, $^{3}H_{6}$, $^{3}I_{6}$, $^{3}I_{6}$, $^{3}I_{6}$, $^{3}I_{6}$, $^{3}I_{6}$, $^{3}I_{6}$, $^{3}K_{6}$, $^{3}K_{6}$, $^{3}K_{6}$, $^{3}K_{6}$, $^{3}K_{6}$, $^{3}K_{6}$, $^{1}I_{6}$, $^{1}I_{6}$, $^{1}I_{6}$, $^{1}I_{6}$, $^{1}I_{6}$, $^{1}I_{6}$, $^{1}I_{6}$, $^{5}H_{7}$, $^{5}H_{7}$, $^{5}I_{7}$, $^{5}I_{7}$, $^{5}K_{7}$, $^{5}L_{7}$, $^{3}I_{7}$, $^{3}I_{7}$, $^{3}I_{7}$, $^{3}I_{7}$, $^{3}I_{7}$, $^{3}I_{7}$, $^{3}K_{7}$, $^{3}K_{7}$, $^{3}K_{7}$, $^{3}K_{7}$, $^{3}K_{7}$, $^{3}K_{7}$, $^{3}L_{7}$, $^{3}L_{7}$, $^{3}L_{7}$, $^{1}K_{7}$, $^{1}K_{7}$, $^{1}K_{7}$, $^{5}I_{8}$, $^{5}I_{8}$, $^{5}K_{8}$, $^{5}L_{8}$, $^{3}K_{8}$, $^{3}K_{8}$, $^{3}K_{8}$, $^{3}K_{8}$, $^{3}K_{8}$, $^{3}K_{8}$, $^{3}L_{8}$, $^{3}L_{8}$, $^{3}L_{8}$, $^{3}M_{8}$, $^{3}M_{8}$, $^{3}M_{8}$, $^{1}L_{8}$, $^{1}L_{8}$, $^{1}L_{8}$, $^{1}L_{8}$, $^{5}K_{9}$, $^{5}L_{9}$, $^{3}L_{9}$, $^{3}L_{9}$, $^{3}L_{9}$, $^{3}M_{9}$, $^{3}M_{9}$, $^{3}M_{9}$, $^{3}N_{9}$, $^{1}M_{9}$, $^{1}M_{9}$, $^{5}L_{10}$, $^{3}M_{10}$, $^{3}M_{10}$, $^{3}M_{10}$, $^{3}N_{10}$, $^{3}O_{10}$, $^{1}N_{10}$, $^{1}N_{10}$, $^{3}N_{11}$, $^{3}O_{11}$, $^{3}O_{12}$, $^{1}Q_{12}$

$\underline{f}^{7}$ (327 LSJ levels)

$^{6}D_{1/2}$, $^{6}F_{1/2}$, $^{4}P_{1/2}$, $^{4}P_{1/2}$, $^{4}D_{1/2}$, $^{4}D_{1/2}$, $^{4}D_{1/2}$, $^{4}D_{1/2}$, $^{4}D_{1/2}$, $^{4}D_{1/2}$, $^{2}S_{1/2}$, $^{2}S_{1/2}$, $^{2}P_{1/2}$, $^{2}P_{1/2}$, $^{2}P_{1/2}$, $^{2}P_{1/2}$, $^{2}P_{1/2}$, $^{6}P_{3/2}$, $^{6}D_{3/2}$, $^{6}F_{3/2}$, $^{6}G_{3/2}$, $^{4}S_{3/2}$, $^{4}S_{3/2}$, $^{4}P_{3/2}$, $^{4}P_{3/2}$, $^{4}D_{3/2}$, $^{4}D_{3/2}$, $^{4}D_{3/2}$, $^{4}D_{3/2}$, $^{4}D_{3/2}$, $^{4}D_{3/2}$, $^{4}F_{3/2}$, $^{4}F_{3/2}$, $^{4}F_{3/2}$, $^{4}F_{3/2}$, $^{4}F_{3/2}$, $^{2}P_{3/2}$, $^{2}P_{3/2}$, $^{2}P_{3/2}$, $^{2}P_{3/2}$, $^{2}P_{3/2}$, $^{2}D_{3/2}$, $^{2}D_{3/2}$, $^{2}D_{3/2}$, $^{2}D_{3/2}$, $^{2}D_{3/2}$, $^{2}D_{3/2}$, $^{2}D_{3/2}$, $^{6}P_{5/2}$, $^{6}D_{5/2}$, $^{6}F_{5/2}$, $^{6}G_{5/2}$, $^{6}H_{5/2}$, $^{4}P_{5/2}$, $^{4}P_{5/2}$, $^{4}D_{5/2}$, $^{4}D_{5/2}$, $^{4}D_{5/2}$, $^{4}D_{5/2}$, $^{4}D_{5/2}$, $^{4}D_{5/2}$, $^{4}F_{5/2}$, $^{4}F_{5/2}$, $^{4}F_{5/2}$, $^{4}F_{5/2}$, $^{4}F_{5/2}$, $^{4}F_{5/2}$, $^{4}G_{5/2}$, $^{4}G_{5/2}$, $^{4}G_{5/2}$, $^{4}G_{5/2}$, $^{4}G_{5/2}$, $^{4}G_{5/2}$, $^{4}G_{5/2}$, $^{2}D_{5/2}$, $^{2}D_{5/2}$, $^{2}D_{5/2}$, $^{2}D_{5/2}$, $^{2}D_{5/2}$, $^{2}D_{5/2}$, $^{2}D_{5/2}$, $^{2}F_{5/2}$, $^{2}F_{5/2}$, $^{2}F_{5/2}$, $^{2}F_{5/2}$, $^{2}F_{5/2}$, $^{2}F_{5/2}$, $^{2}F_{5/2}$, $^{2}F_{5/2}$, $^{2}F_{5/2}$, $^{2}F_{5/2}$, $^{2}F_{5/2}$, $^{8}S_{7/2}$, $^{6}P_{7/2}$, $^{6}D_{7/2}$, $^{6}F_{7/2}$, $^{6}G_{7/2}$, $^{6}H_{7/2}$, $^{6}I_{7/2}$, $^{4}D_{7/2}$, $^{4}D_{7/2}$, $^{4}D_{7/2}$, $^{4}D_{7/2}$, $^{4}D_{7/2}$, $^{4}D_{7/2}$, $^{4}F_{7/2}$, $^{4}F_{7/2}$, $^{4}F_{7/2}$, $^{4}F_{7/2}$, $^{4}F_{7/2}$, $^{4}G_{7/2}$, $^{4}G_{7/2}$, $^{4}G_{7/2}$, $^{4}G_{7/2}$, $^{4}G_{7/2}$, $^{4}G_{7/2}$, $^{4}G_{7/2}$, $^{4}H_{7/2}$, $^{4}H_{7/2}$, $^{4}H_{7/2}$, $^{4}H_{7/2}$, $^{4}H_{7/2}$, $^{2}F_{7/2}$, $^{2}F_{7/2}$, $^{2}F_{7/2}$, $^{2}F_{7/2}$, $^{2}F_{7/2}$, $^{2}F_{7/2}$, $^{2}F_{7/2}$, $^{2}F_{7/2}$, $^{2}F_{7/2}$, $^{2}G_{7/2}$, $^{2}G_{7/2}$, $^{2}G_{7/2}$, $^{2}G_{7/2}$, $^{2}G_{7/2}$, $^{2}G_{7/2}$, $^{2}G_{7/2}$, $^{2}G_{7/2}$, $^{2}G_{7/2}$, $^{2}G_{7/2}$, $^{2}G_{7/2}$, $^{6}D_{9/2}$, $^{6}F_{9/2}$, $^{6}G_{9/2}$, $^{6}H_{9/2}$, $^{6}I_{9/2}$, $^{4}F_{9/2}$, $^{4}F_{9/2}$, $^{4}F_{9/2}$, $^{4}F_{9/2}$, $^{4}F_{9/2}$, $^{4}G_{9/2}$, $^{4}G_{9/2}$, $^{4}G_{9/2}$, $^{4}G_{9/2}$, $^{4}G_{9/2}$, $^{4}G_{9/2}$, $^{4}G_{9/2}$, $^{4}H_{9/2}$, $^{4}H_{9/2}$, $^{4}H_{9/2}$, $^{4}H_{9/2}$, $^{4}H_{9/2}$, $^{4}I_{9/2}$, $^{4}I_{9/2}$, $^{4}I_{9/2}$, $^{4}I_{9/2}$, $^{4}I_{9/2}$, $^{2}G_{9/2}$, $^{2}G_{9/2}$, $^{2}G_{9/2}$, $^{2}G_{9/2}$, $^{2}G_{9/2}$, $^{2}G_{9/2}$, $^{2}G_{9/2}$, $^{2}G_{9/2}$, $^{2}G_{9/2}$, $^{2}G_{9/2}$, $^{2}H_{9/2}$, $^{2}H_{9/2}$, $^{2}H_{9/2}$, $^{2}H_{9/2}$, $^{2}H_{9/2}$, $^{2}H_{9/2}$, $^{2}H_{9/2}$, $^{2}H_{9/2}$, $^{2}H_{9/2}$, $^{6}F_{11/2}$, $^{6}G_{11/2}$, $^{6}H_{11/2}$, $^{6}I_{11/2}$, $^{4}G_{11/2}$, $^{4}G_{11/2}$, $^{4}G_{11/2}$, $^{4}G_{11/2}$, $^{4}G_{11/2}$, $^{4}G_{11/2}$, $^{4}H_{11/2}$, $^{4}H_{11/2}$, $^{4}H_{11/2}$, $^{4}H_{11/2}$, $^{4}H_{11/2}$, $^{4}I_{11/2}$, $^{4}I_{11/2}$, $^{4}I_{11/2}$, $^{4}I_{11/2}$, $^{4}I_{11/2}$, $^{4}K_{11/2}$, $^{4}K_{11/2}$, $^{4}K_{11/2}$, $^{2}H_{11/2}$, $^{2}H_{11/2}$, $^{2}H_{11/2}$, $^{2}H_{11/2}$, $^{2}H_{11/2}$, $^{2}H_{11/2}$, $^{2}H_{11/2}$, $^{2}H_{11/2}$, $^{2}H_{11/2}$, $^{2}I_{11/2}$, $^{2}I_{11/2}$, $^{2}I_{11/2}$, $^{2}I_{11/2}$, $^{2}I_{11/2}$, $^{2}I_{11/2}$, $^{2}I_{11/2}$, $^{2}I_{11/2}$, $^{2}I_{11/2}$, $^{6}G_{13/2}$, $^{6}H_{13/2}$, $^{6}I_{13/2}$, $^{4}H_{13/2}$, $^{4}H_{13/2}$, $^{4}H_{13/2}$, $^{4}H_{13/2}$, $^{4}H_{13/2}$, $^{4}I_{13/2}$, $^{4}I_{13/2}$, $^{4}I_{13/2}$, $^{4}I_{13/2}$, $^{4}I_{13/2}$, $^{4}K_{13/2}$, $^{4}K_{13/2}$, $^{4}K_{13/2}$, $^{4}L_{13/2}$, $^{4}L_{13/2}$, $^{4}L_{13/2}$, $^{2}I_{13/2}$, $^{2}I_{13/2}$, $^{2}I_{13/2}$, $^{2}I_{13/2}$, $^{2}I_{13/2}$, $^{2}I_{13/2}$, $^{2}I_{13/2}$, $^{2}I_{13/2}$, $^{2}K_{13/2}$, $^{2}K_{13/2}$, $^{2}K_{13/2}$, $^{2}K_{13/2}$, $^{2}K_{13/2}$, $^{2}K_{13/2}$, $^{2}K_{13/2}$, $^{6}H_{15/2}$, $^{6}I_{15/2}$, $^{4}I_{15/2}$, $^{4}I_{15/2}$, $^{4}I_{15/2}$, $^{4}I_{15/2}$, $^{4}I_{15/2}$, $^{4}K_{15/2}$, $^{4}K_{15/2}$,

$^4K_{15/2}$, $^4L_{15/2}$, $^4L_{15/2}$, $^4L_{15/2}$, $^4M_{15/2}$, $^2K_{15/2}$, $^2K_{15/2}$, $^2K_{15/2}$, $^2K_{15/2}$, $^2K_{15/2}$, $^2K_{15/2}$, $^2L_{15/2}$, $^2L_{15/2}$, $^2L_{15/2}$, $^2L_{15/2}$, $^2L_{15/2}$, $^6I_{17/2}$, $^4K_{17/2}$, $^4K_{17/2}$, $^4K_{17/2}$, $^4L_{17/2}$, $^4L_{17/2}$, $^4L_{17/2}$, $^4M_{17/2}$, $^4N_{17/2}$, $^2L_{17/2}$, $^2L_{17/2}$, $^2L_{17/2}$, $^2L_{17/2}$, $^2L_{17/2}$, $^2M_{17/2}$, $^2M_{17/2}$, $^2M_{17/2}$, $^2M_{17/2}$, $^4L_{19/2}$, $^4L_{19/2}$, $^4L_{19/2}$, $^4M_{19/2}$, $^4N_{19/2}$, $^2M_{19/2}$, $^2M_{19/2}$, $^2M_{19/2}$, $^2M_{19/2}$, $^2N_{19/2}$, $^2N_{19/2}$, $^4M_{21/2}$, $^4N_{21/2}$, $^2N_{21/2}$, $^2N_{21/2}$, $^2O_{21/2}$, $^4N_{23/2}$, $^2O_{23/2}$, $^2Q_{23/2}$, $^2Q_{25/2}$

$\underline{f}^8$ (295 LSJ levels)

$^7F_0$, $^5D_0$, $^5D_0$, $^5D_0$, $^3P_0$, $^3P_0$, $^3P_0$, $^3P_0$, $^3P_0$, $^3P_0$, $^1S_0$, $^1S_0$, $^1S_0$, $^1S_0$, $^7F_1$, $^5P_1$, $^5D_1$, $^5D_1$, $^5D_1$, $^5F_1$, $^5F_1$, $^3P_1$, $^3P_1$, $^3P_1$, $^3P_1$, $^3P_1$, $^3P_1$, $^3D_1$, $^3D_1$, $^3D_1$, $^3D_1$, $^3D_1$, $^1P_1$, $^7F_2$, $^5S_2$, $^5P_2$, $^5D_2$, $^5D_2$, $^5D_2$, $^5F_2$, $^5F_2$, $^5G_2$, $^5G_2$, $^5G_2$, $^3P_2$, $^3P_2$, $^3P_2$, $^3P_2$, $^3P_2$, $^3P_2$, $^3D_2$, $^3D_2$, $^3D_2$, $^3D_2$, $^3D_2$, $^3F_2$, $^3F_2$, $^3F_2$, $^3F_2$, $^3F_2$, $^3F_2$, $^3F_2$, $^3F_2$, $^3F_2$, $^1D_2$, $^1D_2$, $^1D_2$, $^1D_2$, $^1D_2$, $^1D_2$, $^7F_3$, $^5P_3$, $^5D_3$, $^5D_3$, $^5D_3$, $^5F_3$, $^5F_3$, $^5G_3$, $^5G_3$, $^5G_3$, $^5H_3$, $^5H_3$, $^3D_3$, $^3D_3$, $^3D_3$, $^3D_3$, $^3D_3$, $^3F_3$, $^3F_3$, $^3F_3$, $^3F_3$, $^3F_3$, $^3F_3$, $^3F_3$, $^3F_3$, $^3G_3$, $^3G_3$, $^3G_3$, $^3G_3$, $^3G_3$, $^3G_3$, $^3G_3$, $^1F_3$, $^1F_3$, $^1F_3$, $^1F_3$, $^7F_4$, $^5D_4$, $^5D_4$, $^5D_4$, $^5F_4$, $^5F_4$, $^5G_4$, $^5G_4$, $^5G_4$, $^5H_4$, $^5H_4$, $^5I_4$, $^5I_4$, $^3F_4$, $^3F_4$, $^3F_4$, $^3F_4$, $^3F_4$, $^3F_4$, $^3F_4$, $^3F_4$, $^3F_4$, $^3G_4$, $^3G_4$, $^3G_4$, $^3G_4$, $^3G_4$, $^3G_4$, $^3G_4$, $^3H_4$, $^3H_4$, $^3H_4$, $^3H_4$, $^3H_4$, $^3H_4$, $^3H_4$, $^3H_4$, $^3H_4$, $^1G_4$, $^1G_4$, $^1G_4$, $^1G_4$, $^1G_4$, $^1G_4$, $^1G_4$, $^7F_5$, $^5F_5$, $^5F_5$, $^5G_5$, $^5G_5$, $^5G_5$, $^5H_5$, $^5H_5$, $^5I_5$, $^5I_5$, $^5K_5$, $^3G_5$, $^3G_5$, $^3G_5$, $^3G_5$, $^3G_5$, $^3G_5$, $^3H_5$, $^3H_5$, $^3H_5$, $^3H_5$, $^3H_5$, $^3H_5$, $^3H_5$, $^3H_5$, $^3I_5$, $^3I_5$, $^3I_5$, $^3I_5$, $^3I_5$, $^1H_5$, $^1H_5$, $^1H_5$, $^1H_5$, $^7F_6$, $^5G_6$, $^5G_6$, $^5G_6$, $^5H_6$, $^5H_6$, $^5I_6$, $^5I_6$, $^5K_6$, $^5L_6$, $^3H_6$, $^3H_6$, $^3H_6$, $^3H_6$, $^3H_6$, $^3H_6$, $^3H_6$, $^3H_6$, $^3H_6$, $^3I_6$, $^3I_6$, $^3I_6$, $^3I_6$, $^3I_6$, $^3I_6$, $^3K_6$, $^3K_6$, $^3K_6$, $^3K_6$, $^3K_6$, $^3K_6$, $^1I_6$, $^1I_6$, $^1I_6$, $^1I_6$, $^1I_6$, $^1I_6$, $^1I_6$, $^5H_7$, $^5H_7$, $^5I_7$, $^5I_7$, $^5K_7$, $^5L_7$, $^3I_7$, $^3I_7$, $^3I_7$, $^3I_7$, $^3I_7$, $^3I_7$, $^3K_7$, $^3K_7$, $^3K_7$, $^3K_7$, $^3K_7$, $^3K_7$, $^3L_7$, $^3L_7$, $^3L_7$, $^1K_7$, $^1K_7$, $^1K_7$, $^5I_8$, $^5I_8$, $^5K_8$, $^5L_8$, $^3K_8$, $^3K_8$, $^3K_8$, $^3K_8$, $^3K_8$, $^3K_8$, $^3L_8$, $^3L_8$, $^3L_8$, $^3M_8$, $^3M_8$, $^3M_8$, $^1L_8$, $^1L_8$, $^1L_8$, $^1L_8$, $^5K_9$, $^5L_9$, $^3L_9$, $^3L_9$, $^3L_9$, $^3M_9$, $^3M_9$, $^3M_9$, $^3N_9$, $^1M_9$, $^1M_9$, $^5L_{10}$, $^3M_{10}$, $^3M_{10}$, $^3M_{10}$, $^3N_{10}$, $^3O_{10}$, $^1N_{10}$, $^1N_{10}$, $^3N_{11}$, $^3O_{11}$, $^3O_{12}$, $^1Q_{12}$

$\underline{f}^9$ (198 LSJ levels)

$^6F_{1/2}$, $^4P_{1/2}$, $^4P_{1/2}$, $^4D_{1/2}$, $^4D_{1/2}$, $^4D_{1/2}$, $^2P_{1/2}$, $^2P_{1/2}$, $^2P_{1/2}$, $^2P_{1/2}$, $^6P_{3/2}$, $^6F_{3/2}$, $^4S_{3/2}$, $^4P_{3/2}$, $^4P_{3/2}$, $^4D_{3/2}$, $^4D_{3/2}$, $^4D_{3/2}$, $^4F_{3/2}$, $^4F_{3/2}$, $^4F_{3/2}$, $^4F_{3/2}$, $^2P_{3/2}$, $^2P_{3/2}$, $^2P_{3/2}$, $^2P_{3/2}$, $^2D_{3/2}$, $^2D_{3/2}$, $^2D_{3/2}$, $^2D_{3/2}$, $^2D_{3/2}$, $^6P_{5/2}$, $^6F_{5/2}$, $^6H_{5/2}$, $^4P_{5/2}$, $^4P_{5/2}$, $^4D_{5/2}$, $^4D_{5/2}$, $^4D_{5/2}$, $^4F_{5/2}$, $^4F_{5/2}$, $^4F_{5/2}$, $^4F_{5/2}$, $^4G_{5/2}$, $^4G_{5/2}$, $^4G_{5/2}$, $^4G_{5/2}$, $^2D_{5/2}$, $^2D_{5/2}$, $^2D_{5/2}$, $^2D_{5/2}$, $^2D_{5/2}$, $^2F_{5/2}$, $^2F_{5/2}$, $^2F_{5/2}$, $^2F_{5/2}$, $^2F_{5/2}$, $^2F_{5/2}$, $^2F_{5/2}$, $^6P_{7/2}$, $^6F_{7/2}$, $^6H_{7/2}$, $^4D_{7/2}$, $^4D_{7/2}$, $^4D_{7/2}$, $^4F_{7/2}$, $^4F_{7/2}$, $^4F_{7/2}$, $^4F_{7/2}$, $^4G_{7/2}$, $^4G_{7/2}$, $^4G_{7/2}$, $^4G_{7/2}$, $^4H_{7/2}$, $^4H_{7/2}$, $^4H_{7/2}$, $^2F_{7/2}$, $^2F_{7/2}$, $^2F_{7/2}$, $^2F_{7/2}$, $^2F_{7/2}$, $^2F_{7/2}$, $^2F_{7/2}$, $^2G_{7/2}$, $^2G_{7/2}$, $^2G_{7/2}$, $^2G_{7/2}$, $^2G_{7/2}$, $^2G_{7/2}$, $^6F_{9/2}$, $^6H_{9/2}$, $^4F_{9/2}$, $^4F_{9/2}$, $^4F_{9/2}$, $^4F_{9/2}$, $^4G_{9/2}$, $^4G_{9/2}$, $^4G_{9/2}$, $^4G_{9/2}$, $^4H_{9/2}$, $^4H_{9/2}$, $^4H_{9/2}$, $^4I_{9/2}$, $^4I_{9/2}$, $^4I_{9/2}$, $^2G_{9/2}$, $^2G_{9/2}$, $^2G_{9/2}$, $^2G_{9/2}$, $^2G_{9/2}$, $^2G_{9/2}$, $^2H_{9/2}$, $^2H_{9/2}$, $^2H_{9/2}$, $^2H_{9/2}$, $^2H_{9/2}$, $^2H_{9/2}$, $^2H_{9/2}$, $^6F_{11/2}$, $^6H_{11/2}$, $^4G_{11/2}$, $^4G_{11/2}$, $^4G_{11/2}$, $^4G_{11/2}$, $^4H_{11/2}$, $^4H_{11/2}$, $^4H_{11/2}$, $^4I_{11/2}$, $^4I_{11/2}$, $^4I_{11/2}$, $^4K_{11/2}$, $^4K_{11/2}$, $^2H_{11/2}$, $^2H_{11/2}$, $^2H_{11/2}$, $^2H_{11/2}$, $^2H_{11/2}$, $^2H_{11/2}$, $^2H_{11/2}$, $^2I_{11/2}$, $^2I_{11/2}$, $^2I_{11/2}$, $^2I_{11/2}$, $^2I_{11/2}$, $^6H_{13/2}$, $^4H_{13/2}$, $^4H_{13/2}$, $^4H_{13/2}$, $^4I_{13/2}$, $^4I_{13/2}$, $^4I_{13/2}$, $^4K_{13/2}$, $^4K_{13/2}$, $^4L_{13/2}$, $^2I_{13/2}$, $^2I_{13/2}$, $^2I_{13/2}$, $^2I_{13/2}$, $^2I_{13/2}$, $^2K_{13/2}$, $^2K_{13/2}$, $^2K_{13/2}$, $^2K_{13/2}$, $^2K_{13/2}$, $^6H_{15/2}$, $^4I_{15/2}$, $^4I_{15/2}$, $^4I_{15/2}$, $^4K_{15/2}$, $^4K_{15/2}$, $^4L_{15/2}$, $^4M_{15/2}$, $^2K_{15/2}$, $^2K_{15/2}$, $^2K_{15/2}$, $^2K_{15/2}$, $^2K_{15/2}$, $^2L_{15/2}$, $^2L_{15/2}$, $^2L_{15/2}$, $^4K_{17/2}$, $^4K_{17/2}$, $^4L_{17/2}$, $^4M_{17/2}$, $^2L_{17/2}$, $^2L_{17/2}$, $^2L_{17/2}$, $^2M_{17/2}$, $^2M_{17/2}$, $^4L_{19/2}$, $^4M_{19/2}$, $^2M_{19/2}$, $^2M_{19/2}$, $^2N_{19/2}$, $^4M_{21/2}$, $^2N_{21/2}$, $^2O_{21/2}$, $^2O_{23/2}$

$\underline{f}^{10}$ (107 LSJ levels)

$^5D_0$, $^3P_0$, $^3P_0$, $^3P_0$, $^1S_0$, $^1S_0$, $^5D_1$, $^5F_1$, $^3P_1$, $^3P_1$, $^3P_1$, $^3D_1$, $^3D_1$, $^5S_2$, $^5D_2$, $^5F_2$, $^5G_2$, $^3P_2$, $^3P_2$, $^3P_2$, $^3D_2$, $^3D_2$, $^3F_2$, $^3F_2$, $^3F_2$, $^3F_2$, $^1D_2$, $^1D_2$, $^1D_2$, $^1D_2$, $^5D_3$, $^5F_3$, $^5G_3$, $^3D_3$, $^3D_3$, $^3F_3$, $^3F_3$, $^3F_3$, $^3F_3$, $^3G_3$, $^3G_3$, $^3G_3$, $^1F_3$, $^5D_4$, $^5F_4$, $^5G_4$, $^5I_4$, $^3F_4$, $^3F_4$, $^3F_4$, $^3F_4$, $^3G_4$, $^3G_4$, $^3G_4$, $^3H_4$, $^3H_4$, $^3H_4$, $^3H_4$, $^1G_4$, $^1G_4$, $^1G_4$, $^1G_4$, $^5F_5$, $^5G_5$, $^5I_5$, $^3G_5$, $^3G_5$, $^3G_5$, $^3H_5$, $^3H_5$, $^3H_5$, $^3H_5$, $^3I_5$, $^3I_5$, $^1H_5$, $^1H_5$, $^5G_6$, $^5I_6$, $^3H_6$, $^3H_6$, $^3H_6$, $^3H_6$, $^3I_6$, $^3I_6$, $^3K_6$, $^3K_6$, $^1I_6$, $^1I_6$, $^1I_6$, $^5I_7$, $^3I_7$, $^3I_7$, $^3K_7$, $^3K_7$, $^3L_7$, $^1K_7$, $^5I_8$, $^3K_8$, $^3K_8$, $^3L_8$, $^3M_8$, $^1L_8$, $^1L_8$, $^3L_9$, $^3M_9$, $^3M_{10}$, $^1N_{10}$

$\underline{f}^{11}$ (41 LSJ levels)

$^4D_{1/2}$, $^2P_{1/2}$, $^4S_{3/2}$, $^4D_{3/2}$, $^4F_{3/2}$, $^2P_{3/2}$, $^2D_{3/2}$, $^2D_{3/2}$, $^4D_{5/2}$, $^4F_{5/2}$, $^4G_{5/2}$, $^2D_{5/2}$, $^2D_{5/2}$, $^2F_{5/2}$, $^2F_{5/2}$, $^4D_{7/2}$, $^4F_{7/2}$, $^4G_{7/2}$, $^2F_{7/2}$, $^2F_{7/2}$, $^2G_{7/2}$, $^2G_{7/2}$, $^4F_{9/2}$, $^4G_{9/2}$, $^4I_{9/2}$, $^2G_{9/2}$,

$^2G_{9/2}$, $^2H_{9/2}$, $^2H_{9/2}$, $^4G_{11/2}$, $^4I_{11/2}$, $^2H_{11/2}$, $^2H_{11/2}$, $^2I_{11/2}$, $^4I_{13/2}$, $^2I_{13/2}$, $^2K_{13/2}$, $^4I_{15/2}$, $^2K_{15/2}$, $^2L_{15/2}$, $^2L_{17/2}$

$\underline{f}^{12}$ (13 LSJ levels)
$^3P_0$, $^1S_0$, $^3P_1$, $^3P_2$, $^3F_2$, $^1D_2$, $^3F_3$, $^3F_4$, $^3H_4$, $^1G_4$, $^3H_5$, $^3H_6$, $^1I_6$

$\underline{f}^{13}$ (2 LSJ levels)
$^2F_{5/2}$, $^2F_{7/2}$

The level picture is a much more frugal description of the eigenstates. Not only are the number of basis elements that need to be considered much less than otherwise, but also the diagonalization is more efficient since it can be carried out within subspaces of shared J. One needs, however, to use adequate degeneracy factors in the relevant calculations.

In **qlanth** the function BasisLSJ can be used to retrieve the ordered basis that is used for the intermediate coupling description in terms of levels.

```
BasisLSJ::usage = "BasisLSJ[numE] returns the level basis LSJ. The function returns a list with each element representing the quantum numbers for each basis vector. Each element is of the form {SL (string in spectroscopic notation), J}.
The option ''AsAssociation'' can be set to True to return the basis as an association with the keys being the allowed J values. The default is False.
  ";
Options[BasisLSJ]={"AsAssociation"->False};
BasisLSJ[numE_,OptionsPattern[]] := Module[
  {Js, basis},
  (
    Js    = AllowedJ[numE];
    basis = BasisLSJMJ[numE,"AsAssociation"->False];
    basis = DeleteDuplicates[{#[[1]],#[[2]]}& /@ basis];
    If[OptionValue["AsAssociation"],
      (
        basis = Association @ Table[(J->Select[basis,#[[2]]==J&]),{J, Js}]
      )
    ];
    Return[basis];
  )
];
```

To obtain the blocks (indexed by J) representing the Hamiltonian in the level description, the function LevelSimplerSymbolicHamMatrix is provided in **qlanth**.

```
LevelSimplerSymbolicHamMatrix::usage = "LevelSimplerSymbolicHamMatrix[numE] is a variation of HamMatrixAssembly that returns the diagonal JJ Hamiltonian blocks applying a simplifier and with simplifications adequate for the level description. The keys of the given association correspond to the different values of J that are possible for f^numE, the values are sparse array that are meant to be interpreted in the basis provided by BasisLSJ.
The option ''Simplifier'' is a list of symbols that are set to zero. At a minimum this has to include the crystal field parameters. By default this includes everything except the Slater parameters Fk and the spin orbit coupling ζ.
The option ''Export'' controls whether the resulting association is saved to disk, the default is True and the resulting file is saved to the ./hams/ folder. A hash is appended to the filename that corresponds to the simplifier used in the resulting expression. If the option ''Overwrite'' is set to False then these files may be used to quickly retrieve a previously computed case. The file is saved both in .m and .mx format.
The option ''PrependToFilename'' can be used to append a string to the filename to which the function may export to.
The option ''Return'' can be used to choose whether the function returns the matrix or not.
The option ''Overwrite'' can be used to overwrite the file if it already exists.";
Options[LevelSimplerSymbolicHamMatrix] = {
```

```
  "Export" -> True,
  "PrependToFilename" -> "",
  "Overwrite" -> False,
  "Return" -> True,
  "Simplifier" -> Join[
    {F0,\[Sigma]SS},
    cfSymbols,
    TSymbols,
    casimirSymbols,
    pseudoMagneticSymbols,
    marvinSymbols,
    DeleteCases[magneticSymbols,ζ]
  ]
};
LevelSimplerSymbolicHamMatrix[numE_Integer, OptionsPattern[]] :=
    Module[
  {thisHamAssoc, Js, fname,
  fnamemx, hash, simplifier},
  (
    simplifier = (#->0)&/@Sort[OptionValue["Simplifier"]];
    hash       = Hash[simplifier];
    If[Not[ValueQ[ElectrostaticTable]],LoadElectrostatic[];
    If[Not[ValueQ[SOOandECSOTable]],LoadSOOandECSO[];
    If[Not[ValueQ[SpinOrbitTable]],LoadSpinOrbit[];
    If[Not[ValueQ[SpinSpinTable]],LoadSpinSpin[];
    If[Not[ValueQ[ThreeBodyTable]],LoadThreeBody[];
    fname   = FileNameJoin[{moduleDir,"hams",OptionValue["
    PrependToFilename"]<>"Level-SymbolicMatrix-f"<>ToString[numE]<>"-"
    <>ToString[hash]<>".m"}];
    fnamemx = FileNameJoin[{moduleDir,"hams",OptionValue["
    PrependToFilename"]<>"Level-SymbolicMatrix-f"<>ToString[numE]<>"-"
    <>ToString[hash]<>".mx"}];
    If[Or[FileExistsQ[fname],FileExistsQ[fnamemx]]&&Not[OptionValue["
    Overwrite"]],
    (
      If[OptionValue["Return"],
      (
        Which[FileExistsQ[fnamemx],
        (
          Print["File ",fnamemx," already exists, and option ''
    Overwrite'' is set to False, loading file ..."];
          thisHamAssoc=Import[fnamemx];
          Return[thisHamAssoc];
        ),
        FileExistsQ[fname],
        (
          Print["File ",fname," already exists, and option ''
    Overwrite'' is set to False, loading file ..."];
          thisHamAssoc=Import[fname];
          Print["Exporting to file ",fnamemx," for quicker loading."
    ];
          Export[fnamemx,thisHamAssoc];
          Return[thisHamAssoc];
        )
        ]
      ),
      (
        Print["File ",fname," already exists, skipping ..."];
        Return[Null];
      )
      ]
    )
    ];
    Js           = AllowedJ[numE];
    thisHamAssoc = HamMatrixAssembly[numE,
      "Set t2Switch"->True,
      "IncludeZeeman"->False,
      "ReturnInBlocks"->True
    ];
    thisHamAssoc = Diagonal[thisHamAssoc];
    thisHamAssoc = Map[SparseArray[ReplaceInSparseArray[#,simplifier
    ]]&,thisHamAssoc,{1}];
    thisHamAssoc = FreeHam[thisHamAssoc,numE];
    thisHamAssoc = AssociationThread[Js->thisHamAssoc];
    If[OptionValue["Export"],
      (
```

```
        Print["Exporting to file ",fname," and to ",fnamemx];
        Export[fname,thisHamAssoc];
        Export[fnamemx,thisHamAssoc];
      )
    ];
    If[OptionValue["Return"],
      Return[thisHamAssoc],
      Return[Null]
    ];
  )
];
```

Whereas this description may be calculated without ever making explicit reference to M_J, in **qlanth** what is done is that the more verbose description associated with the $|LSJM_J\rangle$ basis is "downsized" to obtain the description in terms of levels. For this aim the following functions in **qlanth** are instrumental: `EigenLever`, `FreeHam`, `ListRepeater`, and `ListLever`.

The function `LevelSolver` can be used to calculate the level structure for given values of the parameters that one wishes to keep for the level description, which is often simply termed the *free-ion* part of the Hamiltonian.

```
LevelSolver::usage = "LevelSolver[numE, params] puts together (or
    retrieves from disk) the symbolic level Hamiltonian for the f^numE
     configuration and solves it for the given params returning the
    resultant energies and eigenstates.
If the option ''Return as states'' is set to False, then the function
     returns an association whose keys are values for J in f^numE, and
     whose values are lists with two elements. The first element being
     equal to the ordered basis for the corresponding subpsace, given
    as a list of lists of the form {LS string, J}. The second element
    being another list of two elements, the first element being equal
    to the energies and the second being equal to the corresponding
    normalized eigenvectors. The energies given have been subtracted
    the energy of the ground state.
If the option ''Return as states'' is set to True, then the function
    returns a list with three elements. The first element is the
    global level basis for the f^numE configuration, given as a list
    of lists of the form {LS string, J}. The second element are the
    mayor LSJ components in the returned eigenstates. The third
    element is a list of lists with three elements, in each list the
    first element being equal to the energy, the second being equal to
     the value of J, and the third being equal to the corresponding
    normalized eigenvector (given as a row). The energies given have
    been subtracted the energy of the ground state, and the states
    have been sorted in order of increasing energy.
The following options are admitted:
  - ''Overwrite Hamiltonian'', if set to True the function will
    overwrite the symbolic Hamiltonian. Default is False.
  - ''Return as states'', see description above. Default is True.
  - ''Simplifier'', this is a list with symbols that are set to zero
    for defining the parameters kept in the level  description.
";
Options[LevelSolver] = {
  "Overwrite Hamiltonian" -> False,
  "Return as states" -> True,
  "Simplifier" -> Join[
    cfSymbols,
    TSymbols,
    casimirSymbols,
    pseudoMagneticSymbols,
    marvinSymbols,
    DeleteCases[magneticSymbols,ζ]
  ],
  "PrintFun" -> PrintTemporary
};
LevelSolver[numE_Integer, params0_Association, OptionsPattern[]] :=
    Module[
  {ln, simplifier, simpleHam, basis,
  numHam, eigensys, startTime, endTime,
  diagonalTime, params=params0, globalBasis,
  eigenVectors, eigenEnergies, eigenJs,
  states, groundEnergy, allEnergies, PrintFun},
  (
    ln          = theLanthanides[[numE]];
    basis       = BasisLSJ[numE, "AsAssociation"->True];
```

```
    simplifier = OptionValue["Simplifier"];
    PrintFun   = OptionValue["PrintFun"];
    PrintFun["> LevelSolver for ",ln," with ",numE," f-electrons."];
    PrintFun["> Loading the symbolic level Hamiltonian ..."];
    simpleHam  = LevelSimplerSymbolicHamMatrix[numE,
      "Simplifier" -> simplifier,
      "Overwrite"  -> OptionValue["Overwrite Hamiltonian"]
    ];
    (* Everything that is not given is set to zero *)
    PrintFun["> Setting to zero every parameter not given ..."];
    params     = ParamPad[params, "PrintFun" -> PrintFun];
    PrintFun[params];
    (* Create the numeric hamiltonian *)
    PrintFun["> Replacing parameters in the J-blocks of the
    Hamiltonian to produce numeric arrays ..."];
    numHam     = N /@ Map[ReplaceInSparseArray[#, params]&, simpleHam
    ];
    Clear[simpleHam];
    (* Eigensolver *)
    PrintFun["> Diagonalizing the numerical Hamiltonian within each
    separate J-subspace ..."];
    startTime    = Now;
    eigensys     = Eigensystem /@ numHam;
    endTime      = Now;
    diagonalTime = QuantityMagnitude[endTime-startTime,"Seconds"];
    allEnergies  = Flatten[First/@Values[eigensys]];
    groundEnergy = Min[allEnergies];
    eigensys     = Map[Chop[{#[[1]]-groundEnergy,#[[2]]}]&,eigensys];
    eigensys     = Association@KeyValueMap[#1->{basis[#1],#2} &,
    eigensys];
    PrintFun[">> Diagonalization took ",diagonalTime," seconds."];
    If[OptionValue["Return as states"],
      (
        PrintFun["> Padding the eigenvectors to correspond to the
    level basis ..."];
        eigenVectors  = SparseArray @ BlockDiagonalMatrix[Values
    [#[[2, 2]] & /@ eigensys]];
        globalBasis   = Flatten[Values[basis], 1];
        eigenEnergies = Flatten[Values[#[[2, 1]] & /@ eigensys]];
        eigenJs       = Flatten[KeyValueMap[ConstantArray[#1, Length
    [#2[[2, 2]]]] &, eigensys]];
        states        = Transpose[{eigenEnergies, eigenJs,
    eigenVectors}];
        states        = SortBy[states, First];
        eigenVectors  = Last /@ states;
        LSJmultiplets = (RemoveTrailingDigits[#[[1]]] <> ToString[
    InputForm[#[[2]]]]) & /@ globalBasis;
        majorComponentIndices = Ordering[Abs[#]][[-1]] & /@
    eigenVectors;
        levelLabels           = LSJmultiplets[[majorComponentIndices
    ]];
        Return[{globalBasis, levelLabels, states}];
      ),
      Return[{basis, eigensys}]
    ];
  )
];
```

2.4 The coefficients of fractional parentage

In the 1920s and 1930s, when spectroscopic evidence was being studied to inform the emergent quantum mechanics, one conceptual tool that was put forward for the analysis of the complex spectra of ions [BG34] involved using the spectrum of an ion at one stage of ionization to understand another stage. For instance, using the fourth spectrum of oxygen (OIV) in order to understand the third spectrum (OIII) of the same element.

In 1943 Giulio Racah [Rac43] provided a useful extension to this idea. In addition of using the energies of one spectrum to span the energies of another, Racah extended this idea to the wavefunctions themselves, such that from configuration $\underline{\mathrm{f}}^{n-1}$ one can create the wavefunctions for $\underline{\mathrm{f}}^{n}$ with all the required antisymmetry and normalization conditions. In this approach, a given *daughter* term in $\underline{\mathrm{f}}^{n}$ has a number of *parent* terms in $\underline{\mathrm{f}}^{n-1}$, with the coefficients of fractional parentage determining how much of each parent is in the daughter

as a sum over parents

$$|\underline{\ell}^n \alpha LS\rangle = \sum_{\bar{\alpha}\bar{L}\bar{S}} \underbrace{\left(\underline{\ell}^{n-1}\bar{\alpha}\bar{L}\bar{S}\right\}\underline{\ell}^n \alpha LS\right)}_{\substack{\text{How much of parent } |\underline{\ell}^{n-1}\bar{\alpha}\bar{L}\bar{S}\rangle \\ \text{is in daughter} |\underline{\ell}^n \alpha LS\rangle}} \underbrace{|\left(\underline{\ell}^{n-1}\bar{\alpha}\bar{L}\bar{S}, \underline{\ell}\right) \alpha LS\rangle}_{\substack{\text{Couple an additional } \underline{\ell} \\ \text{to the parent } |\underline{\ell}^{n-1}\bar{\alpha}\bar{L}\bar{S}\rangle}} . \tag{14}$$

More importantly for **qlanth**, the coefficients of fractional parentage can be used to evaluate matrix elements of operators, such as in &qn-29, &qn-51, &qn-65, and &qn-41. These formulas realize a convenient calculation advantage: if one knows matrix elements in one configuration, then one can immediately calculate them in any other configuration.

In principle all the data that is needed in order to evaluate the matrix elements that **qlanth** uses can all be derived from coefficients of fractional parentage, tables of 6-j and 3-j coefficients, the LSUW labels for the terms in the $\underline{f}^n$ configurations, reduced matrix elements in $\underline{f}^3$ for the three-body operators, and reduced matrix elements in $\underline{f}^2$ for the magnetic interactions.

The data for the coefficients of fractional parentage we owe to [Vel00] from which the file `B1F_all.txt` originates, and which we use here to extract this useful "escalator" up the $\underline{f}^n$ configurations.

In **qlanth** the function `GenerateCFPTable` is used to parse the data contained in this file. From this data the association `CFP` is generated. This association has keys that represent LS terms for a configuration $\underline{f}^n$ and values that are lists which contain all the parent terms, together with the corresponding coefficients of fractional parentage.

```
GenerateCFPTable::usage = "GenerateCFPTable[] generates the table for the coefficients of fractional parentage. If the optional parameter ''Export'' is set to True then the resulting data is saved to ./data/CFPTable.m.
The data being parsed here is the file attachment B1F_ALL.TXT which comes from Velkov's thesis.";
Options[GenerateCFPTable] = {"Export" -> True};
GenerateCFPTable[OptionsPattern[]] := Module[
  {rawText, rawLines, leadChar, configIndex, line, daughter,
  lineParts, numberCode, parsedNumber, toAppend, CFPTablefname},
  (
    CleanWhitespace[string_]      := StringReplace[string, RegularExpression["\\s+"]->" "];
    AddSpaceBeforeMinus[string_] := StringReplace[string, RegularExpression["(?<!\\s)-"]->" -"];
    ToIntegerOrString[list_]      := Map[If[StringMatchQ[#, NumberString], ToExpression[#], #] &, list];
    CFPTable       = ConstantArray[{},7];
    CFPTable[[1]] = {{"2F",{"1S",1}}};

    (* Cleaning before processing is useful *)
    rawText  = Import[FileNameJoin[{moduleDir, "data", "B1F_ALL.TXT"}]];
    rawLines = StringTrim/@StringSplit[rawText,"\n"];
    rawLines = Select[rawLines,#!=""&];
    rawLines = CleanWhitespace/@rawLines;
    rawLines = AddSpaceBeforeMinus/@rawLines;

    Do[(
      (* the first character can be used to identify the start of a block *)
      leadChar=StringTake[line,{1}];
      (* ..FN, N is at position 50 in that line *)
      If[leadChar=="[",
      (
        configIndex=ToExpression[StringTake[line,{50}]];
        Continue[];
      )
      ];
      (* Identify which daughter term is being listed *)
      If[StringContainsQ[line,"[DAUGHTER TERM]"],
        daughter=StringSplit[line,"["][[1]];
        CFPTable[[configIndex]]=Append[CFPTable[[configIndex]],{daughter}];
        Continue[];
      ];
      (* Once we get here we are already parsing a row with coefficient data *)
      lineParts     = StringSplit[line," "];
```

```
      parent       = lineParts[[1]];
      numberCode   = ToIntegerOrString[lineParts[[3;;]]];
      parsedNumber = SquarePrimeToNormal[numberCode];
      toAppend     = {parent,parsedNumber};
      CFPTable[[configIndex]][[-1]] = Append[CFPTable[[configIndex
    ]][[-1]], toAppend]
    ),
    {line,rawLines}];
    If[OptionValue["Export"],
      (
      CFPTablefname = FileNameJoin[{moduleDir, "data", "CFPTable.m"
    }];
      Export[CFPTablefname, CFPTable];
      )
    ];
    Return[CFPTable];
  )
];
```

The coefficients of fractional parentage are traditionally only provided up to $\underline{\mathrm{f}}^7$ (such is the case in `B1f_all.txt`), tabulating these beyond $\underline{\mathrm{f}}^7$ would be redundant since the coefficients of fractional parentage beyond $\underline{\mathrm{f}}^7$ satisfy relationships with those below $\underline{\mathrm{f}}^7$. According to [NK63]

$$\left(\underline{\ell}^{(14-n)-1}\bar{\alpha}\bar{L}\bar{S}\right\}\underline{\ell}^{(14-n)}\alpha LS\Big) = \xi(-1)^{S+\bar{S}+L+\bar{L}-7/2}\sqrt{\frac{(n+1)[\![\bar{S}]\!][\![\bar{L}]\!]}{(14-n)[\![S]\!][\![L]\!]}}\left(\underline{\ell}^{n-1}\alpha LS\right\}\underline{\ell}^{n}\bar{\alpha}\bar{L}\bar{S}\Big)$$

$$\text{with } \xi = \begin{cases} 1 & \text{if } n \neq 6 \\ (-1)^{(\bar{\nu}-1)/2} & \text{if } n = 6 \end{cases}, \text{ and where } \bar{\boldsymbol{\nu}} \text{ is the seniority of } |\bar{\alpha}\bar{L}\bar{S}\rangle. \quad (15)$$

Under this relationship and phase convention, the matrix elements of operators pick up a global phase which depends on the rank of the operator, namely [NK63]:

$$\langle \underline{\mathrm{f}}^{14-n}\alpha SL\|\hat{U}^{(K)}\|\underline{\mathrm{f}}^{14-n}\alpha' S'L'\rangle = -(-1)^K\langle \underline{\mathrm{f}}^{n}\alpha SL\|\hat{U}^{(K)}\|\underline{\mathrm{f}}^{n}\alpha' S'L'\rangle \quad (16)$$

for a single tensor operator $\hat{U}^{(K)}$ of rank K, and

$$\langle \underline{\mathrm{f}}^{14-n}\alpha SL\|\hat{V}^{(1K)}\|\underline{\mathrm{f}}^{14-n}\alpha' S'L'\rangle = (-1)^K\langle \underline{\mathrm{f}}^{n}\alpha SL\|\hat{V}^{(1K)}\|\underline{\mathrm{f}}^{n}\alpha' S'L'\rangle \quad (17)$$

for a double tensor operator $\hat{V}^{(1K)}$ of rank 1 for spin and rank K for orbit.

2.5 Going beyond $\underline{\mathrm{f}}^7$

In most cases all matrix elements in **qlanth** are only calculated up to and including $\underline{\mathrm{f}}^7$. Beyond $\underline{\mathrm{f}}^7$ adequate changes of sign are enforced to take into account the equivalence that can be made between $\underline{\mathrm{f}}^n$ and $\underline{\mathrm{f}}^{14-n}$ as given by &qn-17 and &qn-16.

This is enforced when the function `HamMatrixAssembly` is called. In there `HoleElectronConjugation` is the function responsible for enforcing a global sign flip for the following operators (or alternatively, to their accompanying coefficients):

$$\begin{aligned} &\zeta, B_q^{(k)} \\ &T^{(2)\prime}, T^{(3)}, T^{(4)}, T^{(6)}, T^{(7)}, T^{(8)} \\ &T^{(11)\prime}, T^{(12)}, T^{(13)}, T^{(14)}, T^{(15)}, T^{(16)}, T^{(17)}, T^{(18)}, T^{(19)}, \end{aligned} \quad (18)$$

$T^{(2)}$ and $T^{(11)}$ must be treated separately since they have a part that changes sign, and another that doesn't.

```
HoleElectronConjugation::usage = "HoleElectronConjugation[params]
    takes the parameters (as an association) that define a
    configuration and converts them so that they may be interpreted as
     corresponding to a complentary hole configuration. Some of this
    can be simply done by changing the sign of the model parameters.
    In the case of the effective three body interaction the
    relationship is more complex and is controlled by the value of the
     isE variable.";
HoleElectronConjugation[params_] := Module[
  {newparams = params},
  (
    flipSignsOf = Join[{ζ} , cfSymbols, TSymbols];
    flipped = Table[
```

```
      (
        flipper -> - newparams[flipper]
      ),
      {flipper, flipSignsOf}
      ];
    nonflipped = Table[
      (
        flipper -> newparams[flipper]
      ),
      {flipper, Complement[Keys[newparams], flipSignsOf]}
      ];
    flippedParams = Association[Join[nonflipped, flipped]];
    flippedParams = Select[flippedParams, FreeQ[#, Missing]&];
    Return[flippedParams];
  )
];
```

2.6 The J-J' block structure

Now that we know how the bases are ordered, we can already understand the structure of how the final Hamiltonian matrix representation in the $|LSJM_J\rangle$ basis is put together.

For a given configuration $\underline{f}^n$ and for each term $\hat{h}$ in the Hamiltonian, **qlanth** first calculates the matrix elements $\langle \alpha LSJM_J|\hat{h}|\alpha' L'S'J'M'_J\rangle$ so that for each interaction an association with keys of the form $\{J, J'\}$ is created. The values being rectangular arrays.

Fig-5 shows roughly this block structure for $\underline{f}^2$. In that figure, the shape of the rectangular blocks is determined by the fact that for $J = 0, 1, 2, 3, 4, 5, 6$ there are (2, 3, 15, 7, 27, 11, 26) corresponding basis states. As such, for example, the first row of blocks consists of blocks of size (2×2), (2×3), (2×15), (2×7), (2×27), (2×11), and (2×26).

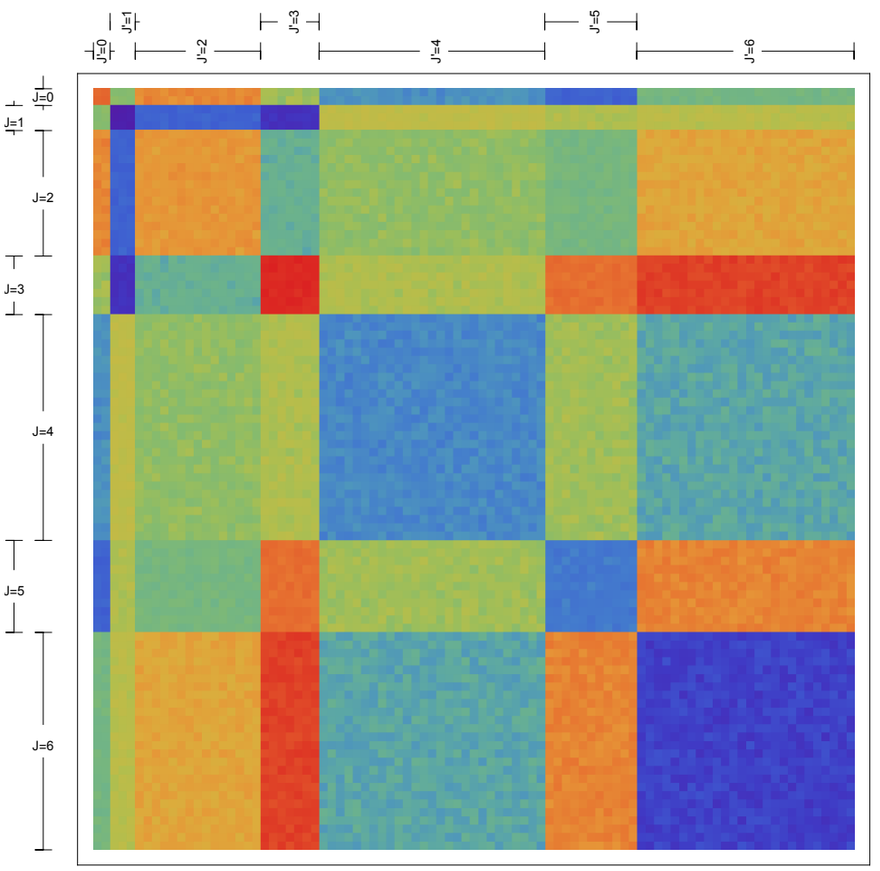


Figure 5: The J-J' block structure for $\underline{f}^2$

In **qlanth** these blocks are put together by the function JJBlockMatrix which adds together the contributions from the different terms in the Hamiltonian.

```
JJBlockMatrix::usage = "For given J, J' in the f^n configuration
    JJBlockMatrix[numE, J, J'] determines all the SL S'L' terms that
    may contribute to them and using those it provides the matrix
    elements <J, LS | H | J', LS'>. H having contributions from the
    following interactions: Coulomb, spin-orbit, spin-other-orbit,
```

```
    electrostatically-correlated-spin-orbit, spin-spin, three-body
    interactions, and crystal-field.";
Options[JJBlockMatrix] = {"Sparse"->True, "ChenDeltas"->False};
JJBlockMatrix[numE_, J_, Jp_, CFTable_, OptionsPattern[]] := Module[
  {NKSLJMs, NKSLJMps, NKSLJM, NKSLJMp,
  SLterm, SpLpterm,
  MJ, MJp,
  subKron, matValue, eMatrix},
  (
    NKSLJMs  = AllowedNKSLJMforJTerms[numE, J];
    NKSLJMps = AllowedNKSLJMforJTerms[numE, Jp];
    eMatrix =
      Table[
        (*Condition for a scalar matrix op*)
        SLterm   = NKSLJM[[1]];
        SpLpterm = NKSLJMp[[1]];
        MJ       = NKSLJM[[3]];
        MJp      = NKSLJMp[[3]];
        subKron  = (
            KroneckerDelta[J, Jp] *
            KroneckerDelta[MJ, MJp]
                );
        matValue =
          If[subKron==0,
            0,
              (
                ElectrostaticTable[{numE, SLterm, SpLpterm}] +
                ElectrostaticConfigInteraction[{SLterm, SpLpterm}] +
                SpinOrbitTable[{numE, SLterm, SpLpterm, J}] +
                MagneticInteractions[{numE, SLterm, SpLpterm, J},
                  "ChenDeltas" -> OptionValue["ChenDeltas"]] +
                ThreeBodyTable[{numE, SLterm, SpLpterm}]
              )
          ];
        matValue += CFTable[{numE, SLterm, J, MJ, SpLpterm, Jp, MJp
    }];
        matValue,
      {NKSLJMp, NKSLJMps},
      {NKSLJM , NKSLJMs}
      ];
  If[OptionValue["Sparse"],
    eMatrix = SparseArray[eMatrix]
  ];
  Return[eMatrix]
)
];
```

Once these blocks have been calculated and saved to disk (in the folder `./hams/`) the function `HamMatrixAssembly` takes them, assembles the arrays in block form, and finally flattens them to provide a sparse rank-2 array. These are the arrays that are finally diagonalized to find energies and eigenstates. Through options, this function can also return the Hamiltonian in block form, which is useful for the level description of the eigenstates.

```
HamMatrixAssembly::usage = "HamMatrixAssembly[numE] returns the
    Hamiltonian matrix for the f^n_i configuration. The matrix is
    returned as a SparseArray.
The function admits an optional parameter ''FilenameAppendix'' which
    can be used to modify the filename to which the resulting array is
     exported to.
It also admits an optional parameter ''IncludeZeeman'' which can be
    used to include the Zeeman interaction. The default is False
The option ''Set t2Switch'' can be used to toggle on or off setting
    the t2 selector automatically or not, the default is True, which
    replaces the parameter according to numE.
The option ''ReturnInBlocks'' can be used to return the matrix in
    block or flattened form. The default is to return it in flattened
    form.";
Options[HamMatrixAssembly] = {
      "FilenameAppendix"->"",
      "IncludeZeeman"->False,
      "Set t2Switch"->True,
      "ReturnInBlocks"->False};
HamMatrixAssembly[nf_, OptionsPattern[]] := Module[
  {numE, ii, jj, howManyJs, Js, blockHam},
  (
```

```
    (*######################################*)
    ImportFun = ImportMZip;
    (*######################################*)
    (*hole-particle equivalence enforcement*)
    numE = nf;
    allVars = {E0, E1, E2, E3, ζ, F0, F2, F4, F6, M0, M2, M4, T2, T2p
    ,
      T3, T4, T6, T7, T8, P0, P2, P4, P6, gs,
      α, β, γ, B02, B04, B06, B12, B14, B16,
      B22, B24, B26, B34, B36, B44, B46, B56, B66, S12, S14, S16, S22
    ,
      S24, S26, S34, S36, S44, S46, S56, S66, T11p, T12, T14, T15,
    T16,
      T17, T18, T19, Bx, By, Bz};
    params0 = AssociationThread[allVars, allVars];
    If[nf > 7,
      (
        numE = 14 - nf;
        params = HoleElectronConjugation[params0];
        If[OptionValue["Set t2Switch"], params[t2Switch] = 0];
      ),
      params = params0;
      If[OptionValue["Set t2Switch"], params[t2Switch] = 1];
    ];
    (* Load symbolic expressions for LS,J,J' energy sub-matrices. *)
    emFname = JJBlockMatrixFileName[numE, "FilenameAppendix" ->
    OptionValue["FilenameAppendix"]];
    JJBlockMatrixTable = ImportFun[emFname];
    (*Patch together the entire matrix representation using J,J'
    blocks.*)
    PrintTemporary["Patching JJ blocks ..."];
    Js         = AllowedJ[numE];
    howManyJs  = Length[Js];
    blockHam   = ConstantArray[0, {howManyJs, howManyJs}];
    Do[
      blockHam[[jj, ii]] = JJBlockMatrixTable[{numE, Js[[ii]], Js[[jj
    ]]}];,
    {ii, 1, howManyJs},
    {jj, 1, howManyJs}
    ];

    (* Once the block form is created flatten it *)
    If[Not[OptionValue["ReturnInBlocks"]],
      (blockHam = ArrayFlatten[blockHam];
      blockHam  = ReplaceInSparseArray[blockHam, params];
      ),
      (blockHam  = Map[ReplaceInSparseArray[#, params]&,blockHam
    ,{2}];)
    ];

    If[OptionValue["IncludeZeeman"],
      (
        PrintTemporary["Including Zeeman terms ..."];
        {magx, magy, magz} = MagDipoleMatrixAssembly[numE, "
    ReturnInBlocks" -> OptionValue["ReturnInBlocks"]];
        blockHam += - teslaToKayser * (Bx * magx + By * magy + Bz *
    magz);
      )
    ];
    Return[blockHam];
  )
];
```

In **qlanth** the reduced matrix elements of all operators, and the subsequent matrix elements of $\hat{\mathcal{H}}$ are calculated exactly. This is in contrast to what is done in older alternatives to **qlanth** such as linuxemp, in which calculations of reduced matrix elements were obtained from tables calculated with finite precision. To underscore this fact, &qn-2.6 shows an example of a J-J block as contained in **qlanth**.

2.7 Kramers' degeneracy

In the odd-electron cases, every energy is at least doubly degenerate. In **qlanth**, except in the case of the experimental data compiled for LaF_3, Kramers' degeneracy is given/expected explicitly.

	$\vert^4\mathrm{F}_{1,-1}\rangle$	$\vert^4\mathrm{F}_{1,0}\rangle$	$\vert^4\mathrm{F}_{1,1}\rangle$
$\langle^4\mathrm{F}_{1,-1}\vert$	$2\alpha+\beta-\frac{B_0^{(2)}}{10}+\gamma$ $-\frac{\zeta}{2}+\frac{14F^{(0)}}{13}+\frac{43F^{(2)}}{195}+\frac{19F^{(4)}}{429}$ $-\frac{875F^{(6)}}{5577}+2m^{(0)}\sigma_{\mathrm{SS}}+\frac{61m^{(0)}}{12}$ $+4m^{(2)}\sigma_{\mathrm{SS}}+\frac{145m^{(2)}}{12}+\frac{50m^{(4)}\sigma_{\mathrm{SS}}}{11}$ $+\frac{1805m^{(4)}}{132}+\frac{43P^{(2)}}{1080}+\frac{19P^{(4)}}{2376}$ $-\frac{875P^{(6)}}{30888}$	$-\frac{\sqrt{3}B_1^{(2)}}{10}-\frac{1}{10}i\sqrt{3}S_2^{(2)}$	$-\frac{1}{5}\sqrt{\frac{3}{2}}B_2^{(2)}-\frac{1}{5}i\sqrt{\frac{3}{2}}S_2^{(2)}$
$\langle^4\mathrm{F}_{1,0}\vert$	$-\frac{\sqrt{3}B_1^{(2)}}{10}+\frac{1}{10}i\sqrt{3}S_2^{(2)}$	$2\alpha+\beta+\frac{B_0^{(2)}}{5}+\gamma$ $-\frac{\zeta}{2}+\frac{14F^{(0)}}{13}+\frac{43F^{(2)}}{195}+\frac{19F^{(4)}}{429}$ $-\frac{875F^{(6)}}{5577}+2m^{(0)}\sigma_{\mathrm{SS}}+\frac{61m^{(0)}}{12}$ $+4m^{(2)}\sigma_{\mathrm{SS}}+\frac{145m^{(2)}}{12}+\frac{50m^{(4)}\sigma_{\mathrm{SS}}}{11}$ $+\frac{1805m^{(4)}}{132}+\frac{43P^{(2)}}{1080}+\frac{19P^{(4)}}{2376}$ $-\frac{875P^{(6)}}{30888}$	$\frac{\sqrt{3}B_1^{(2)}}{10}+\frac{1}{10}i\sqrt{3}S_2^{(2)}$
$\langle^4\mathrm{F}_{1,1}\vert$	$-\frac{1}{5}\sqrt{\frac{3}{2}}B_2^{(2)}+\frac{1}{5}i\sqrt{\frac{3}{2}}S_2^{(2)}$	$\frac{\sqrt{3}B_1^{(2)}}{10}-\frac{1}{10}i\sqrt{3}S_2^{(2)}$	$2\alpha+\beta-\frac{B_0^{(2)}}{10}+\gamma$ $-\frac{\zeta}{2}+\frac{14F^{(0)}}{13}+\frac{43F^{(2)}}{195}+\frac{19F^{(4)}}{429}$ $-\frac{875F^{(6)}}{5577}+2m^{(0)}\sigma_{\mathrm{SS}}+\frac{61m^{(0)}}{12}$ $+4m^{(2)}\sigma_{\mathrm{SS}}+\frac{145m^{(2)}}{12}+\frac{50m^{(4)}\sigma_{\mathrm{SS}}}{11}$ $+\frac{1805m^{(4)}}{132}+\frac{43P^{(2)}}{1080}+\frac{19P^{(4)}}{2376}$ $-\frac{875P^{(6)}}{30888}$

(19)

3 Interactions

3.1 $\hat{\mathcal{H}}_{\mathrm{k}}$: kinetic energy

$$\hat{\mathcal{H}}_{\mathrm{k}} = -\frac{\hbar^2}{2m}\sum_{i=1}^{N}\nabla_i^2 \text{ (kinetic energy of N v-electrons)} \tag{20}$$

Since our description is limited to a single configuration, the kinetic energy simply contributes a constant energy shift, and since all we care about are energy differences, then this term can be omitted from the analysis.

To interpret the range of energies that result from diagonalizing the semi-empirical Hamiltonian, it might be instructive, however, to note that this term imparts an energy of about $10\,\mathrm{eV} \approx 10^6\mathcal{K}$[16] to each electron.

3.2 $\hat{\mathcal{H}}_{\mathrm{e:sn}}$: the central field potential

$$\hat{\mathcal{H}}_{\mathrm{e:sn}} = -e^2\sum_{i=1}^{Z}\frac{1}{r_i} + e^2\underbrace{\sum_{i=1}^{n}\sum_{j=1}^{Z-n}\frac{1}{r_{ij}}}_{\substack{\text{Repulsion between valence}\\ \text{and inner shell}\\ \text{electrons}}} \approx \sum_{i=1}^{n}V_{\mathrm{sn}}(r_i) \text{ (with Z = atomic No.)} \tag{21}$$

In principle, the sum over the Coulomb potential should extend over the nuclear charge and over all the electrons in the atom (not just the valence electrons). However, given the shell structure of the atom, the lanthanide ions "see" the nuclear charge as shielded by a xenon core. Since every closed shell is a singlet, having spherical symmetry, these shields are like spherical shells surrounding the nucleus.

The precise form of $V_{\mathrm{sn}}(r_i)$ is not of our concern here; all that matters is that we assume that it is spherically symmetric so that we can justify the separation of radial and angular parts of the wavefunctions.

3.3 $\hat{\mathcal{H}}_{\mathrm{e:e}}$: e:e repulsion

$$\hat{\mathcal{H}}_{\mathrm{e:e}} = \sum_{i>j}^{n,n}\frac{e^2}{\|\vec{r}_i - \vec{r}_j\|} = \sum_{k=0,2,4,6}F^{(k)}\hat{f}_k = \sum_{k=0,1,2,3}E_k\hat{e}_k \tag{22}$$

This term is the first we will not discard. Calculating this term for the $\underline{\mathrm{f}}^n$ configurations was one of the contributions from Slater, as such the parameters we use to write it up are called *Slater integrals*. After the analysis from Slater, Giulio Racah contributed further to the analysis of this term [Rac49]. The insight that Racah had was that if in a given operator one identifies the parts in it that transform accordingly to the different symmetry groups present in the problem, then calculating the necessary matrix element in all $\underline{\mathrm{f}}^n$ configurations can be greatly simplified.

The functions used in `qlanth` to compute these LS-reduced matrix elements [17] are `Electrostatic` and `fsubk`. In addition to these, the LS-reduced matrix elements of the tensor operators $\hat{C}^{(k)}$ and $\hat{U}^{(k)}$ are also needed. These functions are based in equations 12.16 and 12.17 from [Cow81] as specialized for the case of electrons belonging to a single $\underline{\mathrm{f}}^n$ configuration. By default this term is computed in terms of $F^{(k)}$ Slater integrals, but it can also be computed in terms of the E_k Racah parameters, the functions `EtoF` and `FtoE` are useful for going from one representation to the other.

$$\langle \underline{\mathrm{f}}^n\alpha^{2S+1}\mathrm{L}\|\hat{\mathcal{H}}_{\mathrm{e:e}}\|\underline{\mathrm{f}}^n\alpha'^{2S'+1}\mathrm{L'}\rangle = \sum_{k=0,2,4,6}F^{(f)}{}_k(n,\alpha LS,\alpha' L'S') \tag{23}$$

where

$$f_k(n,\alpha LS,\alpha' L'S') = \frac{1}{2}\delta(S,S')\delta(L,L')\langle\underline{\mathrm{f}}\|\hat{C}^{(k)}\|\underline{\mathrm{f}}\rangle^2\times$$
$$\left\{\frac{1}{2L+1}\sum_{\alpha''L''}\langle\underline{\mathrm{f}}^n\alpha''L''S\|\hat{U}^{(k)}\|\underline{\mathrm{f}}^n\alpha LS\rangle\langle\underline{\mathrm{f}}^n\alpha''L''S\|\hat{U}^{(k)}\|\underline{\mathrm{f}}^n\alpha' LS\rangle - \delta(\alpha,\alpha')\frac{n\,(4\underline{\mathrm{f}}+2-n)}{(2\underline{\mathrm{f}}+1)(4\underline{\mathrm{f}}+1)}\right\}. \tag{24}$$

[16] Note, (Kayser) $\mathcal{K} \equiv \mathrm{cm}^{-1}$, see section on units. [17] An LS-reduced matrix element is ...

```
Electrostatic::usage = "Electrostatic[{numE, NKSL, NKSLp}] returns
    the LS reduced matrix element for repulsion matrix element for
    equivalent electrons. See equation 2-79 in Wybourne (1965). The
    option ''Coefficients'' can be set to ''Slater'' or ''Racah''. If
    set to ''Racah'' then E_k parameters and e^k operators are assumed
    , otherwise the Slater integrals F^k and operators f_k. The
    default is ''Slater''.";
Options[Electrostatic] = {"Coefficients" -> "Slater"};
Electrostatic[{numE_, NKSL_, NKSLp_}, OptionsPattern[]] := Module[
  {fsub0, fsub2, fsub4, fsub6,
   esub0, esub1, esub2, esub3,
   fsup0, fsup2, fsup4, fsup6,
   eMatrixVal, orbital},
  (
    orbital = 3;
    Which[
      OptionValue["Coefficients"] == "Slater",
      (
        fsub0 = fsubk[numE, orbital, NKSL, NKSLp, 0];
        fsub2 = fsubk[numE, orbital, NKSL, NKSLp, 2];
        fsub4 = fsubk[numE, orbital, NKSL, NKSLp, 4];
        fsub6 = fsubk[numE, orbital, NKSL, NKSLp, 6];
        eMatrixVal = fsub0*F0 + fsub2*F2 + fsub4*F4 + fsub6*F6;
      ),
      OptionValue["Coefficients"] == "Racah",
      (
        fsup0 = fsupk[numE, orbital, NKSL, NKSLp, 0];
        fsup2 = fsupk[numE, orbital, NKSL, NKSLp, 2];
        fsup4 = fsupk[numE, orbital, NKSL, NKSLp, 4];
        fsup6 = fsupk[numE, orbital, NKSL, NKSLp, 6];
        esub0 = fsup0;
        esub1 = 9/7*fsup0 +   1/42*fsup2 +   1/77*fsup4 +  1/462*
    fsup6;
        esub2 =             143/42*fsup2 - 130/77*fsup4 + 35/462*
    fsup6;
        esub3 =              11/42*fsup2 + 4/77*fsup4   -  7/462*
    fsup6;
        eMatrixVal = esub0*E0 + esub1*E1 + esub2*E2 + esub3*E3;
      )
    ];
    Return[eMatrixVal];
  )
];
```

```
fsubk::usage = "fsubk[numE, orbital, SL, SLp, k] gives the Slater
    integral f_k for the given configuration and pair of SL terms. See
     equation 12.17 in TASS.";
fsubk[numE_, orbital_, NKSL_, NKSLp_, k_] := Module[
  {terms, S, L, Sp, Lp,
  termsWithSameSpin, SL,
  fsubkVal, spinMultiplicity,
  prefactor, summand1, summand2},
  (
    {S, L}   = FindSL[NKSL];
    {Sp, Lp} = FindSL[NKSLp];
    terms    = AllowedNKSLTerms[numE];
    (* sum for summand1 is over terms with same spin *)
    spinMultiplicity  = 2*S + 1;
    termsWithSameSpin = StringCases[terms, ToString[spinMultiplicity]
     ~~ __];
    termsWithSameSpin = Flatten[termsWithSameSpin];
    If[Not[{S, L} == {Sp, Lp}],
      Return[0]
    ];
    prefactor = 1/2 * Abs[Ck[orbital, k]]^2;
    summand1 = Sum[(
        ReducedUkTable[{numE, orbital, SL, NKSL,  k}] *
        ReducedUkTable[{numE, orbital, SL, NKSLp, k}]
        ),
      {SL, termsWithSameSpin}
    ];
    summand1 = 1 / TPO[L] * summand1;
    summand2 = (
      KroneckerDelta[NKSL, NKSLp] *
        (numE *(4*orbital + 2 - numE)) /
```

```
        ((2*orbital + 1) * (4*orbital + 1))
      );
    fsubkVal = prefactor*(summand1 - summand2);
    Return[fsubkVal];
  )
];
```

```
EtoF::usage = "EtoF[E0, E1, E2, E3] calculates the Slater integral
    parameters {F0, F2, F4, F6} corresponding to the given Racah
    parameters {E0, E1, E2, E3}. This is the inverse of the FtoE
    function.";
EtoF[E0_, E1_, E2_, E3_] := Module[
  {F0, F2, F4, F6},
  (
    F0 = 1/7       (7 E0 + 9 E1);
    F2 = 75/14     (E1 + 143 E2 + 11 E3);
    F4 = 99/7      (E1 - 130 E2 + 4 E3);
    F6 = 5577/350 (E1 + 35 E2 - 7 E3);
    Return[{F0, F2, F4, F6}];
  )
];
```

```
FtoE::usage = "FtoE[F0, F2, F4, F6] calculates the Racah parameters {
    E0, E1, E2, E3} corresponding to the given Slater integrals.
See eqn. 2-80 in Wybourne.
Note that in that equation the subscripted Slater integrals are used
    but since this function assumes the the input values are
    superscripted Slater integrals, it is necessary to convert them
    using Dk.";
FtoE[F0_, F2_, F4_, F6_] := Module[
  {E0, E1, E2, E3},
  (
    E0 = (F0 - 10*F2/Dk[2] - 33*F4/Dk[4] - 286*F6/Dk[6]);
    E1 = (70*F2/Dk[2] + 231*F4/Dk[4] + 2002*F6/Dk[6])/9;
    E2 = (F2/Dk[2] - 3*F4/Dk[4] + 7*F6/Dk[6])/9;
    E3 = (5*F2/Dk[2] + 6*F4/Dk[4] - 91*F6/Dk[6])/3;
    Return[{E0, E1, E2, E3}];
  )
];
```

3.4 $\hat{\mathscr{H}}_{\text{s:o}}$: spin-orbit

The spin-orbit interaction arises from the interaction of the magnetic moment of the electron and the magnetic field that its orbital motion generates. In terms of the central potential $V_{\text{s:n}}$, the spin-orbit term for a single electron is

$$\hat{h}_{\text{s:o}} = \frac{\hbar^2}{2m_e^2c^2}\left(\frac{1}{r}\frac{\mathrm{d}V_{\text{s:n}}}{\mathrm{d}r}\right)\hat{l}\cdot\hat{s} := \zeta(r)\hat{l}\cdot\hat{s}. \tag{25}$$

Adding this term for all the n valence electrons, and replacing $\zeta(r)$ by its radial average ζ then gives

$$\hat{\mathscr{H}}_{\text{s:o}} = \zeta\sum_i^n \hat{l}_i\cdot\hat{s}_i. \tag{26}$$

From equations 2-106 to 2-109 in Wybourne [Wyb63] the matrix elements we need are given by

$$\begin{aligned}\langle\alpha LSJM_J|\hat{\mathscr{H}}_{\text{s:o}}|\alpha' L'S'J'M_{J'}\rangle &= \zeta\delta(J,J')\delta(M_J,M_{J'})\langle\alpha LSJM_J|\sum_i^n \hat{l}_i\cdot\hat{s}_i|\alpha' L'S'JM_J\rangle \\ &= \zeta\delta(J,J')\delta(M_J,M_{J'})(-1)^{J+L+S'}\begin{Bmatrix} L & L' & 1\\ S' & S & J\end{Bmatrix}\langle\alpha LS|\sum_i^n \hat{l}_i\cdot\hat{s}_i|\alpha' L'S'\rangle \\ = \zeta\delta(J,J')\delta(M_J,M_{J'})(-1)^{J+L+S'}&\begin{Bmatrix} L & L' & 1\\ S' & S & J\end{Bmatrix}\sqrt{\underline{\ell}(\underline{\ell}+1)(2\underline{\ell}+1)}\langle\alpha LS\|\hat{V}^{(11)}\|\alpha' L'S'\rangle,\end{aligned} \tag{27}$$

where $\hat{V}^{(11)}$ is a double tensor operator of rank one over spin and orbital parts defined as

$$\hat{V}^{(11)} = \sum_{i=1}^n\left(\hat{s}\hat{u}^{(1)}\right)_i, \tag{28}$$

in which the rank on the spin operator $\hat{s}$ has been omitted, and the rank of the orbital tensor operator given explicitly as 1.

In **qlanth** the reduced matrix elements for this double tensor operator are calculated by ReducedV1k and stored in a static association called ReducedV1kTable. The reduced matrix elements of this operator are calculated using equation 2-101 from Wybourne [Wyb65]:

$$\langle \underline{\ell}^n \psi \| \hat{V}^{(1k)} \| \underline{\ell}^n \psi' \rangle = \langle \underline{\ell}^n \alpha L S \| \hat{V}^{(1k)} \| \underline{\ell}^n \alpha' L' S' \rangle = n\sqrt{\underline{\jmath}(\underline{\jmath}+1)(2\underline{\jmath}+1)}\sqrt{[\![S]\!][\![L]\!][\![S']\!][\![L']\!]}\times$$
$$\sum_{\bar{\psi}} (-1)^{\bar{S}+\bar{L}+S+L+\underline{\ell}+\underline{\jmath}+k+1} \left(\psi \left\{ \left| \bar{\psi} \right) \left(\bar{\psi} \right| \right\} \psi'\right) \begin{Bmatrix} S & S' & 1 \\ \underline{\jmath} & \underline{\jmath} & \bar{S} \end{Bmatrix} \begin{Bmatrix} L & L' & k \\ \underline{\ell} & \underline{\ell} & \bar{L} \end{Bmatrix} \quad (29)$$

In this expression the sum over $\bar{\psi}$ depends on (ψ, ψ') and is over all the states in $\underline{\ell}^{n-1}$ which are common parents to both ψ and ψ'. Also note that in the equation above, since our concern are $\underline{\text{f}}$-electron configurations, we have $\underline{\ell} = 3$ and $\underline{\jmath} = \frac{1}{2}$.

```
ReducedV1k::usage = "ReducedV1k[n, l, SL, SpLp, k] gives the reduced
    matrix element of the spherical tensor operator V^(1k). See
    equation 2-101 in Wybourne 1965.";
ReducedV1k[numE_, SL_, SpLp_, k_] := Module[
  {Vk1, S, L, Sp, Lp,
  Sb, Lb, spin, orbital,
  cfpSL, cfpSpLp,
  SLparents, SpLpparents,
  commonParents, prefactor},
  (
    {spin, orbital} = {1/2, 3};
    {S, L}          = FindSL[SL];
    {Sp, Lp}        = FindSL[SpLp];
    cfpSL           = CFP[{numE, SL}];
    cfpSpLp         = CFP[{numE, SpLp}];
    SLparents       = First /@ Rest[cfpSL];
    SpLpparents     = First /@ Rest[cfpSpLp];
    commonParents = Intersection[SLparents, SpLpparents];
    Vk1 = Sum[(
        {Sb, Lb} = FindSL[\[Psi]b];
        Phaser[(Sb + Lb + S + L + orbital + k - spin)] *
        CFPAssoc[{numE, SL, \[Psi]b}] *
        CFPAssoc[{numE, SpLp, \[Psi]b}] *
        SixJay[{S, Sp, 1}, {spin, spin, Sb}] *
        SixJay[{L, Lp, k}, {orbital, orbital, Lb}]
      ),
    {\[Psi]b, commonParents}
    ];
    prefactor = numE * Sqrt[spin * (spin + 1) * TPO[spin, S, L, Sp,
    Lp] ];
    Return[prefactor * Vk1];
  )
];
```

These reduced matrix elements are then used by the function SpinOrbit.

```
SpinOrbit::usage = "SpinOrbit[numE, SL, SpLp, J] returns the LSJ
    reduced matrix element ζ <SL, J|L.S|SpLp, J>. These are given as a
     function of ζ. This function requires that the association
    ReducedV1kTable be defined.
See equations 2-106 and 2-109 in Wybourne (1965). Equivalently see
    eqn. 12.43 in TASS.";
SpinOrbit[numE_, SL_, SpLp_, J_] := Module[
  {S, L, Sp, Lp, orbital, sign, prefactor, val},
  (
    orbital   = 3;
    {S, L}    = FindSL[SL];
    {Sp, Lp}  = FindSL[SpLp];
    prefactor = Sqrt[orbital * (orbital+1) * (2*orbital+1)] *
                SixJay[{L, Lp, 1}, {Sp, S, J}];
    sign      = Phaser[J + L + Sp];
    val       = sign * prefactor * ζ * ReducedV1kTable[{numE, SL,
    SpLp, 1}];
    Return[val];
  )
];
```

3.5 $\hat{\mathcal{H}}_{\mathcal{SO}(3)}, \hat{\mathcal{H}}_{\mathcal{G}_2}, \hat{\mathcal{H}}_{\mathcal{SO}(7)}$: electrostatic configuration interaction

These are the first terms where we take into account the contributions from *configuration-interaction*. Rajnak and Wybourne [RW63] showed that *configuration-interaction* of the electrostatic interactions corresponding to two-electron excitations from $\underline{\mathrm{f}}^n$ can be represented through the Casimir operators of the groups $\mathcal{SO}(3)$, $\mathcal{G}_2$, and $\mathcal{SO}(7)$. This borrowed from an earlier insight of Trees [Tre52], who realized that an addition of a term proportional to $L(L+1)$ improved the energy calculations for the second spectrum of manganese (Mn-II) and the third spectrum of iron (Fe-III).

One of these Casimir operators is the familiar $\hat{L}^2$ from $\mathcal{SO}(3)$. In analogy to $\hat{L}^2$ in which the quantum number L can be used to determine the eigenvalues, in the cases of $\hat{\mathcal{H}}_{\mathcal{G}_2}$ the necessary state label is the U label of the LS term, and in the case of $\hat{\mathcal{H}}_{\mathcal{SO}(7)}$ the necessary label is W. If $\Lambda_{\mathcal{G}_2}(U)$ is used to note the eigenvalue of the Casimir operator of $\mathcal{G}_2$ corresponding to label U, and $\Lambda_{\mathcal{SO}(7)}(W)$ the eigenvalue corresponding to state label W, then the matrix elements of $\hat{\mathcal{H}}_{\mathcal{SO}(3)}$, $\hat{\mathcal{H}}_{\mathcal{G}_2}$ and $\hat{\mathcal{H}}_{\mathcal{SO}(7)}$ are diagonal in all quantum numbers (see Rajnak and Wybourne [RW63]) and are given by

$$\langle \underline{\ell}^n \alpha S L J M_J | \hat{\mathcal{H}}_{\mathcal{SO}(3)} | \underline{\ell}^n \alpha' S' L' J' M'_J \rangle = \alpha \delta(\alpha S L J M_J, \alpha' S' L' J' M'_J) L(L+1) \tag{30}$$

$$\langle \underline{\ell}^n U \alpha S L J M_J | \hat{\mathcal{H}}_{\mathcal{G}_2} | \underline{\ell}^n U \alpha' S' L' J' M'_J \rangle = \beta \delta(\alpha S L J M_J, \alpha' S' L' J' M'_J) \Lambda_{\mathcal{G}_2}(U) \tag{31}$$

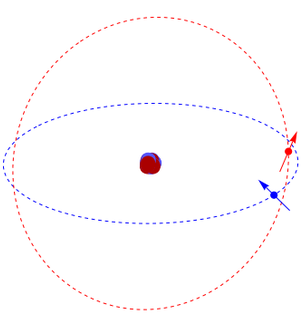
$$\langle \underline{\ell}^n W \alpha S L J M_J | \hat{\mathcal{H}}_{\mathcal{SO}(7)} | \underline{\ell}^n W \alpha' S' L' J' M_J \rangle = \gamma \delta(\alpha S L J M_J, \alpha' S' L' J' M'_J) \Lambda_{\mathcal{SO}(7)}(W) \tag{32}$$

In **qlanth** the role of $\Lambda_{\mathcal{SO}(7)}(W)$ is played by the function `GSO7W`, the role of $\Lambda_{\mathcal{G}_2}(U)$ by `GG2U`, and the role of $\Lambda_{\mathcal{SO}(3)}(L)$ by `CasimirSO3`. These are used by `CasimirG2`, `CasimirSO3`, and `CasimirSO7` which find the corresponding U, W, L labels to the LS terms provided to them. Finally, the function `ElectrostaticConfigInteraction` puts them together.

```
ElectrostaticConfigInteraction::usage = "
    ElectrostaticConfigInteraction[{SL, SpLp}] returns the matrix
    element for configuration interaction as approximated by the
    Casimir operators of the groups R3, G2, and R7. SL and SpLp are
    strings that represent terms under LS coupling.";
ElectrostaticConfigInteraction[{SL_, SpLp_}] := Module[
  {S, L, val},
  (
    {S, L} = FindSL[SL];
    val = (
      If[SL == SpLp,
        CasimirSO3[{SL, SL}] +
        CasimirSO7[{SL, SL}] +
        CasimirG2[{SL, SL}],
        0
      ]
      );
    ElectrostaticConfigInteraction[{S, L}] = val;
    Return[val];
  )
];
```

3.6 $\hat{\mathcal{H}}_{\text{s:s-s:oo}}$: *spin-spin* and *spin-other-orbit*

The calculation of the $\hat{\mathcal{H}}_{\text{s:s-s:oo}}$ is qualitatively different from the previous ones. The previous ones were self-contained in the sense that the reduced matrix elements that we require we also computed on our own. In the case of the interactions that follow from here, we use values from literature for reduced matrix elements either in $\underline{\mathrm{f}}^2$ or in $\underline{\mathrm{f}}^3$ and then we "pull" them up for all $\underline{\mathrm{f}}^n$ configurations with help of the coefficients of fractional parentage.



The analysis of *spin-other-orbit*, and the *spin-spin* contributions used in **qlanth** is that of Judd, Crosswhite, and Crosswhite [JCC68]. Much as the spin-orbit effect can be extracted from the Dirac equation as a relativistic correction, the multi-electron spin-orbit effects can be derived from the Breit operator $\hat{\mathcal{H}}_B$ [BS57] which is a term added to the relativistic description of a many-particle system in order to

account for retardation of the electromagnetic field

$$\hat{\mathcal{H}}_B = -\frac{1}{2}e^2 \sum_{i>j} \left[(\alpha_i \cdot \alpha_j) \frac{1}{r_{ij}} + (\alpha_i \cdot \vec{r}_{ij}) (\alpha_j \cdot \vec{r}_{ij}) \frac{1}{r_{ij}^3} \right]. \tag{33}$$

When this operator is expanded in powers of v/c, a number of non-relativistic inter-electron interactions result. Two of them are the *spin-other-orbit* and *spin-spin* interactions. As usual, the radial part of the Hamiltonian is averaged, which in this case gives appearance to the Marvin integrals

$$M^{(k)} \coloneqq \frac{e^2\hbar^2}{8m^2c^2} \langle (nl)^2 | \frac{r_<^k}{r_>^{k+3}} | (nl)^2 \rangle. \tag{34}$$

With these, the expression for the *spin-spin* term within the single configuration description is [JCC68]

$$\hat{\mathcal{H}}_{s:s} = -2 \sum_{i \neq j} \sum_k M^{(k)} \sqrt{(k+1)(k+2)(2k+3)} \langle \underline{\ell} \| C^{(k)} \| \underline{\ell} \rangle \langle \underline{\ell} \| C^{(k+2)} \| \underline{\ell} \rangle \left\{ \hat{w}_i^{(1,k)} \hat{w}_j^{(1,k+2)} \right\}^{(2,2)0} \tag{35}$$

and the one for *spin-other-orbit*

$$\begin{aligned} \hat{\mathcal{H}}_{s:oo} = \sum_{i \neq j} \sum_k & \sqrt{(k+1)(2\underline{\ell}+k+2)(2\underline{\ell}-k)} \times \\ & \left[\left\{ \hat{w}_i^{(0,k+1)} \hat{w}_j^{(1,k)} \right\}^{(11)0} \left\{ M^{(k-1)} \langle \underline{\ell} \| C^{(k+1)} \| \underline{\ell} \rangle^2 + 2M^{(k)} \langle \underline{\ell} \| C^{(k)} \| \underline{\ell} \rangle^2 \right\} + \right. \\ & \left. \left\{ \hat{w}_i^{(0,k)} \hat{w}_j^{(1,k+1)} \right\}^{(11)0} \left\{ M^{(k)} \langle \underline{\ell} \| C^{(k)} \| \underline{\ell} \rangle^2 + 2M^{(k-1)} \langle \underline{\ell} \| C^{(k+1)} \| \underline{\ell} \rangle^2 \right\} \right]. \end{aligned} \tag{36}$$

In the expressions above $\hat{w}_i^{(\kappa,k)}$ is a double tensor operator of rank κ over spin, of rank k over orbit, and acting on electron i. It is defined by its reduced matrix elements as

$$\langle \underline{\ell} \| \hat{w}^{(\kappa,k)} \| \underline{\ell} \rangle = \sqrt{[\![\kappa]\!][\![k]\!]}. \tag{37}$$

The explicit complexity of the above expressions can be somewhat reduced by identifying them with the scalar part of two new double tensors $\hat{\mathcal{T}}_0^{(11)}$ and $\hat{\mathcal{T}}_0^{(22)}$ such that

$$\sqrt{5}\hat{\mathcal{T}}_0^{(22)} \coloneqq \hat{\mathcal{H}}_{\mathrm{s:s}} \tag{38}$$

$$-\sqrt{3}\hat{\mathcal{T}}_0^{(11)} \coloneqq \hat{\mathcal{H}}_{\mathrm{s:oo}}. \tag{39}$$

In terms of which the reduced matrix elements in the $|LSJ\rangle$ basis can be obtained by

$$\langle \gamma SLJ | \hat{\mathcal{H}} | \gamma' S' L' J' \rangle = \delta(J, J') \begin{Bmatrix} S' & L' & J \\ L & S & t \end{Bmatrix} \langle \gamma SL \| \hat{\mathcal{T}}^{(tt)} \| \gamma' S' L' \rangle. \tag{40}$$

This above relationship is the one effectively used in **qlanth** in the functions `SpinSpin` and `SOOandECSO`.

```
SpinSpin::usage = "SpinSpin[n, SL, SpLp, J] returns the matrix
    element <|SL,J|spin-spin|SpLp,J|> for the spin-spin operator
    within the configuration f^n. This matrix element is independent
    of MJ. This is obtained by querying the relevant reduced matrix
    element from the association T22Table, putting in the adequate
    phase, and 6-j symbol.
This is calculated according to equation (3) in ''Judd, BR, HM
    Crosswhite, and Hannah Crosswhite. ''Intra-Atomic Magnetic
    Interactions for f Electrons.'' Physical Review 169, no. 1 (1968):
     130.''
''.
";
SpinSpin[numE_, SL_, SpLp_, J_] := Module[
  {S, L, Sp, Lp, α, val},
  (
    α = 2;
    {S, L} = FindSL[SL];
    {Sp, Lp} = FindSL[SpLp];
    val = (
            Phaser[Sp + L + J] *
            SixJay[{Sp, Lp, J}, {L, S, α}] *
```

```
            T22Table[{numE, SL, SpLp}]
          );
    Return[val]
  )
];
```

```
SOOandECSO::usage = "SOOandECSO[n, SL, SpLp, J] returns the matrix
    element <|SL,J|spin-spin|SpLp,J|> for the combined effects of the
    spin-other-orbit interaction and the electrostatically-correlated-
    spin-orbit (which originates from configuration interaction
    effects) within the configuration f^n. This matrix element is
    independent of MJ. This is obtained by querying the relevant
    reduced matrix element by querying the association
    SOOandECSOLSTable and putting in the adequate phase and 6-j symbol
    . The SOOandECSOLSTable puts together the reduced matrix elements
    from three operators.
This is calculated according to equation (3) in ''Judd, BR, HM
    Crosswhite, and Hannah Crosswhite. ''Intra-Atomic Magnetic
    Interactions for f Electrons.'' Physical Review 169, no. 1 (1968):
     130.''.
";
SOOandECSO[numE_, SL_, SpLp_, J_] := Module[
  {S, Sp, L, Lp, α, val},
  (
    α = 1;
    {S, L}   = FindSL[SL];
    {Sp, Lp} = FindSL[SpLp];
    val = (
            Phaser[Sp + L + J] *
            SixJay[{Sp, Lp, J}, {L, S, α}] *
            SOOandECSOLSTable[{numE, SL, SpLp}]
          );
    Return[val];
  )
];
```

For two-electron operators such as these, the matrix elements in $\underline{\mathrm{f}}^n$ are related to those in $\underline{\mathrm{f}}^{n-1}$ by equation 4 in Judd *et al.* [JCC68]

$$\langle \underline{\mathrm{f}}^n\psi \| \hat{\mathcal{T}}^{(tt)} \| \underline{\mathrm{f}}^n\psi'\rangle = \frac{n}{n-2}\sum_{\bar{\psi},\bar{\psi}'} (-1)^{\bar{S}+\bar{L}+\underline{s}+\underline{\ell}+S'+L'}\sqrt{[\![S]\!][\![S']\!][\![L]\!][\![L']\!]}\times$$
$$\left(\psi\{|\bar{\psi}\right)\left(\psi'\{|\bar{\psi}'\right)\begin{Bmatrix} S & t & S' \\ \bar{S}' & \underline{s} & \bar{S}\end{Bmatrix}\begin{Bmatrix} L & t & L' \\ \bar{L}' & \underline{\ell} & \bar{L}\end{Bmatrix}\langle \underline{\mathrm{f}}^{n-1}\bar{\psi}\|\hat{\mathcal{T}}^{(tt)}\|\underline{\mathrm{f}}^{n-1}]\bar{\psi}'\rangle, \quad (41)$$

where the sum runs over the terms $\bar{\psi}$ and $\bar{\psi}'$ in $\underline{\mathrm{f}}^{n-1}$ which are parents common to ψ and ψ'. Using these the matrix elements of $\hat{\mathcal{T}}^{(11)}$ and $\hat{\mathcal{T}}^{(22)}$ in $\underline{\mathrm{f}}^2$ can be used to compute all the reduced matrix elements in $\underline{\mathrm{f}}^n$. These could then be used together with Eqn-40 to obtain the matrix elements of $\hat{\mathcal{H}}_{\mathrm{s:s}}$ and $\hat{\mathcal{H}}_{\mathrm{s:oo}}$. This is done for $\hat{\mathcal{H}}_{\mathrm{s:s}}$, but not for $\hat{\mathcal{H}}_{\mathrm{s:oo}}$, because this term is traditionally computed (with a slight modification) at the same time as the electrostically-correlated-spin-orbit (see next section).

These equations are implemented in **qlanth** through the following functions: GenerateT22Table, ReducedT22infn, ReducedT22inf2, ReducedT11inf2. Where ReducedT22inf2 and ReducedT11inf2 provide the reduced matrix elements for $\hat{\mathcal{T}}^{(11)}$ and $\hat{\mathcal{T}}^{(22)}$ in $\underline{\mathrm{f}}^2$ as provided in table II of [JCC68].

```
GenerateT22Table::usage = "GenerateT22Table[nmax] generates the LS
    reduced matrix elements for the double tensor operator T22 in f^n
    up to n=nmax. If the option ''Export'' is set to true then the
    resulting association is saved to the data folder. The values for
    n=1 and n=2 are taken from ''Judd, BR, HM Crosswhite, and Hannah
    Crosswhite. ''Intra-Atomic Magnetic Interactions for f Electrons
    .'' Physical Review 169, no. 1 (1968): 130.'', and the values for
    n>2 are calculated recursively using equation (4) of that same
    paper.
This is an intermediate step to the calculation of the reduced matrix
     elements of the spin-spin operator.";
Options[GenerateT22Table] = {"Export" -> True, "Progress" -> True};
GenerateT22Table[nmax_Integer, OptionsPattern[]] := (
  If[And[OptionValue["Progress"], frontEndAvailable],
    (
      numItersai = Association[Table[numE->Length[AllowedNKSLTerms[
    numE]]^2, {numE, 1, nmax}]];
```

```
      counters = Association[Table[numE->0, {numE, 1, nmax}]];
      totalIters = Total[Values[numItersai[[1;;nmax]]]];
      template1 = StringTemplate["Iteration `numiter` of `totaliter`"];
      template2 = StringTemplate["`remtime` min remaining"];template3 = StringTemplate["Iteration speed = `speed` ms/it"];
      template4 = StringTemplate["Time elapsed = `runtime` min"];
      progBar = PrintTemporary[
        Dynamic[
          Pane[
            Grid[{{Superscript["f", numE]},
                  {template1[<|"numiter"->numiter, "totaliter"->totalIters|>]},
                  {template4[<|"runtime"->Round[QuantityMagnitude[UnitConvert[(Now-startTime), "min"]], 0.1]|>]},
                  {template2[<|"remtime"->Round[QuantityMagnitude[UnitConvert[(Now-startTime)/(numiter)*(totalIters-numiter), "min"]], 0.1]|>]},
                  {template3[<|"speed"->Round[QuantityMagnitude[Now-startTime, "ms"]/(numiter), 0.01]|>]},
                  {ProgressIndicator[Dynamic[numiter], {1, totalIters}]}},
                  Frame->All],
                  Full,
                  Alignment->Center]
              ]
            ];
    )
  ];
  T22Table = <||>;
  startTime = Now;
  numiter = 1;
  Do[
    (
      numiter+= 1;
      T22Table[{numE, SL, SpLp}] = Which[
        numE==1,
        0,
        numE==2,
        SimplifyFun[ReducedT22inf2[SL, SpLp]],
        True,
        SimplifyFun[ReducedT22infn[numE,  SL, SpLp]]
      ];
    ),
  {numE, 1, nmax},
  {SL,   AllowedNKSLTerms[numE]},
  {SpLp, AllowedNKSLTerms[numE]}
  ];
  If[And[OptionValue["Progress"],frontEndAvailable],
    NotebookDelete[progBar]
  ];
  If[OptionValue["Export"],
    (
      fname = FileNameJoin[{moduleDir, "data", "ReducedT22Table.m"}];
      Export[fname, T22Table];
    )
  ];
  Return[T22Table];
);
```

```
ReducedT22infn::usage = "ReducedT22infn[n, SL, SpLp] calculates the reduced matrix element of the T22 operator for the f^n configuration corresponding to the terms SL and SpLp. This is the operator corresponding to the inter-electron between spin.
It does this by using equation (4) of ''Judd, BR, HM Crosswhite, and Hannah Crosswhite. ''Intra-Atomic Magnetic Interactions for f Electrons.'' Physical Review 169, no. 1 (1968): 130.''
";
ReducedT22infn[numE_, SL_, SpLp_] := Module[
  {spin, orbital, t, idx1, idx2, S, L,
  Sp, Lp, cfpSL, cfpSpLp, parentSL,
  parentSpLp, Sb, Lb, Tnkk, phase, Sbp, Lbp},
  (
    {spin, orbital} = {1/2, 3};
    {S, L}   = FindSL[SL];
    {Sp, Lp} = FindSL[SpLp];
```

```
    t = 2;
    cfpSL    = CFP[{numE, SL}];
    cfpSpLp  = CFP[{numE, SpLp}];
    Tnkk = Sum[(
      parentSL   = cfpSL[[idx2, 1]];
      parentSpLp = cfpSpLp[[idx1, 1]];
      {Sb, Lb}   = FindSL[parentSL];
      {Sbp, Lbp} = FindSL[parentSpLp];
      phase = Phaser[Sb + Lb + spin + orbital + Sp + Lp];
      (
        phase *
        cfpSpLp[[idx1, 2]] * cfpSL[[idx2, 2]] *
        SixJay[{S, t, Sp}, {Sbp, spin, Sb}] *
        SixJay[{L, t, Lp}, {Lbp, orbital, Lb}] *
        T22Table[{numE - 1, parentSL, parentSpLp}]
      )
    ),
    {idx1, 2, Length[cfpSpLp]},
    {idx2, 2, Length[cfpSL]}
    ];
    Tnkk *= numE / (numE - 2) * Sqrt[TPO[S,Sp,L,Lp]];
    Return[Tnkk];
  )
];
```

```
ReducedT22inf2::usage = "ReducedT22inf2[SL, SpLp] returns the reduced
    matrix element of the scalar component of the double tensor T22
    for the terms SL, SpLp in f^2.
Data used here for m0, m2, m4 is from Table I of Judd, BR, HM
    Crosswhite, and Hannah Crosswhite. Intra-Atomic Magnetic
    Interactions for f Electrons. Physical Review 169, no. 1 (1968):
    130.
";
ReducedT22inf2[SL_, SpLp_] := Module[
  {statePosition, PsiPsipStates, m0, m2, m4, Tkk2m},
  (
    T22inf2 = <|
    {"3P", "3P"} -> -12 M0 - 24 M2 - 300/11 M4,
    {"3P", "3F"} -> 8/Sqrt[3] (3 M0 + M2 - 100/11 M4),
    {"3F", "3F"} -> 4/3 Sqrt[14] (-M0 + 8 M2 - 200/11 M4),
    {"3F", "3H"} -> 8/3 Sqrt[11/2] (2 M0 - 23/11 M2 - 325/121 M4),
    {"3H", "3H"} -> 4/3 Sqrt[143] (M0 - 34/11 M2 - (1325/1573) M4)
    |>;
    Which[
      MemberQ[Keys[T22inf2],{SL,SpLp}],
        Return[T22inf2[{SL,SpLp}]],
      MemberQ[Keys[T22inf2],{SpLp,SL}],
        Return[T22inf2[{SpLp,SL}]],
      True,
        Return[0]
    ]
  )
];
```

```
Reducedt11inf2::usage = "Reducedt11inf2[SL, SpLp] returns the reduced
    matrix element in f^2 of the double tensor operator t11 for the
    corresponding given terms {SL, SpLp}.
Values given here are those from Table VII of ''Judd, BR, HM
    Crosswhite, and Hannah Crosswhite. ''Intra-Atomic Magnetic
    Interactions for f Electrons.'' Physical Review 169, no. 1 (1968):
    130.''
";
Reducedt11inf2[SL_, SpLp_] := Module[
  {t11inf2},
  (
    t11inf2 = <|
      {"1S", "3P"} -> -2 P0 - 105 P2 - 231 P4 - 429 P6,
      {"3P", "3P"} -> -P0 - 45 P2 - 33 P4 + 1287 P6,
      {"3P", "1D"} -> Sqrt[15/2] (P0 + 32 P2 - 33 P4 - 286 P6),
      {"1D", "3F"} -> Sqrt[10] (-P0 - 9/2 P2 + 66 P4 - 429/2 P6),
      {"3F", "3F"} -> Sqrt[14] (-P0 + 10 P2 + 33 P4 + 286 P6),
      {"3F", "1G"} -> Sqrt[11] (P0 - 20 P2 + 32 P4 - 104 P6),
      {"1G", "3H"} -> Sqrt[10] (-P0 + 55/2 P2 - 23 P4 - 65/2 P6),
      {"3H", "3H"} -> Sqrt[55] (-P0 + 25 P2 + 51 P4 + 13 P6),
      {"3H", "1I"} -> Sqrt[13/2] (P0 - 21 P4 - 6 P6)
      |>;
```

```
    Which[
      MemberQ[Keys[t11inf2],{SL,SpLp}],
        Return[t11inf2[{SL,SpLp}]],
      MemberQ[Keys[t11inf2],{SpLp,SL}],
        Return[t11inf2[{SpLp,SL}]],
      True,
        Return[0]
    ]
  )
];
```

3.7 $\hat{\mathscr{H}}_{\text{ecs:o}}$: *electrostatically-correlated-spin-orbit*

In the same paper [JCC68] that describes the *spin-spin* and *spin-other-orbit* interactions, consideration is also given to the emergence of additional corrections due to configuration interaction as described by the following operator (which is what results from the application of perturbation theory to *second* order) (page. 134 of [JCC68])

$$\hat{\mathscr{H}}_{\text{ci}} = -\sum_{\chi}\sum_{i}\frac{1}{E_\chi}\xi(r_i)\left(\hat{\underline{\jmath}}_i\cdot\hat{\underline{\ell}}_i\right)|\chi\rangle\langle\chi|\hat{\mathfrak{C}} - \frac{1}{E_\chi}\hat{\mathfrak{C}}|\chi\rangle\langle\chi|\xi(r_i)\left(\hat{\underline{\jmath}}_i\cdot\hat{\underline{\ell}}_i\right) \tag{42}$$

where $\xi(r_h)(\hat{\underline{\jmath}}_h\cdot\hat{\underline{\ell}}_h)$ is the customary spin-orbit interaction, E_χ is the energy of state $|\chi\rangle$, i is a label for the valence electrons, $\hat{\mathfrak{C}}$ stands for the Coulomb interaction, and $|\chi\rangle$ are states in the configurations with which one is "interacting". Since this term includes both the electrostatic term and the spin-orbit one, this is called the *electrostatically-correlated-spin-orbit* interaction.

This operator can be identified with the scalar component of a double tensor operator of rank 1 both for the spin and orbital parts of the wavefunction

$$\hat{\mathscr{H}}_{\text{ci}} = -\sqrt{3}\,\hat{t}_0^{(11)}. \tag{43}$$

Judd *et al.* [JCC68] then go on to list the reduced matrix elements of this operator in the $\underline{\text{f}}^2$ configuration. When this is done the Marvin integrals $\mathcal{M}^{(k)}$ appear again, but a second set of parameters, the *pseudo-magnetic* parameters $P^{(k)}$, is also necessary

$$P^{(k)} = 6\sum_{f'}\frac{\zeta_{ff'}}{E_{ff'}}R^{(k)}(ff,ff') \text{ for } k=0,2,4,6. \tag{44}$$

Where f stands for an $\underline{\text{f}}$-electron radial eigenfunction, and f' similarly but for a configuration different from $\underline{\text{f}}^n$. And where

$$\zeta_{ff'} \coloneqq \langle f|\xi(r)|f'\rangle \tag{45}$$

$$R^{(k)}(ff,ff') \coloneqq e^2\langle f_1 f_2|\frac{r_<^k}{r_>^{k+1}}|f_1 f_2'\rangle. \tag{46}$$

In the semi-empirical approach embodied by **qlanth**, calculating these quantities *ab-initio* is not the objective, they are instead to be defined from experiments. Nonetheless, not only these expressions give theoretical justification to the model, but they also serve to justify the ratios between different orders of these quantities, their relative importance, or their sign. Consequently, both the set of three $\mathcal{M}^{(k)}$ and the set of $P^{(k)}$ ultimately rely on a single free parameter each. Such parsimony is desirable given the large number of parameters (about 20) that the Hamiltonian ends up having.

Judd *et al.* further note that $P^{(0)}$ is proportional to the spin orbit operator, and as such its effect is absorbed by the standard spin-orbit parameter ζ. They also developed an alternative approach based on group theory arguments. They put together the *spin-other-orbit* and the *electrostatically-correlated-spin-orbit* as a sum of operators $\hat{z}_i$ with useful transformation rules

$$\langle\psi\|\hat{\mathcal{T}}^{(11)} + \hat{t}^{(11)}\|\psi'\rangle = \sum a_i\langle\psi\|\hat{z}_i\|\psi'\rangle. \tag{47}$$

At this stage a subtle point needs to be raised. As Judd points out, in the sum above, the term $\hat{z}_{13}$ that contributes with a tensorial character equal to that of the regular spin-orbit operator. As such, if the goal is obtaining a parametric Hamiltonian that can be fit with uncorrelated parameters, it is then necessary to subtract this part from $\hat{\mathcal{T}}^{(11)} + \hat{t}^{(11)}$. This point was clarified by Chen *et al.* [Che+08]. Because of this, the final form of the

operator contributing both to *spin-other-orbit* and the *electrostatically-correlated-spin-orbit* is

$$\hat{\mathcal{H}}_{\text{s:oo}} + \hat{\mathcal{H}}_{\text{ecs:o}} = \hat{\mathcal{T}}^{(11)} + \hat{t}^{(11)} - \frac{1}{6} a_{13} \hat{z}_{13} \tag{48}$$

where

$$a_{13} = -33 m^{(0)} + 3 m^{(2)} + \frac{15}{11} m^{(4)} - 6 P^{(0)} + \frac{3}{2} \left(\frac{35}{225} P^{(2)} + \frac{77}{1089} P^{(4)} + \frac{25}{1287} P^{(6)} \right). \tag{49}$$

In **qlanth** the contributions from *spin-spin*, *spin-other-orbit*, and *electrostatically-correlated-spin-orbit* are put together by the function `MagneticInteractions`. That function queries precomputed values from two associations `SpinSpinTable` and `SOOandECSOTable`. In turn these two associations are generated by the functions `GenerateSpinOrbitTable` and `GenerateSOOandECSOTable`. Note that both *spin-spin* and *spin-other-orbit* end up contributing through $m^{(k)}$, however there doesn't seem to be consensus about adding them together, as such **qlanth** allows including or excluding the *spin-spin* contribution, this is done with a control parameter σ_{SS} (1 for including, 0 for excluding).

```
MagneticInteractions::usage = "MagneticInteractions[{numE, SL, SLp, J}] returns the matrix element of the magnetic interaction between the terms SL and SLp in the f^numE configuration for the given value of J. The interaction is given by the sum of the spin-spin, the spin-other-orbit, and the electrostatically-correlated-spin-orbit interactions.
The part corresponding to the spin-spin interaction is provided by SpinSpin[{numE, SL, SLp, J}].
The part corresponding to SOO and ECSO is provided by the function SOOandECSO[{numE, SL, SLp, J}].
The option ''ChenDeltas'' can be used to include or exclude the Chen deltas from the calculation. The default is to exclude them. If this option is used, then the chenDeltas association needs to be loaded into the session with LoadChen[].";
Options[MagneticInteractions] = {"ChenDeltas" -> False};
MagneticInteractions[{numE_, SL_, SLp_, J_}, OptionsPattern[]] := Module[
  {key, ss, sooandecso, total,
  S, L, Sp, Lp, phase, sixjay,
  M0v, M2v, M4v,
  P2v, P4v, P6v},
  (
    key         = {numE, SL, SLp, J};
    ss          = \[Sigma]SS * SpinSpinTable[key];
    sooandecso  = SOOandECSOTable[key];
    total = ss + sooandecso;
    total = SimplifyFun[total];
    If[
      Not[OptionValue["ChenDeltas"]],
      Return[total]
    ];
    (* In the type A errors the wrong values are different *)
    If[MemberQ[Keys[chenDeltas["A"]], {numE, SL, SLp}],
      (
        {S, L}    = FindSL[SL];
        {Sp, Lp}  = FindSL[SLp];
        phase     = Phaser[Sp + L + J];
        sixjay    = SixJay[{Sp, Lp, J}, {L, S, 1}];
        {M0v, M2v, M4v, P2v, P4v, P6v} = chenDeltas["A"][{numE, SL, SLp}]["wrong"];
        total     = (
                        phase * sixjay *
                        (
                          M0v*M0 + M2v*M2 + M4v*M4 +
                          P2v*P2 + P4v*P4 + P6v*P6
                        )
                    );
        total     = wChErrA * total + (1 - wChErrA) * (ss + sooandecso)
      )
    ];
    (* In the type B errors the wrong values are zeros all around *)
    If[MemberQ[chenDeltas["B"], {numE, SL, SLp}],
      (
        total  = (1 - wChErrB) * (ss + sooandecso)
      )
    ];
```

```
    Return[total];
  )
];
```

```
GenerateSpinOrbitTable::usage = "GenerateSpinOrbitTable[nmax]
    computes the matrix elements for the spin-orbit interaction for f^
    n configurations up to n = nmax. The function returns an
    association whose keys are lists of the form {n, SL, SpLp, J}. If
    export is set to True, then the result is exported to the data
    subfolder for the folder in which this package is in. It requires
    ReducedV1kTable to be defined.";
Options[GenerateSpinOrbitTable] = {"Export" -> True};
GenerateSpinOrbitTable[nmax_Integer:7, OptionsPattern[]] := Module[
  {numE, J, SL, SpLp, exportFname},
  (
    SpinOrbitTable =
      Table[
        {numE, SL, SpLp, J} -> SpinOrbit[numE, SL, SpLp, J],
      {numE, 1, nmax},
      {J, MinJ[numE], MaxJ[numE]},
      {SL,   Map[First, AllowedNKSLforJTerms[numE, J]]},
      {SpLp, Map[First, AllowedNKSLforJTerms[numE, J]]}
      ];
    SpinOrbitTable = Association[SpinOrbitTable];

    exportFname = FileNameJoin[{moduleDir, "data", "SpinOrbitTable.m"
    }];
    If[OptionValue["Export"],
      (
        Print["Exporting to file "<>ToString[exportFname]];
        Export[exportFname, SpinOrbitTable];
      )
    ];
    Return[SpinOrbitTable];
  )
];
```

```
GenerateSOOandECSOTable::usage = "GenerateSOOandECSOTable[nmax]
    generates the reduced matrix elements in the |LSJ> basis for the (
    spin-other-orbit + electrostatically-correlated-spin-orbit)
    operator. It returns an association where the keys are of the form
     {n, SL, SpLp, J}. If the option ''Export'' is set to True then
    the resulting object is saved to the data folder. Since this is a
    scalar operator, there is no MJ dependence. This dependence only
    comes into play when the crystal field contribution is taken into
    account.";
Options[GenerateSOOandECSOTable] = {"Export"->False};
GenerateSOOandECSOTable[nmax_, OptionsPattern[]] := (
  SOOandECSOTable = <||>;
  Do[
    SOOandECSOTable[{numE, SL, SpLp, J}] = (SOOandECSO[numE, SL, SpLp
    , J] /. Prescaling);,
  {numE, 1, nmax},
  {J, MinJ[numE], MaxJ[numE]},
  {SL,   First /@ AllowedNKSLforJTerms[numE, J]},
  {SpLp, First /@ AllowedNKSLforJTerms[numE, J]}
  ];
  If[OptionValue["Export"],
  (
    fname = FileNameJoin[{moduleDir, "data", "SOOandECSOTable.m"}];
    Export[fname, SOOandECSOTable];
  )
  ];
  Return[SOOandECSOTable];
);
```

The function GenerateSpinSpinTable calls the function SpinSpin over all possible combinations of the arguments $\{n, SL, S'L', J\}$. In turn the function SpinSpin queries the precomputed values of the the double tensor $\hat{\mathcal{T}}^{(22)}$ which are stored in the association T22Table.

```
GenerateSpinSpinTable::usage = "GenerateSpinSpinTable[nmax] generates
     the reduced matrix elements in the |LSJ> basis for the (spin-
    other-orbit + electrostatically-correlated-spin-orbit) operator.
    It returns an association where the keys are of the form {numE, SL
```

```
    , SpLp, J}. If the option ''Export'' is set to True then the
    resulting object is saved to the data folder. Since this is a
    scalar operator, there is no MJ dependence. This dependence only
    comes into play when the crystal field contribution is taken into
    account.";
Options[GenerateSpinSpinTable] = {"Export"->False};
GenerateSpinSpinTable[nmax_, OptionsPattern[]] :=
  (
    SpinSpinTable = <||>;
    PrintTemporary[Dynamic[numE]];
    Do[
      SpinSpinTable[{numE, SL, SpLp, J}] = (SpinSpin[numE, SL, SpLp,
    J]);,
    {numE, 1, nmax},
    {J, MinJ[numE], MaxJ[numE]},
    {SL,   First /@ AllowedNKSLforJTerms[numE, J]},
    {SpLp, First /@ AllowedNKSLforJTerms[numE, J]}
    ];
    If[OptionValue["Export"],
    (fname = FileNameJoin[{moduleDir, "data", "SpinSpinTable.m"}];
      Export[fname, SpinSpinTable];
      )
    ];
    Return[SpinSpinTable];
  );
```

```
SpinSpin::usage = "SpinSpin[n, SL, SpLp, J] returns the matrix
    element <|SL,J|spin-spin|SpLp,J|> for the spin-spin operator
    within the configuration f^n. This matrix element is independent
    of MJ. This is obtained by querying the relevant reduced matrix
    element from the association T22Table, putting in the adequate
    phase, and 6-j symbol.
This is calculated according to equation (3) in ''Judd, BR, HM
    Crosswhite, and Hannah Crosswhite. ''Intra-Atomic Magnetic
    Interactions for f Electrons.'' Physical Review 169, no. 1 (1968):
     130.''
''.
";
SpinSpin[numE_, SL_, SpLp_, J_] := Module[
  {S, L, Sp, Lp, α, val},
  (
    α = 2;
    {S, L} = FindSL[SL];
    {Sp, Lp} = FindSL[SpLp];
    val = (
            Phaser[Sp + L + J] *
            SixJay[{Sp, Lp, J}, {L, S, α}] *
            T22Table[{numE, SL, SpLp}]
          );
    Return[val]
  )
];
```

The association `T22Table` is computed by the function `GenerateT22Table`. This function populates `T22Table` with keys of the form $\{n, SL, S'L'\}$. It does this by using the function `ReducedT22inf2` in the base case of $\underline{f}^2$, and `ReducedT22infn` for configurations above $\underline{f}^2$. When `ReducedT22infn` is called, the sum in &qn-41 is carried out using $t = 2$. When `ReducedT22inf2` is called, the reduced matrix elements from [JCC68] are used.

```
GenerateT22Table::usage = "GenerateT22Table[nmax] generates the LS
    reduced matrix elements for the double tensor operator T22 in f^n
    up to n=nmax. If the option ''Export'' is set to true then the
    resulting association is saved to the data folder. The values for
    n=1 and n=2 are taken from ''Judd, BR, HM Crosswhite, and Hannah
    Crosswhite. ''Intra-Atomic Magnetic Interactions for f Electrons
    .'' Physical Review 169, no. 1 (1968): 130.'', and the values for
    n>2 are calculated recursively using equation (4) of that same
    paper.
This is an intermediate step to the calculation of the reduced matrix
     elements of the spin-spin operator.";
Options[GenerateT22Table] = {"Export" -> True, "Progress" -> True};
GenerateT22Table[nmax_Integer, OptionsPattern[]] := (
  If[And[OptionValue["Progress"], frontEndAvailable],
    (
      numItersai = Association[Table[numE->Length[AllowedNKSLTerms[
    numE]]^2, {numE, 1, nmax}]];
```

```
      counters = Association[Table[numE->0, {numE, 1, nmax}]];
      totalIters = Total[Values[numItersai[[1;;nmax]]]];
      template1 = StringTemplate["Iteration `numiter` of `totaliter`"];
      template2 = StringTemplate["`remtime` min remaining"];template3 = StringTemplate["Iteration speed = `speed` ms/it"];
      template4 = StringTemplate["Time elapsed = `runtime` min"];
      progBar = PrintTemporary[
        Dynamic[
          Pane[
            Grid[{{Superscript["f", numE]},
                  {template1[<|"numiter"->numiter, "totaliter"->totalIters|>]},
                  {template4[<|"runtime"->Round[QuantityMagnitude[UnitConvert[(Now-startTime), "min"]], 0.1]|>]},
                  {template2[<|"remtime"->Round[QuantityMagnitude[UnitConvert[(Now-startTime)/(numiter)*(totalIters-numiter), "min"]], 0.1]|>]},
                  {template3[<|"speed"->Round[QuantityMagnitude[Now-startTime, "ms"]/(numiter), 0.01]|>]},
                  {ProgressIndicator[Dynamic[numiter], {1, totalIters}]}},
                  Frame->All],
                  Full,
                  Alignment->Center]
              ]
            ];
    )
  ];
  T22Table = <||>;
  startTime = Now;
  numiter = 1;
  Do[
    (
      numiter+= 1;
      T22Table[{numE, SL, SpLp}] = Which[
        numE==1,
        0,
        numE==2,
        SimplifyFun[ReducedT22inf2[SL, SpLp]],
        True,
        SimplifyFun[ReducedT22infn[numE,  SL, SpLp]]
      ];
    ),
  {numE, 1, nmax},
  {SL,   AllowedNKSLTerms[numE]},
  {SpLp, AllowedNKSLTerms[numE]}
  ];
  If[And[OptionValue["Progress"],frontEndAvailable],
    NotebookDelete[progBar]
  ];
  If[OptionValue["Export"],
    (
      fname = FileNameJoin[{moduleDir, "data", "ReducedT22Table.m"}];
      Export[fname, T22Table];
    )
  ];
  Return[T22Table];
);
```

```
ReducedT22infn::usage = "ReducedT22infn[n, SL, SpLp] calculates the reduced matrix element of the T22 operator for the f^n configuration corresponding to the terms SL and SpLp. This is the operator corresponding to the inter-electron between spin.
It does this by using equation (4) of ''Judd, BR, HM Crosswhite, and Hannah Crosswhite. ''Intra-Atomic Magnetic Interactions for f Electrons.'' Physical Review 169, no. 1 (1968): 130.''
";
ReducedT22infn[numE_, SL_, SpLp_] := Module[
  {spin, orbital, t, idx1, idx2, S, L,
  Sp, Lp, cfpSL, cfpSpLp, parentSL,
  parentSpLp, Sb, Lb, Tnkk, phase, Sbp, Lbp},
  (
    {spin, orbital} = {1/2, 3};
    {S, L}   = FindSL[SL];
    {Sp, Lp} = FindSL[SpLp];
```

```
    t = 2;
    cfpSL    = CFP[{numE, SL}];
    cfpSpLp  = CFP[{numE, SpLp}];
    Tnkk = Sum[(
      parentSL   = cfpSL[[idx2, 1]];
      parentSpLp = cfpSpLp[[idx1, 1]];
      {Sb, Lb}   = FindSL[parentSL];
      {Sbp, Lbp} = FindSL[parentSpLp];
      phase = Phaser[Sb + Lb + spin + orbital + Sp + Lp];
      (
        phase *
        cfpSpLp[[idx1, 2]] * cfpSL[[idx2, 2]] *
        SixJay[{S, t, Sp}, {Sbp, spin, Sb}] *
        SixJay[{L, t, Lp}, {Lbp, orbital, Lb}] *
        T22Table[{numE - 1, parentSL, parentSpLp}]
      )
    ),
    {idx1, 2, Length[cfpSpLp]},
    {idx2, 2, Length[cfpSL]}
    ];
    Tnkk *= numE / (numE - 2) * Sqrt[TPO[S,Sp,L,Lp]];
    Return[Tnkk];
  )
];
```

```
ReducedT22inf2::usage = "ReducedT22inf2[SL, SpLp] returns the reduced
     matrix element of the scalar component of the double tensor T22
    for the terms SL, SpLp in f^2.
Data used here for m0, m2, m4 is from Table I of Judd, BR, HM
    Crosswhite, and Hannah Crosswhite. Intra-Atomic Magnetic
    Interactions for f Electrons. Physical Review 169, no. 1 (1968):
    130.
";
ReducedT22inf2[SL_, SpLp_] := Module[
  {statePosition, PsiPsipStates, m0, m2, m4, Tkk2m},
  (
    T22inf2 = <|
    {"3P", "3P"} -> -12 M0 - 24 M2 - 300/11 M4,
    {"3P", "3F"} -> 8/Sqrt[3] (3 M0 + M2 - 100/11 M4),
    {"3F", "3F"} -> 4/3 Sqrt[14] (-M0 + 8 M2 - 200/11 M4),
    {"3F", "3H"} -> 8/3 Sqrt[11/2] (2 M0 - 23/11 M2 - 325/121 M4),
    {"3H", "3H"} -> 4/3 Sqrt[143] (M0 - 34/11 M2 - (1325/1573) M4)
    |>;
    Which[
      MemberQ[Keys[T22inf2],{SL,SpLp}],
        Return[T22inf2[{SL,SpLp}]],
      MemberQ[Keys[T22inf2],{SpLp,SL}],
        Return[T22inf2[{SpLp,SL}]],
      True,
        Return[0]
    ]
  )
];
```

The function GenerateSOOandECSOTable calls the function SOOandECSO over all possible combinations of the arguments $\{n, SL, S'L', J\}$ and uses their values to populate the association SOOandECSOTable. In turn the function SOOandECSO queries the precomputed values of &qn-48 as stored in the association SOOandECSOLSTable.

```
GenerateSOOandECSOTable::usage = "GenerateSOOandECSOTable[nmax]
    generates the reduced matrix elements in the |LSJ> basis for the (
    spin-other-orbit + electrostatically-correlated-spin-orbit)
    operator. It returns an association where the keys are of the form
     {n, SL, SpLp, J}. If the option ''Export'' is set to True then
    the resulting object is saved to the data folder. Since this is a
    scalar operator, there is no MJ dependence. This dependence only
    comes into play when the crystal field contribution is taken into
    account.";
Options[GenerateSOOandECSOTable] = {"Export"->False};
GenerateSOOandECSOTable[nmax_, OptionsPattern[]] := (
  SOOandECSOTable = <||>;
  Do[
    SOOandECSOTable[{numE, SL, SpLp, J}] = (SOOandECSO[numE, SL, SpLp
    , J] /. Prescaling);,
  {numE, 1, nmax},
  {J, MinJ[numE], MaxJ[numE]},
```

```
  {SL,   First /@ AllowedNKSLforJTerms[numE, J]},
  {SpLp, First /@ AllowedNKSLforJTerms[numE, J]}
  ];
  If[OptionValue["Export"],
  (
    fname = FileNameJoin[{moduleDir, "data", "SOOandECSOTable.m"}];
    Export[fname, SOOandECSOTable];
  )
  ];
  Return[SOOandECSOTable];
);
```

```
SOOandECSO::usage = "SOOandECSO[n, SL, SpLp, J] returns the matrix
    element <|SL,J|spin-spin|SpLp,J|> for the combined effects of the
    spin-other-orbit interaction and the electrostatically-correlated-
    spin-orbit (which originates from configuration interaction
    effects) within the configuration f^n. This matrix element is
    independent of MJ. This is obtained by querying the relevant
    reduced matrix element by querying the association
    SOOandECSOLSTable and putting in the adequate phase and 6-j symbol
    . The SOOandECSOLSTable puts together the reduced matrix elements
    from three operators.
This is calculated according to equation (3) in ''Judd, BR, HM
    Crosswhite, and Hannah Crosswhite. ''Intra-Atomic Magnetic
    Interactions for f Electrons.'' Physical Review 169, no. 1 (1968):
     130.''.
";
SOOandECSO[numE_, SL_, SpLp_, J_] := Module[
  {S, Sp, L, Lp, α, val},
  (
    α = 1;
    {S, L}   = FindSL[SL];
    {Sp, Lp} = FindSL[SpLp];
    val = (
             Phaser[Sp + L + J] *
             SixJay[{Sp, Lp, J}, {L, S, α}] *
             SOOandECSOLSTable[{numE, SL, SpLp}]
           );
    Return[val];
  )
];
```

```
SOOandECSO::usage = "SOOandECSO[n, SL, SpLp, J] returns the matrix
    element <|SL,J|spin-spin|SpLp,J|> for the combined effects of the
    spin-other-orbit interaction and the electrostatically-correlated-
    spin-orbit (which originates from configuration interaction
    effects) within the configuration f^n. This matrix element is
    independent of MJ. This is obtained by querying the relevant
    reduced matrix element by querying the association
    SOOandECSOLSTable and putting in the adequate phase and 6-j symbol
    . The SOOandECSOLSTable puts together the reduced matrix elements
    from three operators.
This is calculated according to equation (3) in ''Judd, BR, HM
    Crosswhite, and Hannah Crosswhite. ''Intra-Atomic Magnetic
    Interactions for f Electrons.'' Physical Review 169, no. 1 (1968):
     130.''.
";
SOOandECSO[numE_, SL_, SpLp_, J_] := Module[
  {S, Sp, L, Lp, α, val},
  (
    α = 1;
    {S, L}   = FindSL[SL];
    {Sp, Lp} = FindSL[SpLp];
    val = (
             Phaser[Sp + L + J] *
             SixJay[{Sp, Lp, J}, {L, S, α}] *
             SOOandECSOLSTable[{numE, SL, SpLp}]
           );
    Return[val];
  )
];
```

The association `SOOandECSOLSTable` is computed by the function `GenerateSOOandECSOLSTable`. This function populates `SOOandECSOLSTable` with keys of the form $\{n, SL, S'L'\}$. It does this by using the function `ReducedSOOandECSOinf2` in the base case of $\underline{f}^2$, and

ReducedSOOandECSOinfn for configurations above $\underline{f}^2$. When ReducedSOOandECSOinfn is called the sum in &qn-41 is carried out using $t = 1$. When ReducedSOOandECSOinf2 is called the reduced matrix elements from [JCC68] are used.

```
ReducedSOOandECSOinfn::usage = "ReducedSOOandECSOinfn[numE, SL, SpLp]
    calculates the reduced matrix elements of the (spin-other-orbit +
    ECSO) operator for the f^numE configuration corresponding to the
    terms SL and SpLp. This is done recursively, starting from
    tabulated values for f^2 from ''Judd, BR, HM Crosswhite, and
    Hannah Crosswhite. ''Intra-Atomic Magnetic Interactions for f
    Electrons.'' Physical Review 169, no. 1 (1968): 130.'', and by
    using equation (4) of that same paper.
";
ReducedSOOandECSOinfn[numE_, SL_, SpLp_] := Module[
  {spin, orbital, t, S, L, Sp, Lp,
  idx1, idx2, cfpSL, cfpSpLp, parentSL,
  Sb, Lb, Sbp, Lbp, parentSpLp, funval},
  (
    {spin, orbital} = {1/2, 3};
    {S, L}   = FindSL[SL];
    {Sp, Lp} = FindSL[SpLp];
    t = 1;
    cfpSL    = CFP[{numE, SL}];
    cfpSpLp  = CFP[{numE, SpLp}];
    funval   = Sum[
      (
        parentSL = cfpSL[[idx2, 1]];
        parentSpLp = cfpSpLp[[idx1, 1]];
        {Sb, Lb}   = FindSL[parentSL];
        {Sbp, Lbp} = FindSL[parentSpLp];
        phase = Phaser[Sb + Lb + spin + orbital + Sp + Lp];
        (
          phase *
          cfpSpLp[[idx1, 2]] * cfpSL[[idx2, 2]] *
          SixJay[{S, t, Sp}, {Sbp, spin, Sb}] *
          SixJay[{L, t, Lp}, {Lbp, orbital, Lb}] *
          SOOandECSOLSTable[{numE - 1, parentSL, parentSpLp}]
        )
      ),
    {idx1, 2, Length[cfpSpLp]},
    {idx2, 2, Length[cfpSL]}
    ];
    funval *= numE / (numE - 2) * Sqrt[TPO[S, Sp, L, Lp]];
    Return[funval];
  )
];
```

```
ReducedSOOandECSOinf2::usage = "ReducedSOOandECSOinf2[SL, SpLp]
    returns the reduced matrix element corresponding to the operator (
    T11 + t11 - a13 * z13 / 6) for the terms {SL, SpLp}. This
    combination of operators corresponds to the spin-other-orbit plus
    ECSO interaction.
The T11 operator corresponds to the spin-other-orbit interaction, and
     the t11 operator (associated with electrostatically-correlated
    spin-orbit) originates from configuration interaction analysis. To
     their sum a factor proportional to the operator z13 is subtracted
     since its effect is redundant to the spin-orbit interaction. The
    factor of 1/6 is not on Judd's 1968 paper, but it is on ''Chen,
    Xueyuan, Guokui Liu, Jean Margerie, and Michael F Reid. ''A Few
    Mistakes in Widely Used Data Files for Fn Configurations
    Calculations.'' Journal of Luminescence 128, no. 3 (2008):
    421-27''.
The values for the reduced matrix elements of z13 are obtained from
    Table IX of the same paper. The value for a13 is from table VIII.
Rigurously speaking the Pk parameters here are subscripted. The
    conversion to superscripted parameters is performed elsewhere with
     the Prescaling replacement rules.
";
ReducedSOOandECSOinf2[SL_, SpLp_]  := Module[
  {a13, z13, z13inf2, matElement, redSOOandECSOinf2},
  (
    a13 = (-33 M0 + 3 M2 + 15/11 M4 -
          6 P0 + 3/2 (35 P2 + 77 P4 + 143 P6));
    z13inf2 = <|
        {"1S","3P"} -> 2,
        {"3P","3P"} -> 1,
```

```
        {"3P","1D"} -> -Sqrt[(15/2)],
        {"1D","3F"} -> Sqrt[10],
        {"3F","3F"} -> Sqrt[14],
        {"3F","1G"} -> -Sqrt[11],
        {"1G","3H"} -> Sqrt[10],
        {"3H","3H"} -> Sqrt[55],
        {"3H","1I"} -> -Sqrt[(13/2)]
        |>;
    matElement = Which[
      MemberQ[Keys[z13inf2],{SL,SpLp}],
        z13inf2[{SL,SpLp}],
      MemberQ[Keys[z13inf2],{SpLp,SL}],
        z13inf2[{SpLp,SL}],
      True,
        0
    ];
    redSOOandECSOinf2 = (
        ReducedT11inf2[SL, SpLp] +
        Reducedt11inf2[SL, SpLp] -
        a13 / 6 * matElement
    );
    redSOOandECSOinf2 = SimplifyFun[redSOOandECSOinf2];
    Return[redSOOandECSOinf2];
  )
];
```

3.8 $\hat{\mathcal{H}}_{\text{⅄}}$: three-body effective operators

The three-body operators in the semi-empirical Hamiltonian are due to the *configuration-interaction* effects of the Coulomb repulsion. More specifically, they originate from configuration interaction between the ground configuration $(4\underline{f})^n$ and single electron excitations to the $(4\underline{f})^{n\pm1}(n'\underline{\ell}')^{\mp1}$ configurations.

The operators that can be used to span the resulting effects were initially studied by Wybourne and Rajnak in 1963 [RW63], their analysis was complemented soon after by Judd [Jud66], and revisited again by Judd in 1984 [JS84].

This model interaction is spanned by a set of 14 $\hat{t}_i$ of operators ($\hat{t}$ from *t*hree)

$$\hat{\mathcal{H}}_{\text{⅄}} = T^{\prime(2)}\hat{t}_2{}' + T^{\prime(11)}\hat{t}_{11}{}' \sum_{\substack{k=2,3,4,6,7,8,\\ 11,12,14,15,\\ 16,17,18,19}} T^{(k)}\hat{t}_k, \tag{50}$$

where $\hat{t}_2$ and $\hat{t}_{11}$ are operators that have orthogonal alternatives represented by $\hat{t}_2{}'$ and $\hat{t}_{11}{}'$ (see [JS84]). **qlanth** includes the legacy operator $\hat{t}_2$ since it was used for important work during and before the 1980s.

The omission of some indices in this sum has to do with the fact that the way in which these are defined in terms of their index (see [Jud66]) gives rise to two-body operators which can be absorbed by the two-body terms in the Hamiltonian. As such, it is not so much that they are not included, but rather that their effects are considered to be accounted for elsewhere. This is representative of a common feature of configuration interaction: it gives rise to new intra-configuration operators, but it also contributes to already present operators; this makes it harder to approximate the model parameters *ab-initio*, but is not a practical obstacle for the semi-empirical approach (although it certainly complicates the physical interpretation that each parameter has). Furthermore, it is often the case that the operator set is limited to the subset {2,3,4,6,7,8}; a practice that is justified *post-facto* after seeing that these are sufficient to describe the data.

The calculation of a three body operator matrix elements across the $\underline{f}^n$ configurations is analogous to how a two-body operator is calculated. Except that in this case what is needed are the reduced matrix elements in $\underline{f}^3$ and the equation that is used to propagate these across the other configurations is equation 4 of [Jud66] (here adding the explicit dependence on J and M_J):

$$\langle \underline{f}^n\psi|\hat{t}_i|\underline{f}^n\psi'\rangle = \delta(J,J')\delta(M_J,M_J')\frac{n}{n-3}\sum_{\bar{\psi}\bar{\psi}'}\left(\psi\left\{\bar{\psi}\right)\left(\psi'\left\{\bar{\psi}'\right)\langle \underline{f}^{n-1}\bar{\psi}|\hat{t}_i|\underline{f}^{n-1}\bar{\psi}'\right\rangle. \tag{51}$$

The sum in this expression runs over the parents in $\underline{f}^{n-1}$ that are common to both the daughter terms ψ and ψ' in $\underline{f}^n$. The equation above yielding LSJMJ matrix elements, and being diagonal in J, M_J as is due to a scalar operator.

In **qlanth** this is all implemented in the function GenerateThreeBodyTables. Where the matrix elements in $\underline{f}^3$ are from [JS84], where the data has been digitized in the files Judd1984-1.csv and Judd1984-2.csv, which are parsed through the function ParseJudd1984.

In GenerateThreeBodyTables a special case is made for $\hat{t}_2$ and $\hat{t}_{11}$ which are calculated differently beyond the half-filled shell. In the case of the other $\hat{t}_k$ operators, beyond $\underline{f}^7$ the matrix elements simply see a global sign flip, whereas in the case of $\hat{t}_2$ and $\hat{t}_{11}$ the coefficients of fractional parentage beyond $\underline{f}^7$ are used. This yields the unexpected result that in the $\underline{f}^{12}$ configuration, which corresponds to two holes, there is a non-zero three body operator $\hat{t}_2$. This is an arcane result that was corrected by Judd in 1984 [JS84], but which lingered long enough that important work in the 1980s was calculated with it. When calculations are carried out, if $\hat{t}_2'/\hat{t}_{11}'$ is used then $\hat{t}_2/\hat{t}_{11}$ should not be used and vice versa.

One additional feature of $\hat{t}_2$ that needs to be accounted for, is that it doesn't have the simple relationship for conjugate configurations that all the other $\hat{t}_i$ operators have. For the sake of simplicity, and to avoid having to explicitly store matrix elements beyond $\underline{f}^7$ **qlanth** takes the approach of adding a control parameter t2Switch which needs to be set to 1 if below or at $\underline{f}^7$ and set to 0 if above $\underline{f}^7$.

```
GenerateThreeBodyTables::usage = "This function generates the reduced
     matrix elements for the three body operators using the
    coefficients of fractional parentage, including those beyond f^7."
    ;
Options[GenerateThreeBodyTables] = {"Export" -> False};
GenerateThreeBodyTables[OptionsPattern[]] := (
  tiKeys        = (StringReplace[ToString[#], {"T" -> "t_{", "p" -> "
    }^{'"}] <> "}") & /@ TSymbols;
  TSymbolsAssoc = AssociationThread[tiKeys -> TSymbols];
  juddOperators = ParseJudd1984[];
  (* op3MatrixElement[SL, SpLp, opSymbol] returns the value for the
    reduced matrix element of the operator opSymbol for the terms {SL,
     SpLp} in the f^3 configuration. *)
  op3MatrixElement[SL_, SpLp_, opSymbol_] := (
    jOP = juddOperators[{3, opSymbol}];
    key = {SL, SpLp};
    val = If[MemberQ[Keys[jOP], key],
      jOP[key],
      0];
    Return[val];
  );
  (* ti: This is the implementation of formula (2) in Judd & Suskin
    1984. It computes the reduced matrix elements of ti in f^n by
    using the reduced matrix elements in f^3 and the coefficients of
    fractional parentage. If the option ''Fast'' is set to True then
    the values for n>7 are simply computed as the negatives of the
    values in the complementary configuration; this except for t2 and
    t11 which are treated as special cases. *)
  Options[ti] = {"Fast" -> True};
  ti[nE_, SL_, SpLp_, tiKey_, opOrder_ : 3, OptionsPattern[]] :=
    Module[
    {nn, S, L, Sp, Lp,
    cfpSL, cfpSpLp,
    parentSL, parentSpLp,
    tnk, tnks},
    (
      {S, L}   = FindSL[SL];
      {Sp, Lp} = FindSL[SpLp];
      fast     = OptionValue["Fast"];
      numH     = 14 - nE;
      If[fast && Not[MemberQ[{"t_{2}","t_{11}"},tiKey]] && nE > 7,
        Return[-tktable[{numH, SL, SpLp, tiKey}]]
      ];
      If[(S == Sp && L == Lp),
      (
        cfpSL   = CFP[{nE, SL}];
        cfpSpLp = CFP[{nE, SpLp}];
        tnks = Table[(
            parentSL   = cfpSL[[nn, 1]];
            parentSpLp = cfpSpLp[[mm, 1]];
            cfpSL[[nn, 2]] * cfpSpLp[[mm, 2]] *
            tktable[{nE - 1, parentSL, parentSpLp, tiKey}]
            ),
            {nn, 2, Length[cfpSL]},
            {mm, 2, Length[cfpSpLp]}
```

```
            ];
        tnk = Total[Flatten[tnks]];
        ),
      tnk = 0;
      ];
      Return[ nE / (nE - opOrder) * tnk];
    )
  ];
  (* Calculate the reduced matrix elements of t^i for n up to 14 *)
  tktable = <||>;
  Do[(
    Do[(
      tkValue = Which[numE <= 2,
        (*Initialize n=1,2 with zeros*)
        0,
        numE == 3,
        (* Grab matrix elem in f^3 from Judd 1984 *)
        SimplifyFun[op3MatrixElement[SL, SpLp, opKey]],
        True,
        SimplifyFun[ti[numE, SL, SpLp, opKey, If[opKey == "e_{3}", 2,
   3]]]
        ];
      tktable[{numE, SL, SpLp, opKey}] = tkValue;
      ),
    {SL, AllowedNKSLTerms[numE]},
    {SpLp, AllowedNKSLTerms[numE]},
    {opKey, Append[tiKeys, "e_{3}"]}
    ];
    PrintTemporary[StringJoin["\[ScriptF]", ToString[numE], "
  configuration complete"]];
    ),
    {numE, 1, 14}
  ];

  (* Now use those reduced matrix elements to determine their sum as
    weighted by their corresponding strengths Ti *)
  ThreeBodyTable = <||>;
  Do[
    Do[
    (
      ThreeBodyTable[{numE, SL, SpLp}] = (
        Sum[(
          If[tiKey == "t_{2}", t2Switch, 1] *
          tktable[{numE, SL, SpLp, tiKey}] *
          TSymbolsAssoc[tiKey] +
          If[tiKey == "t_{2}", 1 - t2Switch, 0] *
          (-tktable[{14 - numE, SL, SpLp, tiKey}]) *
          TSymbolsAssoc[tiKey]
          ),
        {tiKey, tiKeys}
        ]
      );
    ),
    {SL, AllowedNKSLTerms[numE]},
    {SpLp, AllowedNKSLTerms[numE]}
    ];
  PrintTemporary[StringJoin["\[ScriptF]", ToString[numE], " matrix
    complete"]];,
  {numE, 1, 7}
  ];

  ThreeBodyTables = Table[(
    terms = AllowedNKSLTerms[numE];
    singleThreeBodyTable =
      Table[
        {SL, SLp} -> ThreeBodyTable[{numE, SL, SLp}],
        {SL, terms},
        {SLp, terms}
      ];
    singleThreeBodyTable  = Flatten[singleThreeBodyTable];
    singleThreeBodyTables = Table[(
        notNullPosition = Position[TSymbols, notNullSymbol][[1, 1]];
        reps = ConstantArray[0, Length[TSymbols]];
        reps[[notNullPosition]] = 1;
        rep = AssociationThread[TSymbols -> reps];
        notNullSymbol -> Association[(singleThreeBodyTable /. rep)]
```

```
        ),
      {notNullSymbol, TSymbols}
      ];
    singleThreeBodyTables = Association[singleThreeBodyTables];
    numE -> singleThreeBodyTables),
    {numE, 1, 7}
];

ThreeBodyTables = Association[ThreeBodyTables];
If[OptionValue["Export"],
  (
    threeBodyTablefname = FileNameJoin[{moduleDir, "data", "
    ThreeBodyTable.m"}];
    Export[threeBodyTablefname, ThreeBodyTable];
    threeBodyTablesfname = FileNameJoin[{moduleDir, "data", "
    ThreeBodyTables.m"}];
    Export[threeBodyTablesfname, ThreeBodyTables];
  )
 ];
Return[{ThreeBodyTable, ThreeBodyTables}];
);
```

```
ParseJudd1984::usage = "This function parses the data from tables 1
    and 2 of Judd from Judd, BR, and MA Suskin. ''Complete Set of
    Orthogonal Scalar Operators for the Configuration f^3''. JOSA B 1,
     no. 2 (1984): 261-65.";
Options[ParseJudd1984] = {"Export" -> False};
ParseJudd1984[OptionsPattern[]] := (
  ParseJuddTab1[str_] := (
    strR = ToString[str];
    strR = StringReplace[strR, ".5" -> "^(1/2)"];
    num = ToExpression[strR];
    sign = Sign[num];
    num = sign*Simplify[Sqrt[num^2]];
    If[Round[num] == num, num = Round[num]];
    Return[num]);

  (* Parse table 1 from Judd 1984 *)
  judd1984Fname1 = FileNameJoin[{moduleDir, "data", "Judd1984-1.csv"
    }];
  data = Import[judd1984Fname1, "CSV", "Numeric" -> False];
  headers = data[[1]];
  data = data[[2 ;;]];
  data = Transpose[data];
  \[Psi] = Select[data[[1]], # != "" &];
  \[Psi]p = Select[data[[2]], # != "" &];
  matrixKeys = Transpose[{\[Psi], \[Psi]p}];
  data = data[[3 ;;]];
  cols = Table[ParseJuddTab1 /@ Select[col, # != "" &], {col, data}];
  cols = Select[cols, Length[#] == 21 &];
  tab1 = Prepend[Prepend[cols, \[Psi]p], \[Psi]];
  tab1 = Transpose[Prepend[Transpose[tab1], headers]];

  (* Parse table 2 from Judd 1984 *)
  judd1984Fname2 = FileNameJoin[{moduleDir, "data", "Judd1984-2.csv"
    }];
  data = Import[judd1984Fname2, "CSV", "Numeric" -> False];
  headers = data[[1]];
  data = data[[2 ;;]];
  data = Transpose[data];
  {operatorLabels, WUlabels, multiFactorSymbols, multiFactorValues} =
     data[[;; 4]];
  multiFactorValues = ParseJuddTab1 /@ multiFactorValues;
  multiFactorValues = AssociationThread[multiFactorSymbols ->
    multiFactorValues];

  (*scale values of table 1 given the values in table 2*)
  oppyS = {};
  normalTable =
    Table[header = col[[1]];
      If[StringContainsQ[header, " "],
        (
          multiplierSymbol = StringSplit[header, " "][[1]];
          multiplierValue = multiFactorValues[multiplierSymbol];
          operatorSymbol = StringSplit[header, " "][[2]];
          oppyS = Append[oppyS, operatorSymbol];
```

```
        ),
        (
          multiplierValue = 1;
          operatorSymbol = header;
        )
      ];
      normalValues = 1/multiplierValue*col[[2 ;;]];
      Join[{operatorSymbol}, normalValues], {col, tab1[[3 ;;]]}
    ];

  (*Create an association for the reduced matrix elements in the f^3
    config*)
  juddOperators = Association[];
  Do[(
    col      = normalTable[[colIndex]];
    opLabel  = col[[1]];
    opValues = col[[2 ;;]];
    opMatrix = AssociationThread[matrixKeys -> opValues];
    Do[(
      opMatrix[Reverse[mKey]] = opMatrix[mKey]
      ),
    {mKey, matrixKeys}
    ];
    juddOperators[{3, opLabel}] = opMatrix),
    {colIndex, 1, Length[normalTable]}
  ];

  (* special case of t2 in f3 *)
  (* this is the same as getting the reduced matrix elements from
    Judd 1966 *)
  numE = 3;
  e3Op      = juddOperators[{3, "e_{3}"}];
  t2prime   = juddOperators[{3, "t_{2}^{'}"}];
  prefactor = 1/(70 Sqrt[2]);
  t2Op = (# -> (t2prime[#] + prefactor*e3Op[#])) & /@ Keys[t2prime];
  t2Op = Association[t2Op];
  juddOperators[{3, "t_{2}"}] = t2Op;

  (*Special case of t11 in f3*)
  t11 = juddOperators[{3, "t_{11}"}];
  eβprimeOp = juddOperators[{3, "e_{\\beta}^{'}"}];
  t11primeOp = (# -> (t11[#] + Sqrt[3/385] eβprimeOp[#])) & /@ Keys[
    t11];
  t11primeOp = Association[t11primeOp];
  juddOperators[{3, "t_{11}^{'}"}] = t11primeOp;
  If[OptionValue["Export"],
    (
      (*export them*)
      PrintTemporary["Exporting ..."];
      exportFname = FileNameJoin[{moduleDir, "data", "juddOperators.m
    "}];
      Export[exportFname, juddOperators];
    )
  ];
  Return[juddOperators];
);
```

3.9 $\hat{\mathcal{H}}_{\mathbf{cf}}$: crystal-field

The crystal-field partially accounts for the influence of the surrounding lattice on the ion. The simplest picture of this influence imagines the lattice as responsible for an electric field felt at the position of the ion. This electric field corresponding to an electrostatic potential described as a multipolar sum of the form:

$$V(r_i, \theta_i, \phi_i) = \sum_{k=1}^{\infty} \sum_{q=-k}^{k} \mathcal{A}_q^{(k)} r_i^k \mathcal{C}_q^{(k)}(\theta_i, \phi_i) \tag{52}$$

where the $\mathcal{C}_q^{(k)}$ are spherical harmonics normalized with the Racah convention

$$\mathcal{C}_q^{(k)} = \sqrt{\frac{4\pi}{2k+1}} Y_q^{(k)}. \tag{53}$$

Here we have chosen a coordinate system with its origin at the position of the nucleus, and in which we only have positive powers of the distance r_i because we have expanded the contributions from all the surrounding ions as a sum over spherical harmonics centered at the position of the nucleus, without r ever large enough to reach any of the positions of the lattice ions.

Furthermore, since we have n valence electrons, then the total crystal field potential is

$$\hat{\mathcal{H}}_{\rm cf}(\vec{r}) = \sum_{i=1}^{n}\sum_{k=0}^{\infty}\sum_{q=-k}^{k} \mathcal{A}_q^{(k)} r_i^k \mathcal{C}_q^{(k)}(\theta_i,\phi_i). \tag{54}$$

And if we average the radial coordinate,

$$\hat{\mathcal{H}}_{\rm cf} = \sum_{i=1}^{n}\sum_{k=1}^{\infty}\sum_{q=-k}^{k} \mathcal{B}_q^{(k)} \mathcal{C}_q^{(k)}(i) \tag{55}$$

where the radial average is included as

$$\mathcal{B}_q^{(k)} := \mathcal{A}_q^{(k)} \langle 4f|r^k|4f\rangle. \tag{56}$$

$\mathcal{B}_q^{(k)}$ may be complex in general. However, since the sum in Eqn-54 needs to result in a real and Hermitian operator, there are restrictions on $\mathcal{B}_q^{(k)}$ that need to be accounted for. Once the behavior of $\mathcal{C}_q^{(k)}$ under complex conjugation is considered, $\mathcal{C}_q^{(k)*} = (-1)^q \mathcal{C}_{-q}^{(k)}$, it is necessary that

$$\mathcal{B}_q^{(k)} = (-1)^q \mathcal{B}_{-q}^{(k)*}. \tag{57}$$

Presently the sum over q spans both its negative and positive values. This can be limited to only the non-negative values of q. Separating the real and imaginary parts of $\mathcal{B}_q^{(k)}$ such that $\mathcal{B}_q^{(k)} = B_q^{(k)} + iS_q^{(k)}$ for $q \neq 0$ and $\mathcal{B}_0^{(k)} = 2B_0^{(k)}$ the sum for the crystal field can then be written as

$$\hat{\mathcal{H}}_{\rm cf}(\vec{r}) = \sum_{i=1}^{n}\sum_{k=0}^{\infty}\sum_{q=0}^{k} B_q^{(k)}\left(\mathcal{C}_q^{(k)} + (-1)^q \mathcal{C}_{-q}^{(k)}\right) + iS_q^{(k)}\left(\mathcal{C}_q^{(k)} - (-1)^q \mathcal{C}_{-q}^{(k)}\right). \tag{58}$$

A staple of the Wigner-Racah algebra is writing up operators of interest in terms of standard ones for which the matrix elements are straightforward. One such operator is the unit tensor operator $\hat{u}^{(k)}$ for a single electron. The Wigner-Eckart theorem – on which all of this algebra is an elaboration – effectively separates the dynamical and geometrical parts of a given interaction; the unit tensor operators isolate the geometric contributions. This irreducible tensor operator $\hat{u}^{(k)}$ is defined as the tensor operator having the following reduced matrix elements (written in terms of the triangular delta, see section on notation):

$$\langle \ell \| \hat{u}^{(k)} \| \ell' \rangle = 1. \tag{59}$$

In terms of this tensor one may then define the symmetric (in the sense that the resulting operator is equitable among all electrons) unit tensor operator for n particles as

$$\hat{U}^{(k)} = \sum_{i}^{n} \hat{u}_i^{(k)}. \tag{60}$$

This tensor is relevant to the calculation of the above matrix elements since

$$\mathcal{C}_q^{(k)} = \langle \underline{\ell} \| C^{(k)} \| \underline{\ell}' \rangle \hat{u}_q^{(k)} = (-1)^{\underline{\ell}} \sqrt{[\![\underline{\ell}]\!][\![\underline{\ell}']\!]} \begin{pmatrix} \underline{\ell} & k & \underline{\ell}' \\ 0 & 0 & 0 \end{pmatrix} \hat{u}_q^{(k)}. \tag{61}$$

With this, the matrix elements of $\hat{\mathcal{H}}_{\rm cf}$ in the $|LSJM_J\rangle$ basis are:

$$\overbrace{\langle \underline{\ell}^n \alpha SLJM_J | \hat{\mathcal{H}}_{\rm cf} | \underline{\ell}^n \alpha' SL'J'M_{J'}\rangle}^{\text{Wybourne eqn. 6-3}} = \sum_{k=1}^{\infty}\sum_{q=-k}^{k} \mathcal{B}_q^{(k)} \langle \underline{\ell}^n \alpha SLJM_J | \hat{U}_q^{(k)} | \underline{\ell}^n \alpha' SL'J'M_{J'}\rangle \langle \underline{\ell} \| \hat{C}^{(k)} \| \underline{\ell}\rangle \tag{62}$$

where the matrix elements of $\hat{U}_q^{(k)}$ can be resolved with a 3j symbol as

$$\overbrace{\langle \underline{\ell}^n \alpha SLJM_J | \hat{U}_q^{(k)} | \underline{\ell}^n \alpha' S'L'J'M_{J'}\rangle}^{\text{Wybourne eqn. 6-4}} = (-1)^{J-M_J} \begin{pmatrix} J & k & J' \\ -M_J & q & M_{J'} \end{pmatrix} \langle \underline{\ell}^n \alpha SLJ \| \hat{U}^{(k)} \| \underline{\ell}^n \alpha' S'L'\rangle \tag{63}$$

and reduced a second time with the inclusion of a 6j symbol resulting in

$$\overbrace{\langle \underline{\ell}^n \alpha SLJ \| \hat{U}^{(k)} \| \underline{\ell}^n \alpha' S' L' \rangle}^{\text{Wybourne eqn. 6-5}} = (-1)^{S+L+J'+k} \sqrt{[\![J]\!][\![J']\!]} \times \begin{Bmatrix} J & J' & k \\ L' & L & S \end{Bmatrix} \langle \underline{\ell}^n \alpha SL \| \hat{U}^{(k)} \| \underline{\ell}^n \alpha' S' L' \rangle. \tag{64}$$

This last reduced matrix element is finally computed by summing over $\bar{\alpha}\bar{L}\bar{S}$ which are the $\underline{\ell}^{n-1}$ parents which are common to $|\alpha LS\rangle$ and $|\alpha' L' S'\rangle$ from the $\underline{\ell}^n$ configuration:

$$\overbrace{\langle \underline{\ell}^n \alpha SL \| \hat{U}^{(k)} \| \underline{\ell}^n \alpha' S' L' \rangle}^{\text{Cowan eqn. 11.53}} = \delta(S,S') n (-1)^{\underline{\ell}+L+k} \sqrt{[\![L]\!][\![L']\!]} \times \sum_{\bar{\alpha}\bar{L}\bar{S}} (-1)^{\bar{L}} \begin{Bmatrix} \underline{\ell} & k & \underline{\ell} \\ L & \bar{L} & L' \end{Bmatrix} \left(\underline{\ell}^n \alpha LS \left\{ \underline{\ell}^{n-1} \bar{\alpha}\bar{L}\bar{S} \right) \left(\underline{\ell}^{n-1} \bar{\alpha}\bar{L}\bar{S} \right\} \underline{\ell}^n \alpha' L' S' \right). \tag{65}$$

From the $\langle \underline{\ell} \| \hat{C}^{(k)} \| \underline{\ell} \rangle$, and given that we are using $\underline{\ell} = \underline{\mathrm{f}} = 3$, we can see that by the triangular condition $\triangleleft(3,k,3)$ the non-zero contributions only come from $k = 0,1,2,3,4,5,6$. An additional selection rule on k comes from considerations of parity. Since both the bra and the ket in $\langle \underline{\ell}^n \alpha SLJM_J | \hat{\mathcal{H}}_{\mathrm{cf}} | \underline{\ell}^n \alpha' SL' J' M_{J'} \rangle$ have the same parity, then the overall parity of the braket is determined by the parity of $\mathcal{C}_q^{(k)}$, and since the parity of $\mathcal{C}_q^{(k)}$ is $(-1)^k$ then for the braket to be non-zero we require that k should also be even. In view of this, in all the above equations for the crystal field the values for k should be limited to $2,4,6$. The value of $k = 0$ having been omitted from the start since this only contributes a common energy shift. Putting everything together:

$$\hat{\mathcal{H}}_{\mathrm{cf}}(\vec{r}) = \sum_{i=1}^{n} \sum_{k=2,4,6} \sum_{q=0}^{k} B_q^{(k)} \left(\mathcal{C}_q^{(k)} + (-1)^q \mathcal{C}_{-q}^{(k)} \right) + i S_q^{(k)} \left(\mathcal{C}_q^{(k)} - (-1)^q \mathcal{C}_{-q}^{(k)} \right). \tag{66}$$

The above equations are implemented in **qlanth** by the function `CrystalField`. This function puts together the symbolic sum in ℰqn-62 by using the function `Cqk`. `Cqk` then uses the diagonal reduced matrix elements of $\mathcal{C}_q^{(k)}$ and the precomputed values for `Uk` (stored in `ReducedUkTable`).

The required reduced matrix elements of $\hat{U}^{(k)}$ are calculated by the function `ReducedUk`, which is used by `GenerateReducedUkTable` to precompute its values.

```
Bqk::usage = "Real part of the Bqk coefficients.";
Bqk[q_, 2] := {B02/2, B12, B22}[[q + 1]];
Bqk[q_, 4] := {B04/2, B14, B24, B34, B44}[[q + 1]];
Bqk[q_, 6] := {B06/2, B16, B26, B36, B46, B56, B66}[[q + 1]];
```

```
Sqk::usage = "Imaginary part of the Bqk coefficients.";
Sqk[q_, 2] := {0, S12, S22}[[q + 1]];
Sqk[q_, 4] := {0, S14, S24, S34, S44}[[q + 1]];
Sqk[q_, 6] := {0, S16, S26, S36, S46, S56, S66}[[q + 1]];
```

```
Cqk::usage = "Cqk[numE, q, k, NKSL, J, M, NKSLp, Jp, Mp]. In Wybourne
    (1965) see equations 6-3, 6-4, and 6-5. Also in TASS see equation
    11.53.";
Cqk[numE_, q_, k_, NKSL_, J_, M_, NKSLp_, Jp_, Mp_] := Module[
  {S, Sp, L, Lp, orbital, val},
  (
    orbital = 3;
    {S, L}   = FindSL[NKSL];
    {Sp, Lp} = FindSL[NKSLp];
    f1  = ThreeJay[{J, -M}, {k, q}, {Jp, Mp}];
    val =
      If[f1==0,
        0,
        (
          f2 = SixJay[{L, J, S}, {Jp, Lp, k}] ;
          If[f2==0,
            0,
            (
              f3 = ReducedUkTable[{numE, orbital, NKSL, NKSLp, k}];
              If[f3==0,
                0,
                (
```

```
                    (
                      Phaser[J - M + S + Lp + J + k] *
                      Sqrt[TPO[J, Jp]] *
                      f1 *
                      f2 *
                      f3 *
                      Ck[orbital, k]
                    )
                  )
                ]
              )
            ]
          )
        ];
      Return[val];
    )
];
```

```
CrystalField::usage = "CrystalField[n, NKSL, J, M, NKSLp, Jp, Mp]
    gives the general expression for the matrix element of the crystal
     field Hamiltonian parametrized with Bqk and Sqk coefficients as a
     sum over spherical harmonics Cqk.
Sometimes this expression only includes Bqk coefficients, see for
    example eqn 6-2 in Wybourne (1965), but one may also split the
    coefficient into real and imaginary parts as is done here, in an
    expression that is patently Hermitian.";
CrystalField[numE_, NKSL_, J_, M_, NKSLp_, Jp_, Mp_] := (
  Sum[
    (
      cqk  = Cqk[numE,  q, k, NKSL, J, M, NKSLp, Jp, Mp];
      cmqk = Cqk[numE, -q, k, NKSL, J, M, NKSLp, Jp, Mp];
      Bqk[q, k]   * (cqk + (-1)^q * cmqk) +
      I*Sqk[q, k] * (cqk - (-1)^q * cmqk)
      ),
  {k, {2, 4, 6}},
  {q, 0, k}
  ]
)
```

```
ReducedUk::usage = "ReducedUk[n, l, SL, SpLp, k] gives the reduced
    matrix element of the symmetric unit tensor operator U^(k). See
    equation 11.53 in TASS.";
ReducedUk[numE_, l_, SL_, SpLp_, k_] := Module[
  {spin, orbital, Uk, S, L,
  Sp, Lp, Sb, Lb, parentSL,
  cfpSL, cfpSpLp, Ukval,
  SLparents, SLpparents,
  commonParents, phase},
    {spin, orbital} = {1/2, 3};
    {S, L}          = FindSL[SL];
    {Sp, Lp}        = FindSL[SpLp];
    If[Not[S == Sp],
      Return[0]
    ];
    cfpSL       = CFP[{numE, SL}];
    cfpSpLp     = CFP[{numE, SpLp}];
    SLparents   = First /@ Rest[cfpSL];
    SLpparents  = First /@ Rest[cfpSpLp];
    commonParents = Intersection[SLparents, SLpparents];
    Uk = Sum[(
      {Sb, Lb} = FindSL[\[Psi]b];
      Phaser[Lb] *
        CFPAssoc[{numE, SL, \[Psi]b}] *
        CFPAssoc[{numE, SpLp, \[Psi]b}] *
        SixJay[{orbital, k, orbital}, {L, Lb, Lp}]
    ),
    {\[Psi]b, commonParents}
    ];
    phase     = Phaser[orbital + L + k];
    prefactor = numE * phase * Sqrt[TPO[L,Lp]];
    Ukval     = prefactor*Uk;
    Return[Ukval];
]
```

Each of the 32 crystallographic point groups requires only a limited number of non-zero crystal field parameters. In **qlanth** these can be queried programatically with the

use of the function `CrystalFieldForm`. These were taken from a table in Benelli and Gatteschi [BG15] and their corresponding expressions (for a single electron) are in the equations below with a table linking to the corresponding equations. Note that these expressions bring with them an implicit choice for the orientation of the coordinate system (see Section 4).

$\mathcal{S}_2$: &qn-67	$\mathcal{C}_s$: &qn-68	$\mathcal{C}_{1h}$: &qn-69	$\mathcal{C}_2$: &qn-70	$\mathcal{C}_{2h}$: &qn-71
$\mathcal{C}_{2v}$: &qn-72	$\mathcal{D}_2$: &qn-73	$\mathcal{D}_{2h}$: &qn-74	$\mathcal{S}_4$: &qn-75	$\mathcal{C}_4$: &qn-76
$\mathcal{C}_{4h}$: &qn-77	$\mathcal{D}_{2d}$: &qn-78	$\mathcal{C}_{4v}$: &qn-79	$\mathcal{D}_4$: &qn-80	$\mathcal{D}_{4h}$: &qn-81
$\mathcal{C}_3$: &qn-82	$\mathcal{S}_6$: &qn-83	$\mathcal{C}_{3h}$: &qn-84	$\mathcal{C}_{3v}$: &qn-85	$\mathcal{D}_3$: &qn-86
$\mathcal{D}_{3d}$: &qn-87	$\mathcal{D}_{3h}$: &qn-88	$\mathcal{C}_6$: &qn-89	$\mathcal{C}_{6h}$: &qn-90	$\mathcal{C}_{6v}$: &qn-91
$\mathcal{D}_6$: &qn-92	$\mathcal{D}_{6h}$: &qn-93	$\mathcal{T}$: &qn-94	$\mathcal{T}_h$: &qn-95	$\mathcal{T}_d$: &qn-96
$\mathcal{O}$: &qn-97	$\mathcal{O}_h$: &qn-98			

Table 1: Expressions for the crystal field in the 32 crystallographic point groups

Crystal field expressions

$$\begin{aligned}\hat{\mathcal{H}}_{\text{cf}}(\mathcal{S}_2) = {} & B_0^{(2)}\mathcal{C}_0^{(2)} + B_1^{(2)}\mathcal{C}_1^{(2)} + \left(B_2^{(2)} + iS_2^{(2)}\right)\mathcal{C}_2^{(2)} + B_0^{(4)}\mathcal{C}_0^{(4)} \\ & + \left(B_1^{(4)} + iS_1^{(4)}\right)\mathcal{C}_1^{(4)} + \left(B_2^{(4)} + iS_2^{(4)}\right)\mathcal{C}_2^{(4)} + \left(B_3^{(4)} + iS_3^{(4)}\right)\mathcal{C}_3^{(4)} + \left(B_4^{(4)} + iS_4^{(4)}\right)\mathcal{C}_4^{(4)} \\ & + B_0^{(6)}\mathcal{C}_0^{(6)} + \left(B_1^{(6)} + iS_1^{(6)}\right)\mathcal{C}_1^{(6)} + \left(B_2^{(6)} + iS_2^{(6)}\right)\mathcal{C}_2^{(6)} + \left(B_3^{(6)} + iS_3^{(6)}\right)\mathcal{C}_3^{(6)} \\ & + \left(B_4^{(6)} + iS_4^{(6)}\right)\mathcal{C}_4^{(6)} + \left(B_5^{(6)} + iS_5^{(6)}\right)\mathcal{C}_5^{(6)} + \left(B_6^{(6)} + iS_6^{(6)}\right)\mathcal{C}_6^{(6)}\end{aligned} \tag{67}$$

$$\begin{aligned}\hat{\mathcal{H}}_{\text{cf}}(\mathcal{C}_s) = {} & B_0^{(2)}\mathcal{C}_0^{(2)} + B_2^{(2)}\mathcal{C}_2^{(2)} + B_0^{(4)}\mathcal{C}_0^{(4)} + \left(B_2^{(4)} + iS_2^{(4)}\right)\mathcal{C}_2^{(4)} \\ & + \left(B_4^{(4)} + iS_4^{(4)}\right)\mathcal{C}_4^{(4)} + B_0^{(6)}\mathcal{C}_0^{(6)} + \left(B_2^{(6)} + iS_2^{(6)}\right)\mathcal{C}_2^{(6)} + \left(B_4^{(6)} + iS_4^{(6)}\right)\mathcal{C}_4^{(6)} \\ & + \left(B_6^{(6)} + iS_6^{(6)}\right)\mathcal{C}_6^{(6)}\end{aligned} \tag{68}$$

$$\begin{aligned}\hat{\mathcal{H}}_{\text{cf}}(\mathcal{C}_{1h}) = {} & B_0^{(2)}\mathcal{C}_0^{(2)} + B_2^{(2)}\mathcal{C}_2^{(2)} + B_0^{(4)}\mathcal{C}_0^{(4)} + \left(B_2^{(4)} + iS_2^{(4)}\right)\mathcal{C}_2^{(4)} \\ & + \left(B_4^{(4)} + iS_4^{(4)}\right)\mathcal{C}_4^{(4)} + B_0^{(6)}\mathcal{C}_0^{(6)} + \left(B_2^{(6)} + iS_2^{(6)}\right)\mathcal{C}_2^{(6)} + \left(B_4^{(6)} + iS_4^{(6)}\right)\mathcal{C}_4^{(6)} \\ & + \left(B_6^{(6)} + iS_6^{(6)}\right)\mathcal{C}_6^{(6)}\end{aligned} \tag{69}$$

$$\begin{aligned}\hat{\mathcal{H}}_{\text{cf}}(\mathcal{C}_2) = {} & B_0^{(2)}\mathcal{C}_0^{(2)} + B_2^{(2)}\mathcal{C}_2^{(2)} + B_0^{(4)}\mathcal{C}_0^{(4)} + \left(B_2^{(4)} + iS_2^{(4)}\right)\mathcal{C}_2^{(4)} \\ & + \left(B_4^{(4)} + iS_4^{(4)}\right)\mathcal{C}_4^{(4)} + B_0^{(6)}\mathcal{C}_0^{(6)} + \left(B_2^{(6)} + iS_2^{(6)}\right)\mathcal{C}_2^{(6)} + \left(B_4^{(6)} + iS_4^{(6)}\right)\mathcal{C}_4^{(6)} \\ & + \left(B_6^{(6)} + iS_6^{(6)}\right)\mathcal{C}_6^{(6)}\end{aligned} \tag{70}$$

$$\begin{aligned}\hat{\mathcal{H}}_{\text{cf}}(\mathcal{C}_{2h}) = {} & B_0^{(2)}\mathcal{C}_0^{(2)} + B_2^{(2)}\mathcal{C}_2^{(2)} + B_0^{(4)}\mathcal{C}_0^{(4)} + \left(B_2^{(4)} + iS_2^{(4)}\right)\mathcal{C}_2^{(4)} \\ & + \left(B_4^{(4)} + iS_4^{(4)}\right)\mathcal{C}_4^{(4)} + B_0^{(6)}\mathcal{C}_0^{(6)} + \left(B_2^{(6)} + iS_2^{(6)}\right)\mathcal{C}_2^{(6)} + \left(B_4^{(6)} + iS_4^{(6)}\right)\mathcal{C}_4^{(6)} \\ & + \left(B_6^{(6)} + iS_6^{(6)}\right)\mathcal{C}_6^{(6)}\end{aligned} \tag{71}$$

$$\begin{aligned}\hat{\mathcal{H}}_{\text{cf}}(\mathcal{C}_{2v}) = {} & B_0^{(2)}\mathcal{C}_0^{(2)} + B_2^{(2)}\mathcal{C}_2^{(2)} + B_0^{(4)}\mathcal{C}_0^{(4)} + B_2^{(4)}\mathcal{C}_2^{(4)} + B_4^{(4)}\mathcal{C}_4^{(4)} \\ & + B_0^{(6)}\mathcal{C}_0^{(6)} + B_2^{(6)}\mathcal{C}_2^{(6)} + B_4^{(6)}\mathcal{C}_4^{(6)} + B_6^{(6)}\mathcal{C}_6^{(6)}\end{aligned} \tag{72}$$

$$\begin{aligned}\hat{\mathcal{H}}_{\text{cf}}(\mathcal{D}_2) = {} & B_0^{(2)}\mathcal{C}_0^{(2)} + B_2^{(2)}\mathcal{C}_2^{(2)} + B_0^{(4)}\mathcal{C}_0^{(4)} + B_2^{(4)}\mathcal{C}_2^{(4)} + B_4^{(4)}\mathcal{C}_4^{(4)} \\ & + B_0^{(6)}\mathcal{C}_0^{(6)} + B_2^{(6)}\mathcal{C}_2^{(6)} + B_4^{(6)}\mathcal{C}_4^{(6)} + B_6^{(6)}\mathcal{C}_6^{(6)}\end{aligned} \tag{73}$$

$$\hat{\mathscr{H}}_{\rm cf}\left(\mathcal{D}_{2h}\right) = B_0^{(2)}\mathcal{C}_0^{(2)} + B_2^{(2)}\mathcal{C}_2^{(2)} + B_0^{(4)}\mathcal{C}_0^{(4)} + B_2^{(4)}\mathcal{C}_2^{(4)} + B_4^{(4)}\mathcal{C}_4^{(4)} + B_0^{(6)}\mathcal{C}_0^{(6)} + B_2^{(6)}\mathcal{C}_2^{(6)} + B_4^{(6)}\mathcal{C}_4^{(6)} + B_6^{(6)}\mathcal{C}_6^{(6)} \tag{74}$$

$$\hat{\mathscr{H}}_{\rm cf}\left(\mathcal{S}_4\right) = B_0^{(2)}\mathcal{C}_0^{(2)} + B_0^{(4)}\mathcal{C}_0^{(4)} + B_4^{(4)}\mathcal{C}_4^{(4)} + B_0^{(6)}\mathcal{C}_0^{(6)} + \left(B_4^{(6)} + iS_4^{(6)}\right)\mathcal{C}_4^{(6)} \tag{75}$$

$$\hat{\mathscr{H}}_{\rm cf}\left(\mathcal{C}_4\right) = B_0^{(2)}\mathcal{C}_0^{(2)} + B_0^{(4)}\mathcal{C}_0^{(4)} + B_4^{(4)}\mathcal{C}_4^{(4)} + B_0^{(6)}\mathcal{C}_0^{(6)} + \left(B_4^{(6)} + iS_4^{(6)}\right)\mathcal{C}_4^{(6)} \tag{76}$$

$$\hat{\mathscr{H}}_{\rm cf}\left(\mathcal{C}_{4h}\right) = B_0^{(2)}\mathcal{C}_0^{(2)} + B_0^{(4)}\mathcal{C}_0^{(4)} + B_4^{(4)}\mathcal{C}_4^{(4)} + B_0^{(6)}\mathcal{C}_0^{(6)} + \left(B_4^{(6)} + iS_4^{(6)}\right)\mathcal{C}_4^{(6)} \tag{77}$$

$$\hat{\mathscr{H}}_{\rm cf}\left(\mathcal{D}_{2d}\right) = B_0^{(2)}\mathcal{C}_0^{(2)} + B_0^{(4)}\mathcal{C}_0^{(4)} + B_4^{(4)}\mathcal{C}_4^{(4)} + B_0^{(6)}\mathcal{C}_0^{(6)} + B_4^{(6)}\mathcal{C}_4^{(6)} \tag{78}$$

$$\hat{\mathscr{H}}_{\rm cf}\left(\mathcal{C}_{4v}\right) = B_0^{(2)}\mathcal{C}_0^{(2)} + B_0^{(4)}\mathcal{C}_0^{(4)} + B_4^{(4)}\mathcal{C}_4^{(4)} + B_0^{(6)}\mathcal{C}_0^{(6)} + B_4^{(6)}\mathcal{C}_4^{(6)} \tag{79}$$

$$\hat{\mathscr{H}}_{\rm cf}\left(\mathcal{D}_4\right) = B_0^{(2)}\mathcal{C}_0^{(2)} + B_0^{(4)}\mathcal{C}_0^{(4)} + B_4^{(4)}\mathcal{C}_4^{(4)} + B_0^{(6)}\mathcal{C}_0^{(6)} + B_4^{(6)}\mathcal{C}_4^{(6)} \tag{80}$$

$$\hat{\mathscr{H}}_{\rm cf}\left(\mathcal{D}_{4h}\right) = B_0^{(2)}\mathcal{C}_0^{(2)} + B_0^{(4)}\mathcal{C}_0^{(4)} + B_4^{(4)}\mathcal{C}_4^{(4)} + B_0^{(6)}\mathcal{C}_0^{(6)} + B_4^{(6)}\mathcal{C}_4^{(6)} \tag{81}$$

$$\hat{\mathscr{H}}_{\rm cf}\left(\mathcal{C}_3\right) = B_0^{(2)}\mathcal{C}_0^{(2)} + B_0^{(4)}\mathcal{C}_0^{(4)} + B_3^{(4)}\mathcal{C}_3^{(4)} + B_0^{(6)}\mathcal{C}_0^{(6)} + \left(B_3^{(6)} + iS_3^{(6)}\right)\mathcal{C}_3^{(6)} + \left(B_6^{(6)} + iS_6^{(6)}\right)\mathcal{C}_6^{(6)} \tag{82}$$

$$\hat{\mathscr{H}}_{\rm cf}\left(\mathcal{S}_6\right) = B_0^{(2)}\mathcal{C}_0^{(2)} + B_0^{(4)}\mathcal{C}_0^{(4)} + B_3^{(4)}\mathcal{C}_3^{(4)} + B_0^{(6)}\mathcal{C}_0^{(6)} + \left(B_3^{(6)} + iS_3^{(6)}\right)\mathcal{C}_3^{(6)} + \left(B_6^{(6)} + iS_6^{(6)}\right)\mathcal{C}_6^{(6)} \tag{83}$$

$$\hat{\mathscr{H}}_{\rm cf}\left(\mathcal{C}_{3h}\right) = B_0^{(2)}\mathcal{C}_0^{(2)} + B_0^{(4)}\mathcal{C}_0^{(4)} + B_0^{(6)}\mathcal{C}_0^{(6)} + B_6^{(6)}\mathcal{C}_6^{(6)} \tag{84}$$

$$\hat{\mathscr{H}}_{\rm cf}\left(\mathcal{C}_{3v}\right) = B_0^{(2)}\mathcal{C}_0^{(2)} + B_0^{(4)}\mathcal{C}_0^{(4)} + B_3^{(4)}\mathcal{C}_3^{(4)} + B_0^{(6)}\mathcal{C}_0^{(6)} + B_3^{(6)}\mathcal{C}_3^{(6)} + B_6^{(6)}\mathcal{C}_6^{(6)} \tag{85}$$

$$\hat{\mathscr{H}}_{\rm cf}\left(\mathcal{D}_3\right) = B_0^{(2)}\mathcal{C}_0^{(2)} + B_0^{(4)}\mathcal{C}_0^{(4)} + B_3^{(4)}\mathcal{C}_3^{(4)} + B_0^{(6)}\mathcal{C}_0^{(6)} + B_3^{(6)}\mathcal{C}_3^{(6)} + B_6^{(6)}\mathcal{C}_6^{(6)} \tag{86}$$

$$\hat{\mathscr{H}}_{\rm cf}\left(\mathcal{D}_{3d}\right) = B_0^{(2)}\mathcal{C}_0^{(2)} + B_0^{(4)}\mathcal{C}_0^{(4)} + B_3^{(4)}\mathcal{C}_3^{(4)} + B_0^{(6)}\mathcal{C}_0^{(6)} + B_3^{(6)}\mathcal{C}_3^{(6)} + B_6^{(6)}\mathcal{C}_6^{(6)} \tag{87}$$

$$\hat{\mathscr{H}}_{\rm cf}\left(\mathcal{D}_{3h}\right) = B_0^{(2)}\mathcal{C}_0^{(2)} + B_0^{(4)}\mathcal{C}_0^{(4)} + B_0^{(6)}\mathcal{C}_0^{(6)} + B_6^{(6)}\mathcal{C}_6^{(6)} \tag{88}$$

$$\hat{\mathscr{H}}_{\rm cf}\left(\mathcal{C}_6\right) = B_0^{(2)}\mathcal{C}_0^{(2)} + B_0^{(4)}\mathcal{C}_0^{(4)} + B_0^{(6)}\mathcal{C}_0^{(6)} + B_6^{(6)}\mathcal{C}_6^{(6)} \tag{89}$$

$$\hat{\mathscr{H}}_{\rm cf}\left(\mathcal{C}_{6h}\right) = B_0^{(2)}\mathcal{C}_0^{(2)} + B_0^{(4)}\mathcal{C}_0^{(4)} + B_0^{(6)}\mathcal{C}_0^{(6)} + B_6^{(6)}\mathcal{C}_6^{(6)} \tag{90}$$

$$\hat{\mathscr{H}}_{\rm cf}\left(\mathcal{C}_{6v}\right) = B_0^{(2)}\mathcal{C}_0^{(2)} + B_0^{(4)}\mathcal{C}_0^{(4)} + B_0^{(6)}\mathcal{C}_0^{(6)} + B_6^{(6)}\mathcal{C}_6^{(6)} \tag{91}$$

$$\hat{\mathscr{H}}_{\rm cf}\left(\mathcal{D}_6\right) = B_0^{(2)}\mathcal{C}_0^{(2)} + B_0^{(4)}\mathcal{C}_0^{(4)} + B_0^{(6)}\mathcal{C}_0^{(6)} + B_6^{(6)}\mathcal{C}_6^{(6)} \tag{92}$$

$$\hat{\mathcal{H}}_{\mathrm{cf}}(\mathcal{D}_{6h}) = B_0^{(2)}\mathcal{C}_0^{(2)} + B_0^{(4)}\mathcal{C}_0^{(4)} + B_0^{(6)}\mathcal{C}_0^{(6)} + B_6^{(6)}\mathcal{C}_6^{(6)} \tag{93}$$

$$\hat{\mathcal{H}}_{\mathrm{cf}}(\mathcal{T}) = B_0^{(4)}\mathcal{C}_0^{(4)} + B_4^{(4)}\mathcal{C}_4^{(4)} + B_0^{(6)}\mathcal{C}_0^{(6)} + B_4^{(6)}\mathcal{C}_4^{(6)} \tag{94}$$

$$\hat{\mathcal{H}}_{\mathrm{cf}}(\mathcal{T}_h) = B_0^{(4)}\mathcal{C}_0^{(4)} + B_4^{(4)}\mathcal{C}_4^{(4)} + B_0^{(6)}\mathcal{C}_0^{(6)} + B_4^{(6)}\mathcal{C}_4^{(6)} \tag{95}$$

$$\hat{\mathcal{H}}_{\mathrm{cf}}(\mathcal{T}_d) = B_0^{(4)}\mathcal{C}_0^{(4)} + B_4^{(4)}\mathcal{C}_4^{(4)} + B_0^{(6)}\mathcal{C}_0^{(6)} + B_4^{(6)}\mathcal{C}_4^{(6)} \tag{96}$$

$$\hat{\mathcal{H}}_{\mathrm{cf}}(\mathcal{O}) = B_0^{(4)}\mathcal{C}_0^{(4)} + B_4^{(4)}\mathcal{C}_4^{(4)} + B_0^{(6)}\mathcal{C}_0^{(6)} + B_4^{(6)}\mathcal{C}_4^{(6)} \tag{97}$$

$$\hat{\mathcal{H}}_{\mathrm{cf}}(\mathcal{O}_h) = B_0^{(4)}\mathcal{C}_0^{(4)} + B_4^{(4)}\mathcal{C}_4^{(4)} + B_0^{(6)}\mathcal{C}_0^{(6)} + B_4^{(6)}\mathcal{C}_4^{(6)} \tag{98}$$

(END) Crystal field expressions (END)

```
CrystalFieldForm::usage = "CrystalFieldForm[symmetryGroup] returns an
     association that describes the crystal field parameters that are
    necessary to desribe a crystal field for the given symmetry group.

The symmetry group must be given as a string in Schoenflies notation
    and must be one of C1, Ci, S2, Cs, C1h, C2, C2h, C2v, D2, D2h, S4,
     C4, C4h, D2d, C4v, D4, D4h, C3, S6, C3h, C3v, D3, D3d, D3h, C6,
    C6h, C6v, D6, D6h, T, Th, Td, O, Oh.

The returned association has three keys:
  ''BqkSqk'' whose values is a list with the nonzero Bqk and Sqk
    parameters;
  ''constraints'' whose value is either an empty list, or a lists of
    replacements rules that are constraints on the Bqk and Sqk
    parameters;
  ''simplifier'' whose value is an association that can be used to
    set to zero the crystal field parameters that are zero for the
    given symmetry group;
  ''aliases'' whose value is a list with the integer by which the
    point group is also known for and an alternate Schoenflies symbol
    if it exists.

This uses data from table 3.3 in Benelli and Gatteschi, 2015.";
CrystalFieldForm[symmetryGroupString_] := (
  If[Not@ValueQ[crystalFieldFunctionalForms],
    crystalFieldFunctionalForms = Import[FileNameJoin[{moduleDir, "
    data", "crystalFieldFunctionalForms.m"}]];
  ];
  cfForm = crystalFieldFunctionalForms[symmetryGroupString];
  simplifier = Association[(# -> 0) &/@ Complement[cfSymbols, cfForm[
    "BqkSqk"]]];
  Return[Join[cfForm, <|"simplifier"->simplifier|>]];
)
```

3.10 $\hat{\mu}$ and $\hat{\mathcal{H}}_{\mathbf{Z}}$: the magnetic dipole operator and the Zeeman term

In Hartree atomic units, the operator associated with the magnetic dipole operator for an electron is

$$\hat{\mu} = -\mu_{\mathrm{B}}\left(\hat{L} + g_s\hat{S}\right)^{(1)}, \text{with } \mu_{\mathrm{B}} = 1/2. \tag{99}$$

Here we have emphasized the fact that the magnetic dipole operator corresponds to a rank-1 spherical tensor operator.

In the $|LSJM_J\rangle$ basis that we use in **qlanth** the LSJ reduced-matrix elements are computed using equation 15.7 in [Cow81]

$$\langle \alpha LSJ \| \left(\hat{L} + g_s\hat{S}\right)^{(1)} \| \alpha' L'S'J' \rangle = \delta(\alpha LSJ, \alpha' L'S'J')\sqrt{J(J+1)(2J+1)} + \delta(\alpha LS, \alpha' L'S')(-1)^{L+S+J+1}\sqrt{[\![J]\!][\![J]\!]}\begin{Bmatrix} L & S & J \\ 1 & J' & S \end{Bmatrix}. \tag{100}$$

Then these reduced matrix elements are used to resolve the M_J components for $q = -1, 0, 1$ through Wigner-Eckart:

$$\langle \alpha LSJM_J | \left(\hat{L} + g_s \hat{S} \right)^{(1)}_q | \alpha' L'S'J'M_{J'} \rangle = (-1)^{J-M_J} \begin{pmatrix} J & 1 & J' \\ -M_J & q & M'_J \end{pmatrix} \langle \alpha LSJ \| \left(\hat{L} + g_s \hat{S} \right)^{(1)} \| \alpha' L'S'J' \rangle. \quad (101)$$

These two above are put together in JJBlockMagDip for given $\{n, J, J'\}$ returning a rank-3 array representing the quantities $\{M_J, M'_J, q\}$.

```
JJBlockMagDip::usage = "JJBlockMagDip[numE, J, Jp] returns an array
    for the LSJM matrix elements of the magnetic dipole operator
    between states with given J and Jp. The option ''Sparse'' can be
    used to return a sparse matrix. The default is to return a sparse
    matrix.
See eqn 15.7 in TASS.
Here it is provided in atomic units in which the Bohr magneton is
    1/2.
\[Mu] = -(1/2) (L + gs S)
We are using the Racah convention for the reduced matrix elements in
    the Wigner-Eckart theorem. See TASS eqn 11.15.
";
Options[JJBlockMagDip]={"Sparse"->True};
JJBlockMagDip[numE_, braJ_, ketJ_, OptionsPattern[]] := Module[
  {braSLJs, ketSLJs,
  braSLJ,   ketSLJ,
  braSL,    ketSL,
  braS,     braL,
  ketS,     ketL,
  braMJ,    ketMJ,
  matValue, magMatrix,
  summand1, summand2,
  threejays},
  (
    braSLJs  = AllowedNKSLJMforJTerms[numE,braJ];
    ketSLJs  = AllowedNKSLJMforJTerms[numE,ketJ];
    magMatrix  = Table[
      braSL     = braSLJ[[1]];
      ketSL     = ketSLJ[[1]];
      {braS, braL}   = FindSL[braSL];
      {ketS, ketL}   = FindSL[ketSL];
      braMJ       = braSLJ[[3]];
      ketMJ       = ketSLJ[[3]];
      summand1    = If[Or[braJ  != ketJ,
                          braSL != ketSL],
        0,
        Sqrt[braJ*(braJ+1)*TPO[braJ]]
      ];
      (* looking at the string includes checking L=L', S=S', and \
   alpha=\alpha'*)
      summand2 = If[braSL!= ketSL,
        0,
        (gs-1) *
          Phaser[braS+braL+ketJ+1] *
            Sqrt[TPO[braJ]*TPO[ketJ]] *
              SixJay[{braJ,1,ketJ},{braS,braL,braS}] *
                Sqrt[braS(braS+1)TPO[braS]]
      ];
      matValue = summand1 + summand2;
      (* We are using the Racah convention for red matrix elements in
    Wigner-Eckart *)
      threejays = (ThreeJay[{braJ, -braMJ}, {1, #}, {ketJ, ketMJ}] &)
    /@ {-1,0,1};
      threejays *= Phaser[braJ-braMJ];
      matValue  = - 1/2 * threejays * matValue;
      matValue,
    {braSLJ, braSLJs},
    {ketSLJ, ketSLJs}
    ];
    If[OptionValue["Sparse"],
      magMatrix = SparseArray[magMatrix]
    ];
    Return[magMatrix];
  )
```

```
];
```

The JJ' blocks that are generated with this function are then put together by MagDipoleMatrixAssembly into the final matrix form and the cartesian components calculated according to

$$\hat{\mu}_x = \frac{\hat{\mu}^{(1)}_{-1} - \hat{\mu}^{(1)}_{+1}}{\sqrt{2}}, \tag{102}$$

$$\hat{\mu}_y = i\frac{\hat{\mu}^{(1)}_{-1} + \hat{\mu}^{(1)}_{+1}}{\sqrt{2}}, \tag{103}$$

$$\hat{\mu}_z = \hat{\mu}^{(1)}_0. \tag{104}$$

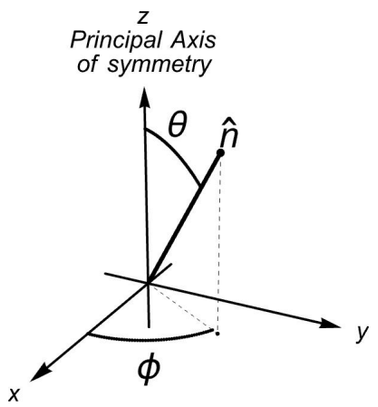
```
MagDipoleMatrixAssembly::usage = "MagDipoleMatrixAssembly[numE]
    returns the matrix representation of the operator - 1/2 (L + gs S)
     in the f^numE configuration. The function returns a list with
    three elements corresponding to the x,y,z components of this
    operator. The option ''FilenameAppendix'' can be used to append a
    string to the filename from which the function imports from in
    order to patch together the array. For numE beyond 7 the function
    returns the same as for the complementary configuration. The
    option ''ReturnInBlocks'' can be used to return the matrices in
    blocks. The default is to return the matrices in flattened form
    and as sparse array.";
Options[MagDipoleMatrixAssembly]={
  "FilenameAppendix"->"",
  "ReturnInBlocks"->False};
MagDipoleMatrixAssembly[nf_Integer, OptionsPattern[]] := Module[
  {ImportFun, numE, appendTo,
  emFname, JJBlockMagDipTable,
  Js, howManyJs, blockOp,
  rowIdx, colIdx},
  (
    ImportFun = ImportMZip;
    numE      = nf;
    numH      = 14 - numE;
    numE      = Min[numE,numH];

    appendTo  = (OptionValue["FilenameAppendix"]<>"-magDip");
    emFname   = JJBlockMatrixFileName[numE,"FilenameAppendix"->
    appendTo];
    JJBlockMagDipTable = ImportFun[emFname];

    Js        = AllowedJ[numE];
    howManyJs = Length[Js];
    blockOp   = ConstantArray[0,{howManyJs,howManyJs}];
    Do[
      blockOp[[rowIdx,colIdx]] = JJBlockMagDipTable[{numE,Js[[rowIdx
    ]],Js[[colIdx]]}],
      {rowIdx,1,howManyJs},
      {colIdx,1,howManyJs}
    ];
    If[OptionValue["ReturnInBlocks"],
      (
        opMinus = Map[#[[1]]&, blockOp, {4}];
        opZero  = Map[#[[2]]&, blockOp, {4}];
        opPlus  = Map[#[[3]]&, blockOp, {4}];
        opX =   (opMinus - opPlus)/Sqrt[2];
        opY = I (opPlus + opMinus)/Sqrt[2];
        opZ = opZero;
      ),
        blockOp = ArrayFlatten[blockOp];
        opMinus = blockOp[[;; , ;; , 1]];
        opZero  = blockOp[[;; , ;; , 2]];
        opPlus  = blockOp[[;; , ;; , 3]];
        opX =   (opMinus - opPlus)/Sqrt[2];
        opY = I (opPlus + opMinus)/Sqrt[2];
        opZ = opZero;
    ];
    Return[{opX, opY, opZ}];
  )
];
```

Using the cartesian components of the magnetic dipole operator, the matrix elements of the Zeeman term can then be evaluated. This term can be included in the Hamiltonian

through an option in HamMatrixAssembly. Since the magnetic dipole operator is calculated in atomic units, and it seeming desirable that the input units of the magnetic field be Tesla, a conversion factor is included so that the final terms be congruent with the energy units assumed in the other terms in the Hamiltonian, namely the energy pseudo-unit Kayser (cm^{-1}). The conversion factor is called teslaToKayser in the file qonstants.m.

4 Coordinate system

Before adding interactions that don't have spherical symmetry, the orientation of the coordinate system is irrelevant. At the point when the crystal field is added, this orientation becomes relevant in the sense that only certain orientations of the coordinate system yield an expression for the crystal field potential in its simplest form[18]. To accomplish this the z-axis needs to be taken as one of the principal axis of symmetry[19]. To complete the orientation of the coodrinate system, the the x-axis. Furthermore, certain choices for the orientation of the coordinate system also allow one to make certain crystal field parameters real, or to fix their sign.



5 Spectroscopic measurements and uncertainty

We may categorize the uncertainty in the parameters fitted to experimental data in three categories: experimental, model, and others.

Before listing the sources that contribute to experimental error, let's briefly recount the types of experiments that are used in order to determine level energies and state labels. The first type is absorption spectroscopy, in which a crystal, adequately doped, is illuminated with a broad spectrum light source, and the wavelength dependent absorption by the crystal thus determined. The crystals absorb radiation depending on the availability of a transition energy between the thermally populated low-lying states and excited levels. This data therefore provides transition energies between the ground multiplet and excited states. Furthermore, from this data one can also estimate the probability that a photon of a given wavelength is absorbed by the ions in the crystal, and from this one estimates the oscillator strength of a given transition.

In order to inform to what two multiplets the transitions belong to, here one may already count how many lines arrange themselves in groups. Alas, this type of absorption spectroscopy is lacking in that it only provides information about transitions between the ground and excited states, and may even elide such transitions that are too weak to be observed. In view of this, some variety of emission spectroscopy becomes relevant. In these, the ions inside of the crystal are excited (thermally, electrically, or radiatively) and the light produced by the relaxing transitions are then registered. This has the benefit that one has now populated other states than the ground state (perhaps with aid of non-radiative transitions inside of the crystal or energy transfer) so that now one can also have information about transitions that depart from a state different than ground. From this type of spectroscopy, given a transition, one may also determine its transition rate, given the availability of time-resolved emission; given this one may then give an upper bound on the spontaneous rate of identified transitions.

[18] Of course, the crystal field potential can be expressed in any rotated coordinate system, but in these the potential would include additional $C_q^{(k)}$ with linear combinations of the $B_q^{(k)}$ [19] A principal axis is a symmetry axis having the most rotational symmetry in the relevant symmetry group. For example, in cubic groups, the principal axis is the 111 diagonal.

In these analyses a few things may not go according to plan:

1. **Several non-equivalent symmetry sites**. Ions may not be located in sites with the same crystal symmetry. As such it will be problematic to interpret their crystal splittings based on the assumption of a single symmetry.

2. **Non-homogeneous crystal field**. Even if they are located in sites with the same point symmetry, it may also be that the crystal field they experience has variations across the bulk of the crystal. As such, the observations would then rather be about an ensemble of crystal fields, instead of a single one.

3. **Crystal impurities**. The doped crystals may contain impurities that will lead to the false identification of transitions to the ion of study. This may be disambiguated from pooling together several experiments.

4. **Non-radiative transitions**, mediated by the crystal, will lead to shifts in transition energies, both in emission, and in absorption. This yields a confounding factor for the *radiative* transition energies that are in principle required to be valid inputs to the model Hamiltonian. Comparison of emission and absorption lines is key to determine the relevance of this.

5. **Spectrometer resolution**. The spectrometers used have a finite resolution. In the setups typically used for this, the nominal resolution might be of the order of 0.1 nm.

6. **Crystal transparency**. Observation of transitions within the ions requires that the crystal be mostly transparent at the relevant wavelengths.

In the works of Carnall and others, the nominal uncertainty in the state energies is of $1\mathcal{K}$, this being the precision to which the used experimental energies are quoted.

With regards to model uncertainties, the following factors may be considered to contribute to it:

1. **Intra-configuration transitions**. When energy levels reach a certain threshold, observations may no longer be intra-configuration transitions, but rather inter-configuration transitions. These transitions should not be included, so care must be taken to exclude them from the analysis.

2. **Unaccounted configuration interaction**. The model makes an attempt at describing configuration interaction effects, but this is only carried to second order in the types of considered interactions, and not all interactions are considered.

Finally, in the "others" category we have the two following:

1. **Numerical precision.** No longer relevant with modern computers, however, at the time at which some of these calculations were done, numerical precision might account for some of the discrepancies one finds when comparing current calculations to old ones.

2. **Errors in tables with reduced matrix elements**. The Crosswhite group at Argonne National Lab produced a set of tables with the reduced matrix elements of operators. However, at some point, these tables became slightly corrupted, and subsequent codes that used them carried those errors with them. In `qlanth` this problem is avoided since all reduced matrix elements are calculated from scratch.

When the model parameters are fitted to experimental data and their uncertainties are being estimated, `qlanth` offers two approaches. In the first approach a given constant uncertainty in the energy levels is assumed, this in turns determines the relevant contour of χ^2, and from this the uncertainties in the model parameters are calculated.

In an alternative approach, the uncertainties are determined *a posteriori*. The model parameters are fit to minimize the square differences between calculated energies and the experimental ones. Then, a single experimental uncertainty is assumed in all the energy levels, and taken equal to the minimum root mean square error, as taken over the available degrees of freedom. This uncertainty σ together with a chosen confidence interval p is then used to determine the contours of χ^2, which in turn determine the corresponding confidence

interval in the model parameters. In a sense, the model is assumed to be valid, and the resulting uncertainties in the model parameters are adjusted to allow for this possibility.

In this dissertation the uncertainty in the experimental data was assumed to be constant and equal to $1\,\mathrm{cm}^{-1}$. And when the data for magnetic dipole transitions was calculated, an uncertainty equal to the σ of the related parametric fit was assumed.

6 Transitions

qlanth can also compute magnetic dipole transition rates within states and levels, as well as forced electric dipole transition rates between levels.

6.1 State description

6.1.1 Magnetic dipole transitions

qlanth can also calculate a few quantities related to magnetic dipole transitions. With $\hat{\mu} = \{\hat{\mu}_x, \hat{\mu}_y, \hat{\mu}_z\}$ the magnetic dipole operator, the line strength between two eigenstates $|\nu\rangle$ and $|\nu'\rangle$ is defined as (see for example equation 14.31 in [Cow81])

$$\hat{S}(\psi, \psi') \coloneqq \left|\langle\psi|\hat{\mu}|\psi'\rangle\right|^2 = \left|\langle\psi|\hat{\mu}_x|\psi'\rangle\right|^2 + \left|\langle\psi|\hat{\mu}_y|\psi'\rangle\right|^2 + \left|\langle\psi|\hat{\mu}_z|\psi'\rangle\right|^2 \tag{105}$$

In **qlanth** this is computed with the function `MagDipLineStrength`, which given a set of eigenvectors computes the sum above, and returns an array that contains all possible pairings of $|\psi\rangle$ and $|\psi'\rangle$ in $\hat{S}(\psi, \psi')$.

```
MagDipLineStrength::usage = "MagDipLineStrength[theEigensys, numE] takes the eigensystem of an ion and the number numE of f-electrons that correspond to it and calculates the line strength array Stot.
The option ''Units'' can be set to either ''SI'' (so that the units of the returned array are (A m^2)^2) or to ''Hartree''.
The option ''States'' can be used to limit the states for which the line strength is calculated. The default, All, calculates the line strength for all states. A second option for this is to provide an index labelling a specific state, in which case only the line strengths between that state and all the others are computed.
The returned array should be interpreted in the eigenbasis of the Hamiltonian. As such the element Stot[[i,i]] corresponds to the line strength states between states |i> and |j>.";
Options[MagDipLineStrength]={"Reload MagOp" -> False, "Units"->"SI", "States" -> All};
MagDipLineStrength[theEigensys_List, numE0_Integer, OptionsPattern[]] := Module[
  {numE, allEigenvecs, Sx, Sy, Sz, Stot, factor},
  (
    numE = Min[14-numE0, numE0];
    (*If not loaded then load it, *)
    If[Or[
        Not[MemberQ[Keys[magOp], numE]],
        OptionValue["Reload MagOp"]],
    (
      magOp[numE] = ReplaceInSparseArray[#, {gs->2}]& /@ MagDipoleMatrixAssembly[numE];
    )
    ];
    allEigenvecs = Transpose[Last /@ theEigensys];
    Which[OptionValue["States"] === All,
      (
        {Sx, Sy, Sz} = (ConjugateTranspose[allEigenvecs].#.allEigenvecs) & /@ magOp[numE];
        Stot         = Abs[Sx]^2+Abs[Sy]^2+Abs[Sz]^2;
      ),
      IntegerQ[OptionValue["States"]],
      (
        singleState  = theEigensys[[OptionValue["States"],2]];
        {Sx, Sy, Sz} = (ConjugateTranspose[allEigenvecs].#.singleState) & /@ magOp[numE];
        Stot         = Abs[Sx]^2+Abs[Sy]^2+Abs[Sz]^2;
      )
    ];
    Which[
      OptionValue["Units"] == "SI",
```

```
        Return[4 \[Mu]B^2 * Stot],
      OptionValue["Units"] == "Hartree",
        Return[Stot],
      True,
      (
        Print["Invalid option for ''Units''. Options are ''SI'' and
    ''Hartree''."];
        Abort[];
      )
    ];
  )
];
```

Using the line strength $\hat{S}$, the transition rate $\mathrm{A_{MD}}$ for the spontaneous transition $|\psi_i\rangle \rightsquigarrow |\psi_f\rangle$ is then given by (from table 7.3 of [TLJ99])

$$\mathrm{A_{MD}}\left(|\psi_i\rangle \rightsquigarrow |\psi_f\rangle\right) = \frac{16\pi^3\mu_0}{3h}\frac{n^3}{\lambda_{if}^3}\frac{\hat{S}(\psi_i,\psi_f)}{g_i}, \tag{106}$$

where λ is the vacuum-equivalent wavelength of the transition between $|\nu\rangle$ and $|\nu'\rangle$, n the refractive index of the medium containing the ion, and g_i the degeneracy of the initial state $|\psi_i\rangle$. At the state level of description, J is no longer a good quantum number so the degeneracy $g_i = 1$.

```
MagDipoleRates::usage = "MagDipoleRates[eigenSys, numE] calculates
    the magnetic dipole transition rate array for the provided
    eigensystem. The option ''Units'' can be set to ''SI'' or to ''
    Hartree''. If the option ''Natural Radiative Lifetimes'' is set to
     true then the reciprocal of the rate is returned instead.
    eigenSys is a list of lists with two elements, in each list the
    first element is the energy and the second one the corresponding
    eigenvector.
Based on table 7.3 of Thorne 1999, using g2=1.
The energy unit assumed in eigenSys is kayser.
The returned array should be interpreted in the eigenbasis of the
    Hamiltonian. As such the element AMD[[i,i]] corresponds to the
    transition rate (or the radiative lifetime, depending on options)
    between eigenstates |i> and |j>.
By default this assumes that the refractive index is unity, this may
    be changed by setting the option ''RefractiveIndex'' to the
    desired value.
The option ''Lifetime'' can be used to return the reciprocal of the
    transition rates. The default is to return the transition rates.";
Options[MagDipoleRates]={"Units"->"SI", "Lifetime"->False, "
    RefractiveIndex"->1};
MagDipoleRates[eigenSys_List, numE0_Integer,OptionsPattern[]] :=
    Module[
  {AMD, Stot, eigenEnergies,
  transitionWaveLengthsInMeters, nRefractive},
  (
    nRefractive   = OptionValue["RefractiveIndex"];
    numE          = Min[14-numE0, numE0];
    Stot          = MagDipLineStrength[eigenSys, numE, "Units" ->
    OptionValue["Units"]];
    eigenEnergies = Chop[First/@eigenSys];
    energyDiffs   = Outer[Subtract, eigenEnergies, eigenEnergies];
    energyDiffs   = ReplaceDiagonal[energyDiffs, Indeterminate];
    (* Energies assumed in kayser.*)
    transitionWaveLengthsInMeters = 0.01/energyDiffs;

    unitFactor    = Which[
    OptionValue["Units"]=="Hartree",
    (
      (* The bohrRadius factor in SI needed to convert the
    wavelengths which are assumed in m*)
      16 \[Pi]^3 (\[Mu]0Hartree /(3 hPlanckFine)) * bohrRadius^3
    ),
    OptionValue["Units"]=="SI",
    (
      16 \[Pi]^3 \[Mu]0/(3 hPlanck)
    ),
    True,
    (
      Print["Invalid option for ''Units''. Options are ''SI'' and ''
    Hartree''."];
```

```
      Abort[];
    )
    ];
    AMD = unitFactor / transitionWaveLengthsInMeters^3 * Stot *
    nRefractive^3;
    Which[OptionValue["Lifetime"],
      Return[1/AMD],
      True,
      Return[AMD]
    ]
  )
];
```

A final quantity of interest is the oscillator strength for the transition between the ground state $|\psi_g\rangle$ and an excited state $|\psi_e\rangle$. The oscillator strength is a dimensionless quantity which is indicative of how strong absorption is. The oscillator strength may be defined for other initial states than the ground state, but since this is the state most likely to be populated in ordinary experimental conditions, this is the initial state that is of most frequent interest. The oscillator strength is given by [CFW65]

$$\mathrm{f_{MD}}\left(|\psi_g\rangle \rightsquigarrow |\psi_e\rangle\right) = \frac{8\pi^2 m_e}{3\,hc\,e^2}\frac{n}{\lambda_{ge}}\frac{\hat{\mathcal{S}}(\psi_g,\psi_e)}{g_g} \tag{107}$$

where g_g is the degeneracy of the ground state. At the level of detail that the eigenstates are described in **qlanth** where J is no longer a good quantum number, $g_g = 1$.

In **qlanth** the function GroundMagDipoleOscillatorStrength implements the calculation of the oscillator strengths from the ground state to all the excited ones.

```
GroundMagDipoleOscillatorStrength::usage = "
    GroundMagDipoleOscillatorStrength[eigenSys, numE] calculates the
    magnetic diople oscillator strengths between the ground state and
    the excited states as given by eigenSys.
Based on equation 8 of Carnall 1965, removing the 2J+1 factor since
    this degeneracy has been removed by the crystal field.
eigenSys is a list of lists with two elements, in each list the first
     element is the energy and the second one the corresponding
    eigenvector.
The energy unit assumed in eigenSys is Kayser.
The oscillator strengths are dimensionless.
The returned array should be interpreted in the eigenbasis of the
    Hamiltonian. As such the element fMDGS[[i]] corresponds to the
    oscillator strength between ground state and eigenstate |i>.
By default this assumes that the refractive index is unity, this may
    be changed by setting the option ''RefractiveIndex'' to the
    desired value.";
Options[GroundMagDipoleOscillatorStrength]={"RefractiveIndex"->1};
GroundMagDipoleOscillatorStrength[eigenSys_List, numE_Integer,
    OptionsPattern[]] := Module[
  {eigenEnergies, SMDGS, GSEnergy, energyDiffs,
  transitionWaveLengthsInMeters, unitFactor, nRefractive},
  (
    eigenEnergies     = First/@eigenSys;
    nRefractive       = OptionValue["RefractiveIndex"];
    SMDGS             = MagDipLineStrength[eigenSys,numE, "Units"->"SI
    ", "States"->1];
    GSEnergy          = eigenSys[[1,1]];
    energyDiffs       = eigenEnergies-GSEnergy;
    energyDiffs[[1]] = Indeterminate;
    transitionWaveLengthsInMeters = 0.01/energyDiffs;
    unitFactor        = (8\[Pi]^2 me)/(3 hPlanck eCharge^2 cLight);
    fMDGS             = unitFactor / transitionWaveLengthsInMeters *
    SMDGS * nRefractive;
    Return[fMDGS];
  )
];
```

6.2 Level description

6.2.1 Forced electric dipole transitions

Any two eigenfunctions that are approximated within the limits of a single configuration cannot help but have the same parity as they are spanned by basis vectors with definite and shared parity. Analysis of the amplitudes for different transition operators can then

inform as to what transitions are forbidden, which are those in which the product of the parity of the two participating wavefunctions and that of the transition operator results in odd parity. As such, within the single configuration approximation, since the product of the two participating wavefunctions is always even, then any transition described by an operator of odd parity is forbidden. This is the content of Laporte's parity selection rule. Since the parity of the magnetic dipole operator is even [20], then this operator allows for intra-configuration transitions, and since the parity of the electric dipole operator is odd, then these types of intra-configuration transitions are forbidden.

However, much as configuration interaction is an essential component in the description of the electronic structure, it has a bearing on the energy spectrum and the intra-configuration wavefunctions themselves. Configuration interaction may also be used to bring back into the analysis the fact that the *actual* wavefunctions will also have at least a small part of them in other configurations, even if most of them may be within the ground configuration. It is therefore the case that the *actual* parity of the wavefunctions is mixed, and therefore intra-configuration [21] electric dipole transitions are actually allowed. These electric dipole transitions are called *forced* electric dipole transitions.

Judd [Jud62] and Ofelt [Ofe62] came separately to similar versions of this analysis, and showed after a series of approximations that the forced electric dipole transitions could be described by the intra-configuration matrix elements of the multi-electron unit operators $\hat{U}^{(k)}$ (for k=2,4,6) together with a set of three accompanying coefficients $\{\Omega_{(2)}, \Omega_{(4)}, \Omega_{(6)}\}$. These coefficients have a definite form related to the overlap between the mixed parity parts of the corrected wavefunctions, but they can also be considered as additional phenomenological parameters.

Judd-Ofelt theory is based on the level description, and its mathematical expression is the following. Given two intermediate coupling levels $|\alpha SLJ\rangle$ and $|\alpha' S'L'J'\rangle$, the oscillator strength between them is approximated as [Jud62]

$$\mathrm{f}_{\text{f-ED}}\left(|\alpha LSJ\rangle \rightsquigarrow |\alpha' S'L'J'\rangle\right) = \mathcal{R}\frac{8\pi^2 m_e}{3h}\frac{\nu}{2J+1}\frac{\chi}{n}\sum_{k=2,4,6}\Omega_{(k)}\left|\langle \underline{\mathrm{f}}^n \alpha SLJ \| \hat{U}^{(k)} \| \underline{\mathrm{f}}^n \alpha' S'L'J'\rangle\right|^2, \tag{108}$$

where ν is the frequency of the transition, χ the local field correction, n the refractive index of the crystal host, and $\mathcal{R} = 1$ in the case of absorption and $\mathcal{R} = n^2$ in the case of emission.

The local field correction χ accounts for the difference between the macroscopic and microscopic electric fields, in the case of ions embedded for crystals the most common choice is

$$\chi = \frac{n^2+2}{3} \tag{109}$$

and for other environments (or emitters other than ions such as molecules) different alternatives are relevant (see [DR06]).

In **qlanth** Judd-Ofelt theory is implemented with help of the functions JuddOfeltUkSquared and LevelElecDipoleOscillatorStrength.

```
JuddOfeltUkSquared::usage = "JuddOfeltUkSquared[numE, params]
    calculates the matrix elements of the Uk operator in the level
    basis. These are calculated according to equation (7) in Carnall
    1965.
The function returns a list with the following elements:
  - basis : A list with the allowed {SL, J} terms in the f^numE
    configuration. Equal to BasisLSJ[numE].
  - eigenSys : A list with the eigensystem of the Hamiltonian for the
     f^n configuration.
  - levelLabels : A list with the labels of the major components of
    the level eigenstates.
  - LevelUkSquared : An association with the squared matrix elements
    of the Uk operators in the level eigenbasis. The keys being {2, 4,
     6} corresponding to the rank of the Uk operator. The basis in
    which the matrix elements are given is the one corresponding to
    the level eigenstates given in eigenSys and whose major SLJ
    components are given in levelLabels. The matrix is symmetric and
    given as a SymmetrizedArray.
  The function admits the following options:
  ''PrintFun'' : A function that will be used to print the progress
    of the calculations. The default is PrintTemporary.";
```

[20] The parity of the electric quadrupole operator is also even, but we haven't included it in **qlanth**

[21] Calling these *intra*-configuration transitions is somewhat of a misnomer since their nature is tied to the fact that the single-configuration description is wanting.

```
Options[JuddOfeltUkSquared] = {"PrintFun" -> PrintTemporary};
JuddOfeltUkSquared[numE_, params_, OptionsPattern[]] := Module[
  {eigenChanger, numEH, basis, eigenSys,
  Js, Ukmat, LevelUkSquared, kRank,
  S, L, Sp, Lp, J, Jp, phase,
  braTerm, ketTerm, levelLabels,
  eigenVecs, majorComponentIndices},
  (
    If[Not[ValueQ[ReducedUkTable]],
      LoadUk[]
    ];
    numEH = Min[numE, 14-numE];
    PrintFun = OptionValue["PrintFun"];
    PrintFun["> Calculating the levels for the given parameters ..."
    ];
    {basis, eigenSys} = LevelSolver[numE, params];
    (* The change of basis matrix to the eigenstate basis *)
    eigenChanger = Transpose[Last /@ eigenSys];
    PrintFun["Calculating the matrix elements of Uk in the physical
    coupling basis ..."];
    LevelUkSquared = <||>;
    Do[(
      Ukmat = Table[(
          {S, L}   = FindSL[braTerm[[1]]];
          J        = braTerm[[2]];
          Jp       = ketTerm[[2]];
          {Sp, Lp} = FindSL[ketTerm[[1]]];
          phase    = Phaser[S + Lp + J + kRank];
          Simplify @ (
            phase *
            Sqrt[TPO[J]*TPO[Jp]] *
            SixJay[{J, Jp, kRank}, {Lp, L, S}] *
            ReducedUkTable[{numEH, 3, braTerm[[1]], ketTerm[[1]],
    kRank}]
            )
          ),
        {braTerm, basis},
        {ketTerm, basis}
      ];
      Ukmat = (Transpose[eigenChanger] . Ukmat . eigenChanger)^2;
      Ukmat = Chop@Ukmat;
      LevelUkSquared[kRank] = SymmetrizedArray[Ukmat, Dimensions[
    eigenChanger], Symmetric[{1, 2}]];
      ),
      {kRank, {2, 4, 6}}
    ];
    LSJmultiplets = (RemoveTrailingDigits[#[[1]]] <> ToString[
    InputForm[#[[2]]]]) & /@ basis;
    eigenVecs = Last /@ eigenSys;
    majorComponentIndices = Ordering[Abs[#]][[-1]] & /@ eigenVecs;
    levelLabels = LSJmultiplets[[majorComponentIndices]];
    Return[{basis, eigenSys, levelLabels, LevelUkSquared}];
  )
];
```

```
LevelElecDipoleOscillatorStrength::usage = "
    LevelElecDipoleOscillatorStrength[numE, levelParams,
    juddOfeltParams] uses Judd-Ofelt theory to estimate the forced
    electric dipole oscillator strengths ions whose level description
    is determined by levelParams.
The third parameter juddOfeltParams is an asssociation with keys
    equal to the three Judd-Ofelt intensity parameters {\[CapitalOmega
    ]2, \[CapitalOmega]4, \[CapitalOmega]6} and corresponding values
    in cm^2.
The local field correction implemented here corresponds to the one
    given by the virtual cavity model of Lorentz.
The function returns a list with the following elements:
  - basis : A list with the allowed {SL, J} terms in the f^numE
    configuration. Equal to BasisLSJ[numE].
  - eigenSys : A list with the eigensystem of the Hamiltonian for the
     f^n configuration in the level description.
  - levelLabels : A list with the labels of the major components of
    the calculated levels.
  - oStrengthArray : A square array whose elements represent the
    oscillator strengths between levels such that the element
    oStrengthArray[[i,j]] is the oscillator strength between the
```

```
    levels |Subscript[\[Psi], i]> and |Subscript[\[Psi], j]>. In this
    array, the elements below the diagonal represent emission
    oscillator strengths, and elements above the diagonal represent
    absorption oscillator strengths.
The function admits the following three options:
  ''PrintFun'' : A function that will be used to print the progress
    of the calculations. The default is PrintTemporary.
  ''RefractiveIndex'' : The refractive index of the medium where the
    transitions are taking place. This may be a number or a function.
    If a number then the oscillator strengths are calculated for
    assuming a wavelength-independent refractive index. If a function
    then the refractive indices are calculated accordingly to the
    wavelength of each transition (the function must admit a single
    argument equal to the wavelength in nm). The default is 1.
  ''LocalFieldCorrection'' : The local field correction to be used.
    The default is ''VirtualCavity''. The options are: ''VirtualCavity
    '' and ''EmptyCavity''.
The equation implemented here is the one given in eqn. 29 from the
    review article of Hehlen (2013). See that same article for a
    discussion on the local field correction.
";
Options[LevelElecDipoleOscillatorStrength]={
  "PrintFun"        -> PrintTemporary,
  "RefractiveIndex" -> 1,
  "LocalFieldCorrection" -> "VirtualCavity"
};
LevelElecDipoleOscillatorStrength[numE_, levelParams_Association,
    juddOfeltParams_Association, OptionsPattern[]] := Module[
  {PrintFun, basis, eigenSys, levelLabels,
  LevelUkSquared, eigenEnergies, energyDiffs,
  oStrengthArray, nRef, \[Chi], nRefs,
  \[Chi]OverN, groundLevel, const,
  transitionFrequencies, wavelengthsInNM,
  fieldCorrectionType},
  (
    PrintFun = OptionValue["PrintFun"];
    nRef     = OptionValue["RefractiveIndex"];
    PrintFun["Calculating the Uk^2 matrix elements for the given
    parameters ..."];
    {basis, eigenSys, levelLabels, LevelUkSquared} =
    JuddOfeltUkSquared[numE, levelParams, "PrintFun"->PrintFun];
    eigenEnergies = First/@eigenSys;
    const         = (8\[Pi]^2)/3 me/hPlanck;
    energyDiffs   = Transpose@Outer[Subtract,eigenEnergies,
    eigenEnergies];
    (* since energies are assumed in Kayser, speed of light needs to
    be in cm/s, so that the frequencies are in 1/s *)
    transitionFrequencies = energyDiffs*cLight*100;
    (* grab the J for each level *)
    levelJs        = #[[2]] & /@ eigenSys;
    oStrengthArray = (
      juddOfeltParams[\[CapitalOmega]2]*LevelUkSquared[2]+
      juddOfeltParams[\[CapitalOmega]4]*LevelUkSquared[4]+
      juddOfeltParams[\[CapitalOmega]6]*LevelUkSquared[6]
    );
    oStrengthArray = Abs@(const * transitionFrequencies *
    oStrengthArray);
    (* it is necessary to divide each oscillator strength by the
    degeneracy of the initial level *)
    oStrengthArray = MapIndexed[1/(2 levelJs[[#2[[1]]]]+1) #1 &,
    oStrengthArray,{2}];
    (* including the effects of the refractive index *)
    fieldCorrectionType = OptionValue["LocalFieldCorrection"];
    Which[
      nRef === 1,
        True,
      NumberQ[nRef],
      (
        \[Chi] = Which[
          fieldCorrectionType == "VirtualCavity",
          (
            ( (nRef^2 + 2) / 3 )^2
          ),
          fieldCorrectionType == "EmptyCavity",
          (
            ( 3 * nRef^2 / ( 2 * nRef^2 + 1 ) )^2
```

```
          )
        ];
        \[Chi]OverN    = \[Chi] / nRef;
        oStrengthArray = \[Chi]OverN * oStrengthArray;
        (* the refractive index participates differently in
    absorption and in emission *)
        aFunction      = If[#2[[1]]>#2[[2]], #1 * nRef^2, #1]&;
        oStrengthArray = MapIndexed[aFunction, oStrengthArray, {2}];
      ),
      True,
      (
        wavelengthsInNM = Abs[1 / energyDiffs] * 10^7;
        nRefs           = Map[nRef, wavelengthsInNM];
        Print["Calculating the oscillator strengths for the given
    refractive index ..."];
        \[Chi] = Which[
          fieldCorrectionType == "VirtualCavity",
          (
            ( (nRefs^2 + 2) / 3 )^2
          ),
          fieldCorrectionType == "EmptyCavity",
          (
            ( 3 * nRefs^2 / ( 2*nRefs^2 + 1 ) )^2
          )
        ];
        \[Chi]OverN     = \[Chi] / nRefs;
        oStrengthArray  = \[Chi]OverN * oStrengthArray
      )
    ];
    Return[{basis, eigenSys, levelLabels, oStrengthArray}];
  )
];
```

6.2.2 Magnetic dipole transitions

In Hartree atomic units, the magnetic dipole line strength between levels $|\alpha LSJ\rangle$ and $|\alpha' S' L' J'\rangle$ is given by

$$\hat{S}(|\alpha LSJ\rangle, |\alpha' S' L' J'\rangle) = \left| \langle \alpha LSJ \| \frac{1}{2}(\hat{L} + g\hat{S}) \| \alpha' S' L' J' \rangle \right|^2 \tag{110}$$

In **qlanth** the line strength can be calculated using the function LevelMagDipoleLineStrength.

```
LevelMagDipoleLineStrength::usage = "LevelMagDipoleLineStrength[
    eigenSys, numE] calculates the magnetic dipole line strengths for
    an ion whose level description is determined by levelParams. The
    function returns a square array whose elements represent the
    magnetic dipole line strengths between the levels given in
    eigenSys such that the element magDipoleLineStrength[[i,j]] is the
     line strength between the levels |Subscript[\[Psi], i]> and |
    Subscript[\[Psi], j]>. Eigensys must be such that it consists of a
     lists of lists where in each list the last element corresponds to
     the eigenvector of a level (given as a row) in the standard basis
     for levels of the f^numE configuration.
The function admits the following options:
  ''Units'' : The units in which the line strengths are given. The
    default is ''SI''. The options are ''SI'' and ''Hartree''. If ''SI
    '' then the unit of the line strength is (A m^2)^2 = (J/T)^2. If
    ''Hartree'' then the line strength is given in units of 2 \[Mu]B."
    ;
Options[LevelMagDipoleLineStrength] = {
  "Units"->"SI"
  };
LevelMagDipoleLineStrength[theEigensys_List, numE0_Integer,
    OptionsPattern[]] := Module[
  {numE, levelMagOp, allEigenvecs, magDipoleLineStrength, units},
  (
    numE          = Min[14-numE0,numE0];
    levelMagOp    = LevelMagDipoleMatrixAssembly[numE];
    allEigenvecs  = Transpose[Last/@theEigensys];
    units         = OptionValue["Units"];
    magDipoleLineStrength          = Transpose[allEigenvecs].
    levelMagOp.allEigenvecs;
    magDipoleLineStrength          = Abs[magDipoleLineStrength]^2;
```

```
    Which[
      units=="SI",
        Return[4 \[Mu]B^2 * magDipoleLineStrength],
      units=="Hartree",
        Return[magDipoleLineStrength]
    ];
  )
];
```

In atomic units, the magnetic dipole oscillator strength for a transition between level $|\alpha LSJ\rangle$ and an excited level $|\alpha' S' L' J'\rangle$ is given by [Rud07]

$$\mathrm{f_{MD}}\left(|\alpha LSJ\rangle \rightsquigarrow |\alpha' S' L' J'\rangle\right) = \frac{2n}{3}\frac{\mathcal{E}(|\alpha' S' L' J'\rangle) - \mathcal{E}(|\alpha LSJ)\rangle}{2J+1}\alpha^2 \hat{\mathcal{S}}\left(|\alpha LSJ\rangle, |\alpha' S' L' J'\rangle\right) \quad (111)$$

where $\mathcal{E}(|\alpha LSJ\rangle)$ is the energy of level $|\alpha LSJ\rangle$, n is the refractive index of the medium, and α is the fine structure constant. In obtaining this expression one considers the transition from one state of the initial level into another single state of the final level. Furthermore, here it is assumed that all the states of the initial level are equally populated.

In **qlanth** the function LevelMagDipoleOscillatorStrength can be used to calculate these.

```
LevelMagDipoleOscillatorStrength::usage = "
    LevelMagDipoleOscillatorStrength[eigenSys, numE] calculates the
    magnetic dipole oscillator strengths for an ion whose level
    description is determined by levelParams. The refractive index of
    the medium is relevant, but here it is assumed to be 1, this can
    be changed through the option ''RefractiveIndex''. eigenSys must
    consist of a lists of lists with three elements: the first element
     being the energy of the level, the second element being the J of
    the level, and the third element being the eigenvector of the
    level.
  The function returns a list with the following elements:
    - basis : A list with the allowed {SL, J} terms in the f^numE
    configuration. Equal to BasisLSJ[numE].
    - eigenSys : A list with the eigensystem of the Hamiltonian for
    the f^n configuration in the level description.
    - levelLabels : A list with the labels of the major components of
     the calculated levels.
    - magDipoleOstrength : A square array whose elements represent
    the magnetic dipole oscillator strengths between the levels given
    in eigenSys such that the element magDipoleOstrength[[i,j]] is the
     oscillator strength between the levels |Subscript[\[Psi], i]> and
     |Subscript[\[Psi], j]>. In this array the elements below the
    diagonal represent emission oscillator strengths, and elements
    above the diagonal represent absorption oscillator strengths. The
    emission oscillator strengths are negative. The oscillator
    strength is a dimensionless quantity.
  The function admits the following option:
    ''RefractiveIndex'' : The refractive index of the medium where
    the transitions are taking place. This may be a number or a
    function. If a number then the oscillator strengths are calculated
     assuming a wavelength-independent refractive index as given. If a
     function then the refractive indices are calculated accordingly
    to the vaccum wavelength of each transition (the function must
    admit a single argument equal to the wavelength in nm). The
    default is 1.
  For reference see equation (27.8) in Rudzikas (2007). The
    expression for the line strenght is the simplest when using atomic
     units, (27.8) is missing a factor of \[Alpha]^2.";
Options[LevelMagDipoleOscillatorStrength]={
  "RefractiveIndex" -> 1
};
LevelMagDipoleOscillatorStrength[eigenSys_, numE_, OptionsPattern[]]
    := Module[
  {eigenEnergies, eigenVecs, levelJs,
  energyDiffs, magDipoleOstrength, nRef,
  wavelengthsInNM, nRefs, degenDivisor},
  (
    basis          = BasisLSJ[numE];
    eigenEnergies  = First/@eigenSys;
    nRef           = OptionValue["RefractiveIndex"];
    eigenVecs      = Last/@eigenSys;
    levelJs        = #[[2]]&/@eigenSys;
    energyDiffs    = -Outer[Subtract,eigenEnergies,eigenEnergies];
```

```
    energyDiffs  *= kayserToHartree;
    magDipoleOstrength = LevelMagDipoleLineStrength[eigenSys, numE, "
    Units"->"Hartree"];
    magDipoleOstrength = 2/3 * αFine^2 * energyDiffs *
    magDipoleOstrength;
    degenDivisor       = #1 / ( 2 * levelJs[[#2[[1]]]] + 1 ) &;
    magDipoleOstrength = MapIndexed[degenDivisor, magDipoleOstrength,
     {2}];
    Which[nRef===1,
      True,
      NumberQ[nRef],
        (
          magDipoleOstrength = nRef * magDipoleOstrength;
        ),
      True,
        (
          wavelengthsInNM    = Abs[kayserToHartree / energyDiffs] *
    10^7;
          nRefs              = Map[nRef, wavelengthsInNM];
          magDipoleOstrength = nRefs * magDipoleOstrength;
        )
    ];
    Return[{basis, eigenSys, magDipoleOstrength}];
  )
];
```

A final quantity of interest is the spontaneous magnetic dipole decay rate from one level to a lower lying one. In atomic units this rate is determined by

$$\Gamma_{\mathrm{MD}}\left(|\alpha LSJ\rangle \rightsquigarrow |\alpha' S' L' J'\rangle\right) = \frac{4n^3}{3}\frac{\left(\mathcal{E}(|\alpha LSJ\rangle) - \mathcal{E}(|\alpha' S' L' J'\rangle)\right)^3}{2J+1}\hat{\alpha}^5\hat{\mathcal{S}}\left(|\alpha LSJ\rangle, |\alpha' S' L' J'\rangle\right). \tag{112}$$

In **qlanth** the spontaneous decay rates may be calculated through the function LevelMagDipoleSpotaneousDecayRates.

```
LevelMagDipoleSpotaneousDecayRates::usage = "
    LevelMagDipoleSpotaneousDecayRates[eigenSys, numE] calculates the
    spontaneous emission rates for the magnetic dipole transitions
    between the levels given in eigenSys. The function returns a
    square array whose elements represent the spontaneous emission
    rates between the levels given in eigenSys such that the element
    [[i,j]] of the returned array is the rate of spontaneous emission
    from the level |Subscript[\[Psi], i]> to the level |Subscript[\[
    Psi], j]>. In this array the elements below the diagonal represent
     emission rates, and elements above the diagonal are identically
    zero.
The function admits two optional arguments:
  + \"Units\" : The units in which the rates are given. The default
    is \"SI\". The options are \"SI\" and \"Hartree\". If \"SI\" then
    the rates are given in s^-1. If \"Hartree\" then the rates are
    given in the atomic unit of frequency.
  + \"RefractiveIndex\" : The refractive index of the medium where
    the transitions are taking place. This may be a number or a
    function. If a number then the rates are calculated assuming a
    wavelength-independent refractive index as given. If a function
    then the refractive indices are calculated accordingly to the
    vaccum wavelength of each transition (the function must admit a
    single argument equal to the wavelength in nm). The default is 1."
    ;
Options[LevelMagDipoleSpotaneousDecayRates] = {
  "Units" -> "SI",
  "RefractiveIndex" -> 1};
LevelMagDipoleSpotaneousDecayRates[eigenSys_List, numE_Integer,
    OptionsPattern[]] := Module[
  {
    levMDlineStrength, eigenEnergies, energyDiffs, levelJs,
    spontaneousRatesInHartree, spontaneousRatesInSI, degenDivisor,
    units,
    nRef, nRefs, wavelengthsInNM
  },
  (
    nRef               = OptionValue["RefractiveIndex"];
    units              = OptionValue["Units"];
    levMDlineStrength = LowerTriangularize@LevelMagDipoleLineStrength
    [eigenSys,numE,"Units"->"Hartree"];
    levMDlineStrength = SparseArray[levMDlineStrength];
```

```
    eigenEnergies      = First /@ eigenSys;
    energyDiffs        = Outer[Subtract, eigenEnergies, eigenEnergies
    ];
    energyDiffs        = kayserToHartree * energyDiffs;
    energyDiffs        = SparseArray[LowerTriangularize[energyDiffs]];
    levelJs            = #[[2]]& /@ eigenSys;
    spontaneousRatesInHartree = 4/3 αFine^5 * energyDiffs^3 *
    levMDlineStrength;
    degenDivisor               = #1 / (2*levelJs[[#2[[1]]]] + 1)&;
    spontaneousRatesInHartree = MapIndexed[degenDivisor,
    spontaneousRatesInHartree, {2}];
    Which[nRef===1,
      True,
      NumberQ[nRef],
        (
          spontaneousRatesInHartree = nRef^3 *
    spontaneousRatesInHartree;
        ),
      True,
        (
          wavelengthsInNM    = Abs[kayserToHartree / energyDiffs] *
    10^7;
          nRefs              = Map[nRef, wavelengthsInNM];
          spontaneousRatesInHartree = nRefs^3 *
    spontaneousRatesInHartree;
        )
    ];
    If[units == "SI",
      (
        spontaneousRatesInSI = 1/hartreeTime *
    spontaneousRatesInHartree;
        Return[SparseArray@spontaneousRatesInSI];
      ),
      Return[SparseArray@spontaneousRatesInHartree];
    ];
  )
];
```

7 Parameter constraints

When there is a scarcity of experimental data, one useful strategy to reduce the number of free parameters is to enforce some constraints between ratios of Slater integrals $F^{(k)}$, Marvin integrals $\mathcal{M}^{(k)}$, and pseudo-magnetic parameters $P^{(k)}$.

For the Slater integrals one may leave only $F^{(2)}$ as free parameter, and fix the ratios $F^{(4)}/F^{(2)}$ and $F^{(6)}/F^{(2)}$.

For the Marvin integrals one often leaves only a single free parameter $\mathcal{M}^{(0)}$, and give values to $\mathcal{M}^{(2)}$ and $\mathcal{M}^{(4)}$, by fixing the ratios $\mathcal{M}^{(2)}/\mathcal{M}^{(0)}$ and $\mathcal{M}^{(4)}/\mathcal{M}^{(0)}$.

For the pseudo-magnetic parameters again the common practice is to only leave a single free parameter $P^{(2)}$, and give values to $P^{(4)}$ and $P^{(6)}$, by fixing the ratios $P^{(4)}/P^{(2)}$ and $P^{(6)}/P^{(2)}$.

The values for all these ratios were historically obtained by using the integral expressions for the corresponding parameters, and calculating them using Hartree-Fock solutions to the radial parts of the wavefunctions. Examples of these ratios can be seen in the sections with data for LaF_3 and $LiYF_4$.

8 Fitting experimental data

qlanth also has the capacity to fit the semi-empirical Hamiltonian to experimental data. This is included in the sub-module `fittings.m` (see Appendix 17.2). This sub-module includes the function `ClassicalFit` which uses a truncated Hamiltonian (based on free-ion energies) to fit a given subset of the model parameters to given experimental data. It yields an extensive set of results, including fitted parameters and uncertainties. If the truncation energy parameter is set to infinity, then the fitting is performed with no truncation.

This function, however, is specifically used for fitting data for a single ion in a specific host. In the case of fitting data for several ions, it may be necessary to use parameter trends $\mathcal{P}(n)$. This is necessary since not only there might be some ions where there is no

data (and where one would then propose a "synthetic" solution), but also since there are cases where there are too few data points to justify varying all of the model parameters.[22]

In these cases where one is fitting data for all or most of the lanthanide ions in a given host, it is useful to first fit the model in cases where there are the most data points, and to build up a parameter model $\mathscr{P}(n)$ for each parameter as the fitting of all the ions progresses. One feature often used in fitting for several ions (see Carnall *et al.* [Car+89] and Cheng *et al.* [Che+16]) is that when there is scarcity of data (as mentioned above), one can then use the trends in the $\mathscr{P}(n)$ in order to fix some parameter values at a given column (and proceed to vary others to fit the data to the model).[23]

Here below is a detailed explanation of the parameters required by `ClassicalFit`. The code for this function `ClassicalFit` may be found in Appendix 17.2.

- `numE`: number of electrons in the system, specifying the electronic configuration.
- `expData`: experimental data, a list of lists where each sublist represents an energy level and associated parameters. The first element of the sublists must represent energies, the other elements in the sublists are ignored but can be given to be kept together with the fitted data. The data must be ordered in increasing order of energy. **IMPORTANT:** if there are known unknown levels, these should be made explicit, anything other than a number will be interpreted as a level of undetermined energy in the corresponding gap. **ALSO IMPORTANT:** in the case of odd electron cases, `expData` needs to explicitly include the duplicate energies corresponding to Kramers' degeneracy; the gaps also need to be adequately duplicated in these cases.
- `excludeDataIndices`: indices in `expData` to be excluded from the fitting process. This can be used to exclude experimental data which is present, but which is considered dubious. In the case of odd electron configurations, these indices need to explicitly include the double degeneracy of Kramers doublets.
- `problemVars`: symbols representing the parameters to be fitted, some of which may be constrained (set fixed or proportional to others). **IMPORTANT:** if `problemVars` is a proper subset of all the parameters needed to evaluate the simplified Hamiltonian, the values for the other necessary parameters are taken from the Carnall *et al.* [Car+89] systematic study of LaF_3.
- `startValues`: an association with the initial values for the independent parameters given in `problemVars`. Independent parameters are those that remain once the constraints have been accounted for.
- σ`exp`: estimated uncertainty in the energy level differences between experimental and calculated values.
- `constraints`: a list of replacement rules defining constraints on the parameters. These constraints can either pin down a value, or apply proportionality ratios between them. If constrained by proportionally factors, these ratios are usually taken from Hartree-Fock calculations.

Here is a description of the different steps that this algorithm implements.

1. **Initialization**: sets initial conditions, processes options, and prepares data structures. Manages settings like the truncation energy, logging preferences, and computational accuracy goals.
2. **Data Preparation**: determines valid data points, excluding specified indices, and establishes truncation energy for the model.
3. **Hamiltonian Assembly and Simplification**: constructs the Hamiltonian while preserving its block structure, applies simplification rules, and processes the diagonal blocks to retain only free-ion parameters.
4. **Level Calculation**: determines the level description using free-ion parameters.

[22] The extreme case of this scarcity being Yb and Ce, where there are only 7 non-degenerate energies, but where the crystal-field alone might require more parameters than these (for instance in C_{2v} symmetry one needs 9 $B_q^{(k)}$ parameters). [23] For example, in the Table **??** for LaF_3, in the case of Yb, only two parameters are varied (ζ and ϵ) and the values for the crystal field obtained from linear fits to the previously fitted $B_q^{(k)}$ in Pr, Nd, Dy, Sm*, Ho*, Er, and Tm. (* not all $B_q^{(k)}$)

5. **Compilation and Truncation of Hamiltonian**: compiles the Hamiltonian and truncates it based on the set truncation energy, optimizing for computational efficiency.

6. **Fitting Process Initialization**: prepares variables and functions for optimization, including eigenvalue calculations and difference evaluations.

7. **Optimization**: employs the Levenberg-Marquardt method to optimize parameters, minimizing the discrepancy between calculated and experimental energy levels.

8. **Post-Processing**: calculates the Hamiltonian's eigensystem at the solution, deriving statistics like RMS deviation, parameter uncertainties, and covariance matrix.

9. **Output Compilation**: aggregates all relevant data and results into the output association `solCompendium`, documenting the fitting process and outcomes.

10. **Logging and Return**: saves the comprehensive fitting results to a log file and returns the detailed output data.

This function admits several options. Importantly here one may permit the model to have a constant shift to all the levels and the truncation energy can be set. Here one can also provide simplification rules that are applied to the compiled version of the Hamiltonian.

- `Energy Uncertainty in K`: used for error estimation, it can be either `Automatic` in which case the (σ of the fit is used as the uncertainty of the energies) or a numeric value in which case that is the value used for error propagation.

- `TruncationEnergy`: determines the energy level at which the Hamiltonian is truncated. If set to `Automatic`, the truncation energy is derived from the maximum energy present in the experimental data (`expData`). Otherwise, it can be manually set to a specific value.

- `MagneticSimplifier`: provides a list of replacement rules to simplify the magnetic parameters in the Hamiltonian, aiding in the reduction of computational complexity.

- `MagFieldSimplifier`: offers a list of replacement rules to specify a magnetic field, enhancing the flexibility in modeling magnetic effects within the system.

- `SymmetrySimplifier`: A list of replacement rules used to simplify the crystal field components of the Hamiltonian, facilitating a more efficient fitting process.

- `OtherSimplifier`: an additional list of replacement rules applied to the Hamiltonian before computation, allowing for further customization and simplification of the model, such as disabling specific interactions or effects. **IMPORTANT**: here the default is that the spin-spin contribution (as controlled by the σSS parameter) for the Marvin integrals is *not* included.

- `MaxHistory`: this option controls the length of the logs for the solver, enabling users to adjust the amount of log data retained during the fitting process.

- `MaxIterations`: sets the maximum number of iterations that the fitting algorithm (`NMinimize`) will execute, allowing control over the computational effort spent on the fitting.

- `FilePrefix`: specifies the prefix for the filenames under which the fitting results are saved. By default, the prefix is set to "calcs", and the files are saved in the "log/calcs" directory.

- `AddConstantShift`: if set to `True`, this option allows for a constant shift in the energy levels during the fitting process. This is particularly useful for fine-tuning the model to better match experimental data.

- `AccuracyGoal`: defines the accuracy goal for the `NMinimize` function used in the fitting process, allowing users to set the desired level of precision for the fit.

- `PrintFun`: specifies the function used to print progress messages during the fitting process. The default is `PrintTemporary`, which displays temporary output that can be useful for monitoring the fitting's progress.

- SlackChannel: names the Slack channel to which progress messages will be sent. If set to None, this feature is disabled, and no messages are sent to Slack.
- ProgressView: controls whether a progress window is displayed during the fitting process. When set to True, it provides an auxiliary notebook is created automatically with plots showing the progress of NMinimize.
- SignatureCheck: if True, the function ends prematurely and prints the list of the symbols that define the Hamiltonian after all basic simplifications have been applied without considering the given constraints.
- SaveEigenvectors: determines whether both the eigenvectors and eigenvalues of the fitted model are saved. If set to False, only the energies are saved.
- AppendToLogFile: what is provided here is appended to the log file under the "Appendix" key, enabling additional data to be stored alongside the fitting results.

The function returns an association with the following keys.

- bestRMS: the best root mean square deviation found during the fitting process.
- bestParams: the optimal set of parameters found through the fitting process.
- paramSols: a list of the parameter solutions at each step of the fitting algorithm.
- timeTaken/s: the total time taken to complete the fitting process, measured in seconds.
- simplifier: the replacement rules used to reduce the define the free-ion Hamiltonian.
- excludeDataIndices: the indices that were excluded from the fitting process as specified in the input.
- startValues: the initial values for the problem variables as given in the input.
- freeIonSymbols: symbols used in the intermediate coupling level calculation.
- truncationEnergy: the energy level at which the Hamiltonian was truncated.
- numE: the number of electrons in the f^{numE} configuration.
- expData: the experimental data used for the fitting process.
- problemVars: the variables considered during the fitting process.
- maxIterations: the maximum number of iterations used in the fitting process.
- hamDim: the dimension of the full Hamiltonian before simplifications or truncations.
- allVars: all the symbols defining the Hamiltonian under the applied simplifications.
- freeBies: the free-ion parameters used to calculate the intermediate coupling levels.
- truncatedDim: the dimension of the truncated Hamiltonian.
- compiledIntermediateFname: the file name of the compiled function used for the truncated Hamiltonian.
- fittedLevels: the number of levels that were fitted.
- actualSteps: the actual number of steps taken by the fitting algorithm.
- solWithUncertainty: a list of replacement rules showing the best fit value and its uncertainty for each parameter.
- rmsHistory: as list of the RMS values found during the fitting process.
- Appendix: an association appended to the log file under the "Appendix" key.
- presentDataIndices: the indices in expData that were used for fitting.
- states: a list of eigenvalues and eigenvectors for the fitted model, available if eigenvectors were saved.
- energies: a list of the energies of the fitted levels, adjusted if an energy shift was included in the fitting.

9 Accompanying notebooks

The code for this dissertation is accompanied by the following auxiliary *Mathematica* notebooks, which either document the functions included in the code, or serve as aids in the calculation of matrix elements.

- 🖫 /notebooks/qlanth.nb: gives an overview of functions included in **qlanth**.
- 🖫 /notebooks/qlanth - Table Generator.nb: generates the basic tables on which every calculation is based. This means that LS-reduced matrix elements are used to calculate matrix elements in the $|LSJM_J\rangle$ basis.
- 🖫 /notebooks/qlanth - JJBlock Calculator.nb: can be used to generate the J-J' blocks for the different interactions. The data files produced here are necessary for HamMatrixAssembly to work. These blocks are creating by putting together matrix elements from different interactions.
- 🖫 /notebooks/The Lanthanides in LaF3.nb: runs **qlanth** over the lanthanide ions in LaF_3 and compares the results against the published values from Carnall *et al.* [Car+89]. It also calculates magnetic dipole transition rates and oscillator strengths.

10 Compiled data for LaF_3:Ln^{3+} and $LiYF_4$:Ln^{3+}

The study of Carnall *et al.* [Car+89] on lanthanum fluoride was a systematic review of trivalent lanthanide ions in LaF_3. In this work they fitted the experimental data for all of the lanthanide ions using the single-configuration effective Hamiltonian. In their appendices one can find their calculated values, together with the experimental values that they used for their least squares fittings. In **qlanth** this data can be accessed by invoking the command LoadCarnall which brings into the session an association that has keys that have as values the tables and appendices from this article. 𝓕ig-6 shows the results of a calculation done with **qlanth** for the energy levels in LaF_3. Additionally the function LoadLaF3Parameters can be used to query the data for the fitted parameters, which may serve as a useful starting point for the description of the lanthanides ions in hosts other than LaF_3.

Similarly, Cheng *et al.* [Che+16] compiled data for $LiYF_4$. In **qlanth** model parameters for $LiYF_4$ can be obtained by calling the function LoadLiYF4Parameters. 𝓕ig-7 shows the results of a calculation done with **qlanth** for the energy levels in $LiYF_4$.

```
Carnall::usage = "Association of data from Carnall et al (1989) with
    the following keys: {data, annotations, paramSymbols, elementNames
    , rawData, rawAnnotations, annnotatedData, appendix:Pr:Association
    , appendix:Pr:Calculated, appendix:Pr:RawTable, appendix:Headings}
    ";
```

```
LoadCarnall::usage = "LoadCarnall[] loads data for trivalent
    lanthanides in LaF3 using the data from Bill Carnall's 1989 paper.
    ";
LoadCarnall[] := (
  If[ValueQ[Carnall], Return[]];
  carnallFname = FileNameJoin[{moduleDir, "data", "Carnall.m"}];
  If[!FileExistsQ[carnallFname],
    (PrintTemporary[">> Carnall.m not found, generating ..."];
      Carnall = ParseCarnall[];
    ),
    Carnall = Import[carnallFname];
  ];
);
```

```
LoadLaF3Parameters::usage = "LoadLaF3Parameters[ln] takes a string
    with the symbol the element of a trivalent lanthanide ion and
    returns model parameters for it. It is based on the data for LaF3.
     If the option ''Free Ion'' is set to True then the function sets
    all crystal field parameters to zero. Through the option ''gs'' it
     allows modyfing the electronic gyromagnetic ratio. For
    completeness this function also computes the E parameters using
    the F parameters quoted on Carnall.";
Options[LoadLaF3Parameters] = {
```

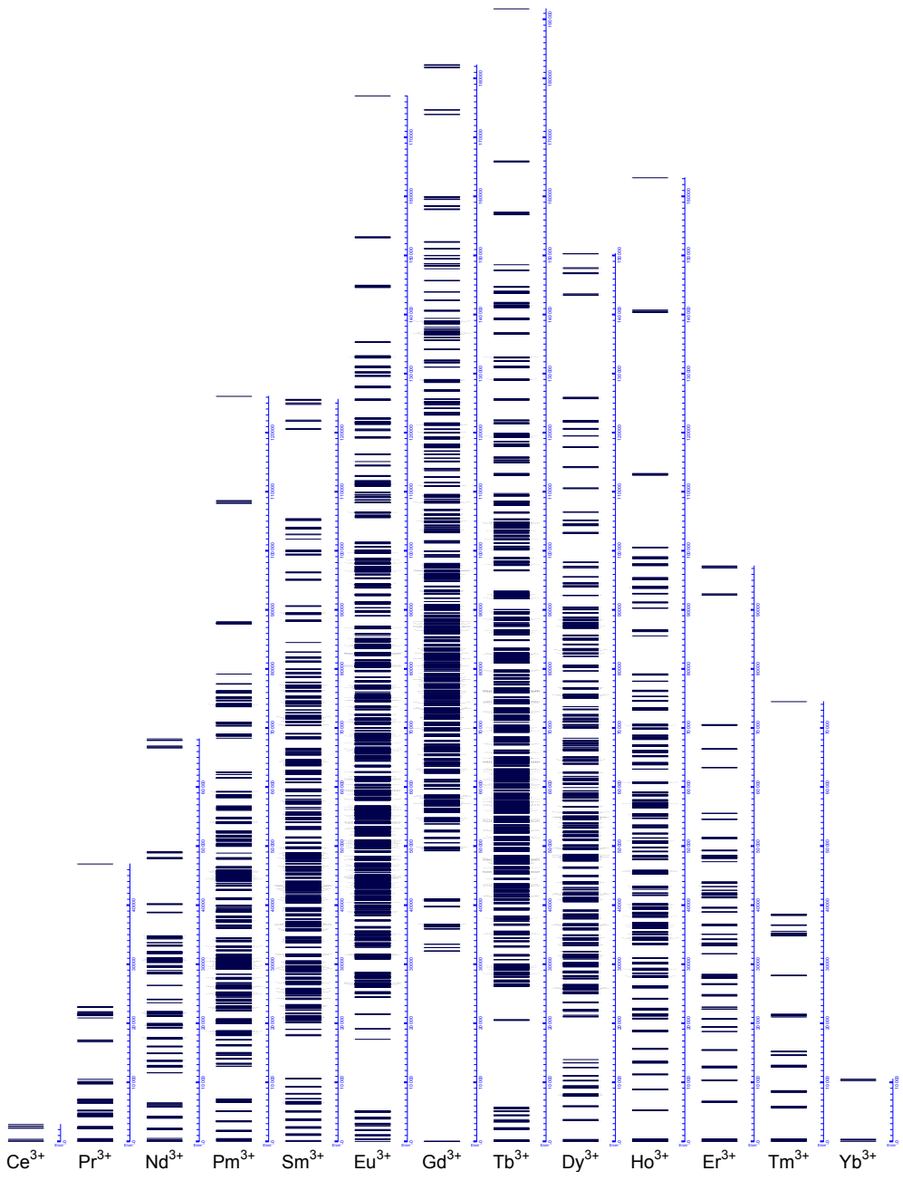


Figure 6: Energy levels in LaF_3.

```
    "Free Ion"->False,
    "gs"->2.002319304386,
    "With Uncertainties"->False
    };
LoadLaF3Parameters[Ln_String, OptionsPattern[]] := Module[
  {params, uncertain,
  uncertainKeys, uncertainRules},
  (
    If[Not[ValueQ[Carnall]],
      LoadCarnall[];
    ];
    params = Association[Carnall["data"][Ln]];
    (*If a free ion then all the parameters from the crystal field
    are set to zero*)
    If[OptionValue["Free Ion"],
      Do[params[cfSymbol] = 0, {cfSymbol, cfSymbols}]
    ];
    params[F0] = 0;
    params[M2] = 0.56 * params[M0]; (*See Carnall 1989,Table I,
    caption,probably fixed based on HF values*)
    params[M4] = 0.31 * params[M0]; (*See Carnall 1989,Table I,
    caption,probably fixed based on HF values*)
    params[P0] = 0;
    params[P4] = 0.5 * params[P2];  (*See Carnall 1989,Table I,
    caption,probably fixed based on HF values*)
    params[P6] = 0.1 * params[P2];  (*See Carnall 1989,Table I,
    caption,probably fixed based on HF values*)
```

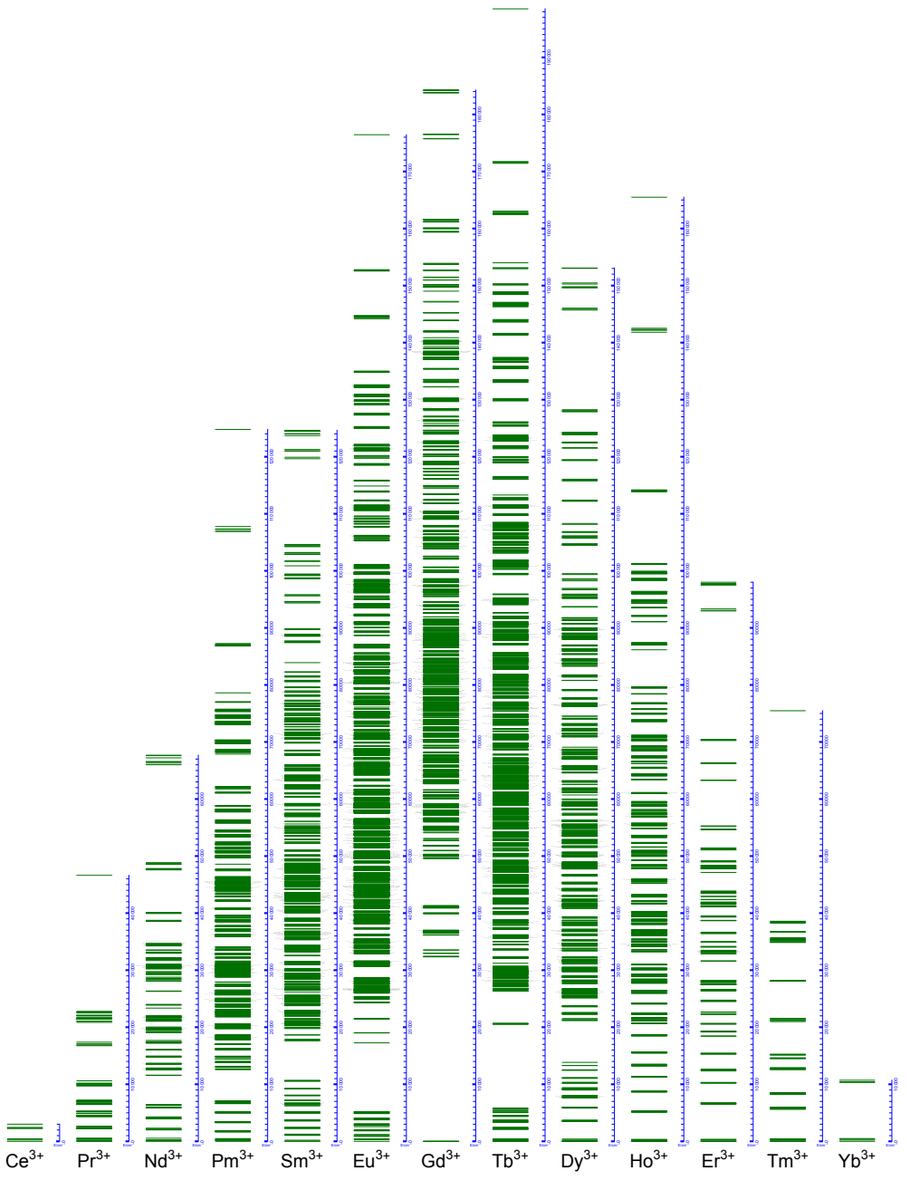


Figure 7: Energy levels in $LiYF_4$.

```
    params[gs] = OptionValue["gs"];
    {params[E0], params[E1], params[E2], params[E3]} = FtoE[params[F0
], params[F2], params[F4], params[F6]];
    params[E0] = 0;
    If[
      Not[OptionValue["With Uncertainties"]],
      Return[params],
      (
        uncertain     = Association[Carnall["annotations"][Ln]];
        uncertainKeys = Keys[uncertain];
        uncertain     = If[# == "Not allowed to vary in fitting." ||
# == "Interpolated",
            0., #] & /@ uncertain;
        paramKeys = Keys[params];
        uncertainVals = Sort[Intersection[paramKeys, uncertainKeys]]
/. Association[uncertain];
        uncertainRules = MapThread[Rule, {Sort[uncertainKeys],
uncertainVals}];
        Which[
          MemberQ[{"Ce", "Yb"}, Ln],
          (
            subsetL = {F0};
            subsetR = {0};
          ),
          True,
          (
          subsetL = {F0, M2, M4, P0, P4, P6, E0, E1, E2, E3};
```

```
48            subsetR = {0, M0*0.65, M0*0.31, 0, P2*0.5, P2*0.1,
49              0,
50              Sqrt[(196 F2^2)/164025 + (49 F4^2)/88209 + (122500 F6^2)
    /134165889],
51              Sqrt[F2^2/4100625 + F4^2/10673289 + (30625 F6^2)
    /2743558264161],
52              Sqrt[F2^2/18225 + (4 F4^2)/1185921 + (30625 F6^2)
    /1803785841]};
53            )
54          ];
55          uncertainRules = Join[uncertainRules, MapThread[Rule, {
    subsetL,subsetR /. uncertainRules}]];
56          uncertainRules = Association[uncertainRules];
57          Which[
58            Ln == "Eu",
59            (
60              uncertainRules[F4] = 12.121;
61              uncertainRules[F6] = 15.872;
62            ),
63            Ln == "Gd",
64            (
65              uncertainRules[F4] = 12.07;
66            ),
67            Ln == "Tb",
68            (
69              uncertainRules[F4] = 41.006;
70            )
71          ];
72          If[MemberQ[{"Eu","Gd","Tb"},Ln],
73            (
74              uncertainRules[E1] = Sqrt[(196 F2^2)/164025 + (49 F4^2)
    /88209 + (122500 F6^2)/134165889] /. uncertainRules;
75              uncertainRules[E2] = Sqrt[F2^2/4100625 + F4^2/10673289 +
    (30625 F6^2)/2743558264161] /. uncertainRules;
76              uncertainRules[E3] = Sqrt[F2^2/18225 + (4 F4^2)/1185921 +
     (30625 F6^2)/1803785841] /. uncertainRules;
77            )
78          ];
79          uncertainKeys = First /@ Normal[uncertainRules];
80          fullParams = Association[MapThread[Rule, {uncertainKeys,
    MapThread[Around, {uncertainKeys /. params, uncertainKeys /.
    uncertainRules}]}]];
81          Return[Join[params, fullParams]]
82        )
83        ];
84    )
85  ];
```

```
1  LoadLiYF4Parameters::usage="LoadLiYF4Parameters[ln] takes a string
       with the symbol the element of a trivalent lanthanide ion and
       returns model parameters for it. It return the data for LiYF4 from
        Cheng et al.";
2  LoadLiYF4Parameters[ln_, OptionsPattern[]]:=(
3    If[!ValueQ[paramsLiYF4],
4      paramsChengLiYF4 = Import[FileNameJoin[{moduleDir,"data","
       chengLiYF4.m"}]];
5    ];
6    Return[paramsChengLiYF4[ln]];
7  )
```

11 sparsefn.py

qlanth is also accompanied by seven Python scripts sparsef[1-7].py. Each of these contains a single function effective_hamiltonian_f[1-7] which returns a sparse array for given values for the model parameters.

There is an eight Python script called basisLSJMJ.py which contains a dictionary whose keys are f1, f2, f3, f4, f5, f6, and f7, and whose values are lists that contain the ordered basis in which the array produced by the sparsefn.py should be understood to be in. Each basis vector is a list with three elements {LS string in NK notation, J, M_J}.

In those it is left up to the user to make the adequate change of signs in the parameters for configurations above $\underline{f}^7$. These include changing the signs of all in &qn-18 and setting t2Switch to 0. For configurations at or below $\underline{f}^7$ it is necessary to set t2Switch to 1.

12 Data sources

The data (and their provenance) upon which **qlanth** bases its calculations is the following:

- Coefficients of fractional parentage and seniority numbers from Velkov [Vel00].
- Terms labels from $\underline{f}^1$ to $\underline{f}^7$ from Nielson and Koster [NK63].
- 3j-symbol [Wol24b] and 6j-symbol [Wol24a] values from *Mathematica* (v 13.2),
- Reduced matrix elements for the three body operators from Judd [JS84].
- Reduced matrix elements for the magnetic interactions from Judd [JCC68].

13 Other details

- Fitting the experimental data for the entire row might take about 45 minutes, if run for the first time, but takes much less time once compiled functions from the truncated (or not truncated) Hamiltonian have been saved to disk.
- The code was run in *Mathematica* version 13.2 on MacOS Sonoma 14.5.

14 Units

Following the tradition of the spectroscopic community, all the matrix elements of the Hamiltonian are calculated using the Kayser ($\mathcal{K} \equiv \mathrm{cm}^{-1}$) as the (pseudo) energy unit. All the parameters (except the magnetic field which is in Tesla) in the effective Hamiltonian are assumed to be in this unit. As is customary, the angular momentum operators assume atomic units in which $\hbar = 1$.

Some constants and conversion values are included in the file `qonstants.m`.

```
BeginPackage["qonstants`"];

(* Physical Constants*)
bohrRadius = 5.29177210903 * 10^-9;
ee         = 1.602176634 * 10^-19;

(* Spectroscopic niceties*)
theLanthanides = {"Ce", "Pr", "Nd", "Pm", "Sm", "Eu", "Gd", "Tb", "Dy
    ", "Ho", "Er", "Tm", "Yb"};
theActinides   = {"Ac", "Th", "Pa", "U", "Np", "Pu", "Am", "Cm", "Bk"
    , "Cf", "Es", "Fm", "Md", "No", "Lr"};
theTrivalents  = {"Pr", "Nd", "Pm", "Sm", "Eu", "Gd", "Tb", "Dy", "Ho
    ", "Er", "Tm"};
specAlphabet   = "SPDFGHIKLMNOQRTUV";
complementaryNumE = {1,13,2,12,3,11,4,10,5,9,6,8,7};

(* SI *)
hPlanck = 6.62607015 * 10^-34;          (* Planck's constant in J s
    *)
hBar    = hPlanck    / (2 \[Pi]);       (* reduced Planck's constant
    in J s *)
\[Mu]B  = 9.2740100783 * 10^-24;        (* Bohr magneton in SI *)
me      = 9.1093837015 * 10^-31;        (* electron mass in kg *)
cLight  = 2.99792458   * 10^8;          (* speed of light in m/s *)
eCharge = 1.602176634  * 10^-19;        (* elementary charge in SI *)
\[Epsilon]0  = 8.8541878128 * 10^-12;   (* electric permittivity in
    vacuum in SI *)
\[Mu]0  = 4 \[Pi] * 10^-7;              (* magnetic permeability in
    vacuum in SI *)
αFine = 1/137.036;                (* fine structure constant *)

bohrRadius    = 5.29177*10^-11;         (* Bohr radius in m *)
hartreeEnergy = hBar^2 / (me * bohrRadius^2); (* Hartree energy in J
    *)
hartreeTime   = hBar / hartreeEnergy; (* Hartree time in s *)

(* Hartree atomic units *)
hPlanckHartree = 2 \[Pi]; (* Planck's constant in Hartree *)
meHartree      = 1;       (* electron mass in Hartree *)
cLightHartree  = 137.036; (* speed of light in Hartree *)
eChargeHartree = 1;       (* elementary charge in Hartree *)
```

```
\[Mu]0Hartree  = αFine^2; (* magnetic permeability in vacuum in
    Hartree *)

(* some conversion factors *)
eVToJoule       = eCharge;
jouleToeV       = 1 / eVToJoule;
jouleToHartree  = 1 / hartreeEnergy;
eVToKayser      = eCharge /( hPlanck * cLight * 100 ); (* 1 eV =
    8065.54429 cm^-1 *)
kayserToeV      = 1 / eVToKayser;
teslaToKayser   = 2 * \[Mu]B / hPlanck / cLight / 100;
kayserToHartree = kayserToeV * eVToJoule * jouleToHartree;
hartreeToKayser = 1 / kayserToHartree;

EndPackage[];
```

15 Notation

orbital angular momentum operator of a single electron

$$\hat{l} \tag{113}$$

total orbital angular momentum operator

$$\hat{L} \tag{114}$$

spin angular momentum operator of a single electron

$$\hat{s} \tag{115}$$

total spin angular momentum operator

$$\hat{S} \tag{116}$$

Shorthand for all other quantum numbers

$$\Lambda \tag{117}$$

orbital angular momentum number

$$\underline{\ell} \tag{118}$$

spinning angular momentum number

$$\underline{\jmath} \tag{119}$$

Coulomb non-central potential

$$\hat{\mathfrak{C}} \tag{120}$$

LS-reduced matrix element of operator $\hat{O}$ between ΛLS and $\Lambda' L' S'$

$$\langle \Lambda LS \| \hat{O} \| \Lambda' L' S' \rangle \tag{121}$$

LSJ-reduced matrix element of operator $\hat{O}$ between ΛLSJ and $\Lambda' L' S' J'$

$$\langle \Lambda LSJ \| \hat{O} \| \Lambda' L' S' J' \rangle \tag{122}$$

Spectroscopic term αLS in Russel-Saunders notation

$$^{2S+1}\alpha \mathrm{L} \equiv |\alpha LS\rangle \tag{123}$$

spherical tensor operator of rank k

$$\hat{X}^{(k)} \tag{124}$$

q-component of the spherical tensor operator $\hat{X}^{(k)}$

$$\hat{X}^{(k)}_q \tag{125}$$

The coefficient of fractional parentage from the parent term $|\underline{\ell}^{n-1} \alpha' L' S'\rangle$ for the daughter term $|\underline{\ell}^n \alpha LS\rangle$

$$\left(\underline{\ell}^{n-1} \alpha' L' S' \middle\} \underline{\ell}^n \alpha LS \right) \tag{126}$$

16 Definitions

$$\overbrace{[\![x]\!]}^{\text{two plus one}} \coloneqq 2x+1 \tag{127}$$

$$\overbrace{\hat{u}^{(k)}}^{\text{irreducible unit tensor operator of rank k}} \tag{128}$$

$$\overbrace{\hat{U}^{(k)} \coloneqq \sum_{i=1}^{n} \hat{u}^{(k)}}^{\text{symmetric unit tensor operator for n equivalent electrons}} \tag{129}$$

$$\overbrace{C_q^{(k)} \coloneqq \sqrt{\frac{4\pi}{2k+1}} \mathrm{Y}_q^{(k)}}^{\text{Renormalized spherical harmonics}} \tag{130}$$

$$\overbrace{\triangleleft(j_1,j_2,j_3) \coloneqq \begin{cases} 1 & \text{if } j_1 = (j_2+j_3), (j_2+j_3-1), \ldots, |j_2-j_3| \\ 0 & \text{otherwise} \end{cases}}^{\text{Triangle “delta” between } j_1, j_2, j_3} \tag{131}$$

17 code

17.1 qlanth.m

This file encapsulates the main functions in **qlanth** and contains all the physics related functions.

```
(* ------------------------------------------------------------------
+--------------------------------------------------------------------+
|                                                                    |
|                                                                    |
|                      __                          __     __         |
|              ____ _    / /  ____ _    ____      / /_   / /_        |
|           / __ `/  / /  / __ `/  / __ \    / __/  / __ \          |
|          / /_/ /  / /  / /_/ /  / / / /  / /_    / / / /          |
|          \__, /  /_/   \__, _/  /_/ /_/   \__/  /_/ /_/          |
|            /_/                                                     |
|                                                                    |
|                                                                    |
+--------------------------------------------------------------------+
This code was initially authored by Christopher M. Dodson and Rashid
Zia, and then rewritten and expanded by Juan David Lizarazo Ferro in
the years 2022-2024 under the advisory of Dr. Rashid Zia. It has
also benefited from the discussions with Tharnier Puel.

It uses an effective Hamiltonian to describe the electronic
structure of lanthanide ions in crystals. This effective Hamiltonian
includes terms representing the following interactions/relativistic
corrections: spin-orbit, electrostatic repulsion, spin-spin, crystal
field, and spin-other-orbit.

The Hilbert space used in this effective Hamiltonian is limited to
single f^n configurations. The inaccuracy of this single
configuration description is partially compensated by the inclusion
of configuration interaction terms as parametrized by the Casimir
operators of SO(3), G(2), and SO(7), and by three-body effective
operators ti.

The parameters included in this model are listed in the string
paramAtlas.

The notebook "qlanth.nb" contains a gallery with many of the
functions included in this module with some simple use cases.

The notebook "The Lanthanides in LaF3.nb" is an example in which the
results from this code are compared against the published results by
Carnall et. al for the energy levels of lanthinde ions in crystals
of lanthanum trifluoride.

VERSION: AUGUST 2024

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```

```
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------------------------------------------------------------------- *)

BeginPackage["qlanth`"];
Needs["qonstants`"];
Needs["qplotter`"];
Needs["misc`"];

paramAtlas = "
E0: linear combination of F_k, see eqn. (2-80) in Wybourne 1965
E1: linear combination of F_k, see eqn. (2-80) in Wybourne 1965
E2: linear combination of F_k, see eqn. (2-80) in Wybourne 1965
E3: linear combination of F_k, see eqn. (2-80) in Wybourne 1965

ζ: spin-orbit strength parameter.

F0: Direct Slater integral F^0, produces an overall shift of all
    energy levels.
F2: Direct Slater integral F^2
F4: Direct Slater integral F^4, possibly constrained by ratio to F^2
```

```
F6: Direct Slater integral F^6, possibly constrained by ratio to F^2

M0: 0th Marvin integral
M2: 2nd Marvin integral
M4: 4th Marvin integral
\[Sigma]SS: spin-spin override, if 0 spin-spin is omitted, if 1 then
    spin-spin is included

T2:  three-body effective operator parameter T^2  (non-orthogonal)
T2p: three-body effective operator parameter T^2' (orthogonalized T2)
T3:  three-body effective operator parameter T^3
T4:  three-body effective operator parameter T^4
T6:  three-body effective operator parameter T^6
T7:  three-body effective operator parameter T^7
T8:  three-body effective operator parameter T^8

T11p: three-body effective operator parameter T^11' (orthogonalized
    T11)
T12:  three-body effective operator parameter T^12
T14:  three-body effective operator parameter T^14
T15:  three-body effective operator parameter T^15
T16:  three-body effective operator parameter T^16
T17:  three-body effective operator parameter T^17
T18:  three-body effective operator parameter T^18
T19:  three-body effective operator parameter T^19

P0: pseudo-magnetic parameter P^0
P2: pseudo-magnetic parameter P^2
P4: pseudo-magnetic parameter P^4
P6: pseudo-magnetic parameter P^6

gs: electronic gyromagnetic ratio

α: Trees' parameter α describing configuration interaction via the
    Casimir operator of SO(3)
β: Trees' parameter β describing configuration interaction via the
    Casimir operator of G(2)
γ: Trees' parameter γ describing configuration interaction via the
    Casimir operator of SO(7)

B02: crystal field parameter B_0^2 (real)
B04: crystal field parameter B_0^4 (real)
B06: crystal field parameter B_0^6 (real)
B12: crystal field parameter B_1^2 (real)
B14: crystal field parameter B_1^4 (real)

B16: crystal field parameter B_1^6 (real)
B22: crystal field parameter B_2^2 (real)
B24: crystal field parameter B_2^4 (real)
B26: crystal field parameter B_2^6 (real)
B34: crystal field parameter B_3^4 (real)

B36: crystal field parameter B_3^6 (real)
B44: crystal field parameter B_4^4 (real)
B46: crystal field parameter B_4^6 (real)
B56: crystal field parameter B_5^6 (real)
B66: crystal field parameter B_6^6 (real)

S12: crystal field parameter S_1^2 (real)
S14: crystal field parameter S_1^4 (real)
S16: crystal field parameter S_1^6 (real)
S22: crystal field parameter S_2^2 (real)

S24: crystal field parameter S_2^4 (real)
S26: crystal field parameter S_2^6 (real)
S34: crystal field parameter S_3^4 (real)
S36: crystal field parameter S_3^6 (real)

S44: crystal field parameter S_4^4 (real)
S46: crystal field parameter S_4^6 (real)
S56: crystal field parameter S_5^6 (real)
S66: crystal field parameter S_6^6 (real)

\[Epsilon]: ground level baseline shift
t2Switch: controls the usage of the t2 operator beyond f7 (1 for f7
    or below, 0 for f8 or above)
```

```
wChErrA: If 1 then the type-A errors in Chen are used, if 0 then not.
wChErrB: If 1 then the type-B errors in Chen are used, if 0 then not.

Bx: x component of external magnetic field (in T)
By: y component of external magnetic field (in T)
Bz: z component of external magnetic field (in T)

\[CapitalOmega]2: Judd-Ofelt intensity parameter k=2 (in cm^2)
\[CapitalOmega]4: Judd-Ofelt intensity parameter k=4 (in cm^2)
\[CapitalOmega]6: Judd-Ofelt intensity parameter k=6 (in cm^2)

nE: number of electrons in a configuration
";
paramSymbols    = StringSplit[paramAtlas, "\n"];
paramSymbols    = Select[paramSymbols, # != ""& ];
paramSymbols    = ToExpression[StringSplit[#, ":"][[1]]] & /@
    paramSymbols;
Protect /@ paramSymbols;

(* Parameter families *)
Unprotect[racahSymbols, chenSymbols, slaterSymbols, controlSymbols,
    cfSymbols, TSymbols, pseudoMagneticSymbols, marvinSymbols,
    casimirSymbols, magneticSymbols, juddOfeltIntensitySymbols];
racahSymbols    = {E0, E1, E2, E3};
chenSymbols     = {wChErrA, wChErrB};
slaterSymbols   = {F0, F2, F4, F6};
controlSymbols  = {t2Switch, \[Sigma]SS};
cfSymbols       = {B02, B04, B06, B12, B14, B16, B22, B24, B26, B34,
    B36,
                   B44, B46, B56, B66,
                   S12, S14, S16, S22, S24, S26, S34, S36, S44, S46,
    S56, S66};
TSymbols        = {T2, T2p, T3, T4, T6, T7, T8, T11p, T12, T14, T15,
    T16, T17, T18, T19};
pseudoMagneticSymbols = {P0, P2, P4, P6};
marvinSymbols         = {M0, M2, M4};
magneticSymbols       = {Bx, By, Bz, gs, ζ};
casimirSymbols        = {α, β, γ};
juddOfeltIntensitySymbols = {\[CapitalOmega]2, \[CapitalOmega]4, \[
    CapitalOmega]6};
paramFamilies         = Hold[{racahSymbols, chenSymbols,
    slaterSymbols, controlSymbols, cfSymbols, TSymbols,
    pseudoMagneticSymbols, marvinSymbols, casimirSymbols,
    magneticSymbols, juddOfeltIntensitySymbols}];
ReleaseHold[Protect /@ paramFamilies];
crystalGroups = {"C1","Ci","C2","Cs","C2h","D2","C2v","D2h","C4","S4"
    ,"C4h","D4","C4v","D3d","D4h","C3","C3i","D3","C3v","D3d","C6","
    C3h","C6h","D6","C6v","D3h","D6h","T","Th","O","Td","Oh"};

(* Parameter usage *)
paramLines = Select[StringSplit[paramAtlas, "\n"], # != "" &];
usageTemplate = StringTemplate["`paramSymbol`::usage=\"`paramSymbol`
    : `paramUsage`\";"];
Do[(
  {paramString, paramUsage} = StringSplit[paramLine, ":"];
  paramUsage                = StringTrim[paramUsage];
  expressionString          = usageTemplate[<|"paramSymbol" ->
    paramString, "paramUsage" -> paramUsage|>];
  ToExpression[usageTemplate[<|"paramSymbol" -> paramString, "
    paramUsage" -> paramUsage|>]]
),
{paramLine, paramLines}
];

AllowedJ;
AllowedMforJ;
AllowedNKSLJMforJMTerms;
AllowedNKSLJMforJTerms;
AllowedNKSLJTerms;

AllowedNKSLTerms;
AllowedNKSLforJTerms;
AllowedSLJMTerms;
AllowedSLJTerms;
AllowedSLTerms;

```

```
BasisLSJ;
BasisLSJMJ;
BasisTableGenerator;
Bqk;
CFP;

CFPAssoc;
CFPTable;
CFPTerms;
Carnall;
CasimirG2;

CasimirSO3;
CasimirSO7;
Cqk;
CrystalField;
CrystalFieldForm;

Dk;
EigenLever;
Electrostatic;
ElectrostaticConfigInteraction;
ElectrostaticTable;

EnergyLevelDiagram;
EnergyStates;
EtoF;
ExportMZip;
ExportmZip;

FindNKLSTerm;
FindSL;
FreeHam;
FreeIonTable;
FromArrayToTable;
FtoE;

GG2U;
GSO7W;
GenerateCFP;
GenerateCFPAssoc;
GenerateCFPTable;

GenerateCrystalFieldTable;
GenerateElectrostaticTable;
GenerateFreeIonTable;
GenerateReducedUkTable;
GenerateReducedV1kTable;
GenerateSOOandECSOLSTable;

GenerateSOOandECSOTable;
GenerateSpinOrbitTable;
GenerateSpinSpinTable;
GenerateT22Table;
GenerateThreeBodyTables;

Generator;
GroundMagDipoleOscillatorStrength;
HamMatrixAssembly;
HamiltonianForm;

HamiltonianMatrixPlot;
HoleElectronConjugation;
ImportMZip;
IonSolver;
JJBlockMagDip;

JJBlockMatrix;
JJBlockMatrixFileName;
JJBlockMatrixTable;
JuddOfeltUkSquared;
LabeledGrid;

LevelElecDipoleOscillatorStrength;
LevelJJBlockMagDipole;
LevelMagDipoleLineStrength;
```

```
LevelMagDipoleMatrixAssembly;
LevelMagDipoleOscillatorStrength;

LevelMagDipoleSpontaneousDecayRates;
LevelSimplerSymbolicHamMatrix;
LevelSolver;
ListRepeater;
LoadAll;

LoadCFP;
LoadCarnall;
LoadChenDeltas;
LoadElectrostatic;
LoadFreeIon;
LoadGuillotParameters;

LoadLaF3Parameters;
LoadLiYF4Parameters;
LoadSOOandECSO;
LoadSOOandECSOLS;
LoadSpinOrbit;
LoadSpinSpin;

LoadSymbolicHamiltonians;
LoadT11;
LoadT22;
LoadTermLabels;
LoadThreeBody;

LoadUk;
LoadV1k;
MagDipLineStrength;
MagDipoleMatrixAssembly;
MagDipoleRates;

MagneticInteractions;
MapToSparseArray;
MaxJ;
MinJ;
NKCFPPhase;

ParamPad;
ParseBenelli2015;
ParseStates;
ParseStatesByNumBasisVecs;
ParseStatesByProbabilitySum;

ParseTermLabels;
Phaser;
PrettySaundersSL;
PrettySaundersSLJ;
PrettySaundersSLJmJ;

PrintL;
PrintSLJ;
PrintSLJM;
ReducedSOOandECSOinf2;
ReducedSOOandECSOinfn;

ReducedT11inf2;
ReducedT22inf2;
ReducedT22infn;
ReducedUk;
ReducedUkTable;

ReducedV1kTable;
Reducedt11inf2;
ReplaceInSparseArray;
ScalarLSJMFromLS;
SOOandECSO;
SOOandECSOLSTable;

SOOandECSOTable;
ScalarOperatorProduct;
Seniority;
ShiftedLevels;
```

```
SimplerSymbolicHamMatrix;

SixJay;
SpinOrbit;
SpinOrbitTable;
SpinSpin;
SpinSpinTable;

Sqk;
SquarePrimeToNormal;
TPO;
TabulateJJBlockMagDipTable;
TabulateJJBlockMatrixTable;

TabulateManyJJBlockMagDipTables;
TabulateManyJJBlockMatrixTables;
ThreeBodyTable;
ThreeBodyTables;
ThreeJay;

TotalCFIters;
chenDeltas;
fK;
fnTermLabels;
fsubk;

fsupk;
moduleDir;
symbolicHamiltonians;

(* this selects the function that is applied to calculated matrix
   elements which helps keep down the complexity of the resulting
   algebraic expressions *)
SimplifyFun = Expand;

Begin["`Private`"]

  moduleDir = DirectoryName[$InputFileName];
  frontEndAvailable = (Head[$FrontEnd] === FrontEndObject);

  (* ############################################################ *)
  (* ########################### MISC ########################### *)

  TPO::usage = "TPO[x, y, ...] gives the product of 2x+1, 2y+1, ...";
  TPO[args__] := Times @@ ((2*# + 1) & /@ {args});

  Phaser::usage = "Phaser[x] gives (-1)^x.";
  Phaser[exponent_] := ((-1)^exponent);

  TriangleCondition::usage = "TriangleCondition[a, b, c] evaluates
    the triangle condition on a, b, and c.";
  TriangleCondition[a_, b_, c_] := (Abs[b - c] <= a <= (b + c));

  TriangleAndSumCondition::usage = "TriangleAndSumCondition[a, b, c]
    evaluates the joint satisfaction of the triangle and sum
    conditions.";
  TriangleAndSumCondition[a_, b_, c_] := (
    And[
      Abs[b - c] <= a <= (b + c),
      IntegerQ[a + b + c]
      ]
    );

  SquarePrimeToNormal::usage = "SquarePrimeToNormal[squarePrime]
    evaluates the standard representation of a number from the squared
     prime representation given in the list squarePrime. For
    squarePrime of the form {c0, c1, c2, c3, ...} this function
    returns the number c0 * Sqrt[p1^c1 * p2^c2 * p3^c3 * ...] where pi
     is the ith prime number. Exceptionally some of the ci might be
    letters in which case they have to be one of \"A\", \"B\", \"C\",
    \"D\" with them corresponding to 10, 11, 12, and 13, respectively.
    ";
  SquarePrimeToNormal[squarePrime_] :=
  (
    radical = Product[Prime[idx1 - 1] ^ Part[squarePrime, idx1], {
    idx1, 2, Length[squarePrime]}];
```

```
    radical = radical /. {"A" -> 10, "B" -> 11, "C" -> 12, "D" ->
    13};
    val = squarePrime[[1]] * Sqrt[radical];
    Return[val];
  );

  ParamPad::usage = "ParamPad[params] takes an association params
    whose keys are a subset of paramSymbols. The function returns a
    new association where all the keys not present in paramSymbols,
    will now be included in the returned association with their values
     set to zero.
  The function additionally takes an option \"Print\" that if set to
    True, will print the symbols that were not present in the given
    association. The default is True.";
  Options[ParamPad] = {"PrintFun" -> PrintTemporary};
  ParamPad[params_, OptionsPattern[]] := (
    notPresentSymbols = Complement[paramSymbols, Keys[params]];
    PrintFun = OptionValue["PrintFun"];
    PrintFun["Following symbols were not given and are being set to
    0: ",
      notPresentSymbols];
    newParams = Transpose[{paramSymbols, ConstantArray[0, Length[
    paramSymbols]]}];
    newParams = (#[[1]] -> #[[2]]) & /@ newParams;
    newParams = Association[newParams];
    newParams = Join[newParams, params];
    Return[newParams];
    )

  (* ############################################################ *)
  (* ###################### Racah Algebra ###################### *)

  ReducedUk::usage = "ReducedUk[n, l, SL, SpLp, k] gives the reduced
    matrix element of the symmetric unit tensor operator U^(k). See
    equation 11.53 in TASS.";
  ReducedUk[numE_, l_, SL_, SpLp_, k_] := Module[
    {spin, orbital, Uk, S, L,
    Sp, Lp, Sb, Lb, parentSL,
    cfpSL, cfpSpLp, Ukval,
    SLparents, SLpparents,
    commonParents, phase},
      {spin, orbital} = {1/2, 3};
      {S, L}          = FindSL[SL];
      {Sp, Lp}        = FindSL[SpLp];
      If[Not[S == Sp],
        Return[0]
      ];
      cfpSL      = CFP[{numE, SL}];
      cfpSpLp    = CFP[{numE, SpLp}];
      SLparents  = First /@ Rest[cfpSL];
      SLpparents = First /@ Rest[cfpSpLp];
      commonParents = Intersection[SLparents, SLpparents];
      Uk = Sum[(
        {Sb, Lb} = FindSL[\[Psi]b];
        Phaser[Lb] *
          CFPAssoc[{numE, SL, \[Psi]b}] *
          CFPAssoc[{numE, SpLp, \[Psi]b}] *
          SixJay[{orbital, k, orbital}, {L, Lb, Lp}]
      ),
      {\[Psi]b, commonParents}
      ];
      phase     = Phaser[orbital + L + k];
      prefactor = numE * phase * Sqrt[TPO[L,Lp]];
      Ukval     = prefactor*Uk;
      Return[Ukval];
  ]

  Ck::usage = "Ck[orbital, k] gives the diagonal reduced matrix
    element <l||C^(k)||l> where the Subscript[C, q]^(k) are
    renormalized spherical harmonics. See equation 11.23 in TASS with
    l=l'.";
  Ck[orbital_, k_] := (-1)^orbital * TPO[orbital] * ThreeJay[{orbital
    , 0}, {k, 0}, {orbital, 0}];

  SixJay::usage = "SixJay[{j1, j2, j3}, {j4, j5, j6}] provides the
    value for SixJSymbol[{j1, j2, j3}, {j4, j5, j6}] with memorization
```

```
    of computed values and short-circuiting values based on triangle
    conditions.";
SixJay[{j1_, j2_, j3_}, {j4_, j5_, j6_}] := (
  sixJayval = Which[
    Not[TriangleAndSumCondition[j1, j2, j3]],
    0,
    Not[TriangleAndSumCondition[j1, j5, j6]],
    0,
    Not[TriangleAndSumCondition[j4, j2, j6]],
    0,
    Not[TriangleAndSumCondition[j4, j5, j3]],
    0,
    True,
    SixJSymbol[{j1, j2, j3}, {j4, j5, j6}]];
  SixJay[{j1, j2, j3}, {j4, j5, j6}] = sixJayval);

ThreeJay::usage = "ThreeJay[{j1, m1}, {j2, m2}, {j3, m3}] gives the
    value of the Wigner 3j-symbol and memorizes the computed value.";
ThreeJay[{j1_, m1_}, {j2_, m2_}, {j3_, m3_}] := (
 threejval = Which[
   Not[(m1 + m2 + m3) == 0],
   0,
   Not[TriangleCondition[j1,j2,j3]],
   0,
   True,
   ThreeJSymbol[{j1, m1}, {j2, m2}, {j3, m3}]
   ];
 ThreeJay[{j1, m1}, {j2, m2}, {j3, m3}] = threejval);

ReducedV1k::usage = "ReducedV1k[n, l, SL, SpLp, k] gives the
  reduced matrix element of the spherical tensor operator V^(1k).
  See equation 2-101 in Wybourne 1965.";
ReducedV1k[numE_, SL_, SpLp_, k_] := Module[
  {Vk1, S, L, Sp, Lp,
  Sb, Lb, spin, orbital,
  cfpSL, cfpSpLp,
  SLparents, SpLpparents,
  commonParents, prefactor},
  (
    {spin, orbital} = {1/2, 3};
    {S, L}          = FindSL[SL];
    {Sp, Lp}        = FindSL[SpLp];
    cfpSL           = CFP[{numE, SL}];
    cfpSpLp         = CFP[{numE, SpLp}];
    SLparents       = First /@ Rest[cfpSL];
    SpLpparents     = First /@ Rest[cfpSpLp];
    commonParents = Intersection[SLparents, SpLpparents];
    Vk1 = Sum[(
        {Sb, Lb} = FindSL[\[Psi]b];
        Phaser[(Sb + Lb + S + L + orbital + k - spin)] *
        CFPAssoc[{numE, SL, \[Psi]b}] *
        CFPAssoc[{numE, SpLp, \[Psi]b}] *
        SixJay[{S, Sp, 1}, {spin, spin, Sb}] *
        SixJay[{L, Lp, k}, {orbital, orbital, Lb}]
      ),
    {\[Psi]b, commonParents}
    ];
    prefactor = numE * Sqrt[spin * (spin + 1) * TPO[spin, S, L, Sp,
   Lp] ];
    Return[prefactor * Vk1];
  )
];

GenerateReducedUkTable::usage = "GenerateReducedUkTable[numEmax]
  can be used to generate the association of reduced matrix elements
   for the unit tensor operators Uk from f^1 up to f^numEmax. If the
   option \"Export\" is set to True then the resulting data is saved
   to ./data/ReducedUkTable.m.";
Options[GenerateReducedUkTable] = {"Export" -> True, "Progress" ->
  True};
GenerateReducedUkTable[numEmax_Integer:7, OptionsPattern[]] := (
  numValues = Total[Length[AllowedNKSLTerms[#]]*Length[
  AllowedNKSLTerms[#]]&/@Range[1, numEmax]] * 4;
  Print["Calculating " <> ToString[numValues] <> " values for Uk k
  =0,2,4,6."];
  counter = 1;
```

```
    If[And[OptionValue["Progress"], frontEndAvailable],
    progBar = PrintTemporary[
        Dynamic[Row[{ProgressIndicator[counter, {0, numValues}], " ",
          counter}]]]
      ];
    ReducedUkTable = Table[
      (
        counter = counter+1;
        {numE, 3, SL, SpLp, k} -> SimplifyFun[ReducedUk[numE, 3, SL,
    SpLp, k]]
      ),
      {numE, 1, numEmax},
      {SL,   AllowedNKSLTerms[numE]},
      {SpLp, AllowedNKSLTerms[numE]},
      {k, {0, 2, 4, 6}}
    ];
    ReducedUkTable = Association[Flatten[ReducedUkTable]];
    ReducedUkTableFname = FileNameJoin[{moduleDir, "data", "
    ReducedUkTable.m"}];
    If[And[OptionValue["Progress"], frontEndAvailable],
      NotebookDelete[progBar]
    ];
    If[OptionValue["Export"],
      (
        Print["Exporting to file " <> ToString[ReducedUkTableFname]];
        Export[ReducedUkTableFname, ReducedUkTable];
      )
    ];
    Return[ReducedUkTable];
  )

  GenerateReducedV1kTable::usage = "GenerateReducedV1kTable[nmax]
    calculates values for Vk1 and returns an association where the
    keys are lists of the form {n, SL, SpLp, 1}. If the option \"
    Export\" is set to True then the resulting data is saved to ./data
    /ReducedV1kTable.m.";
  Options[GenerateReducedV1kTable] = {"Export" -> True, "Progress" ->
     True};
  GenerateReducedV1kTable[numEmax_Integer:7, OptionsPattern[]] := (
    numValues = Total[Length[AllowedNKSLTerms[#]]*Length[
    AllowedNKSLTerms[#]]&/@Range[1, numEmax]];
    Print["Calculating " <> ToString[numValues] <> " values for Vk1."
    ];
    counter = 1;
    If[And[OptionValue["Progress"], frontEndAvailable],
    progBar = PrintTemporary[
        Dynamic[Row[{ProgressIndicator[counter, {0, numValues}], " ",
          counter}]]]
      ];
    ReducedV1kTable = Table[
      (
        counter = counter+1;
        {n, SL, SpLp, 1} -> SimplifyFun[ReducedV1k[n, SL, SpLp, 1]]
      ),
      {n, 1, numEmax},
      {SL, AllowedNKSLTerms[n]},
      {SpLp, AllowedNKSLTerms[n]}
    ];
    ReducedV1kTable = Association[ReducedV1kTable];
    If[And[OptionValue["Progress"], frontEndAvailable],
      NotebookDelete[progBar]
    ];
    exportFname = FileNameJoin[{moduleDir, "data", "ReducedV1kTable.m
    "}];
    If[OptionValue["Export"],
      (
        Print["Exporting to file "<>ToString[exportFname]];
        Export[exportFname, ReducedV1kTable];
      )
    ];
    Return[ReducedV1kTable];
  )

  (* ###################### Racah Algebra ###################### *)
  (* ########################################################### *)
```

```
(* ############################################################ *)
(* ###################### Electrostatic ###################### *)

fsubk::usage = "fsubk[numE, orbital, SL, SLp, k] gives the Slater integral f_k for the given configuration and pair of SL terms. See equation 12.17 in TASS.";
fsubk[numE_, orbital_, NKSL_, NKSLp_, k_] := Module[
  {terms, S, L, Sp, Lp,
  termsWithSameSpin, SL,
  fsubkVal, spinMultiplicity,
  prefactor, summand1, summand2},
  (
    {S, L}   = FindSL[NKSL];
    {Sp, Lp} = FindSL[NKSLp];
    terms    = AllowedNKSLTerms[numE];
    (* sum for summand1 is over terms with same spin *)
    spinMultiplicity  = 2*S + 1;
    termsWithSameSpin = StringCases[terms, ToString[spinMultiplicity] ~~ __];
    termsWithSameSpin = Flatten[termsWithSameSpin];
    If[Not[{S, L} == {Sp, Lp}],
      Return[0]
    ];
    prefactor = 1/2 * Abs[Ck[orbital, k]]^2;
    summand1 = Sum[(
        ReducedUkTable[{numE, orbital, SL, NKSL,  k}] *
        ReducedUkTable[{numE, orbital, SL, NKSLp, k}]
        ),
      {SL, termsWithSameSpin}
    ];
    summand1 = 1 / TPO[L] * summand1;
    summand2 = (
      KroneckerDelta[NKSL, NKSLp] *
        (numE *(4*orbital + 2 - numE)) /
        ((2*orbital + 1) * (4*orbital + 1))
      );
    fsubkVal = prefactor*(summand1 - summand2);
    Return[fsubkVal];
  )
];

fsupk::usage = "fsupk[numE, orbital, SL, SLp, k] gives the superscripted Slater integral f^k = Subscript[f, k] * Subscript[D, k].";
fsupk[numE_, orbital_, NKSL_, NKSLp_ ,k_] := (
  Dk[k] * fsubk[numE, orbital, NKSL, NKSLp, k]
  )

Dk::usage = "D[k] gives the ratio between the super-script and sub-scripted Slater integrals (F^k / F_k). k must be even. See table 6-3 in TASS, and also section 2-7 of Wybourne (1965). See also equation 6.41 in TASS.";
Dk[k_] := {1, 225, 1089, 184041/25}[[k/2+1]];

FtoE::usage = "FtoE[F0, F2, F4, F6] calculates the Racah parameters {E0, E1, E2, E3} corresponding to the given Slater integrals.
See eqn. 2-80 in Wybourne.
Note that in that equation the subscripted Slater integrals are used but since this function assumes the the input values are superscripted Slater integrals, it is necessary to convert them using Dk.";
FtoE[F0_, F2_, F4_, F6_] := Module[
  {E0, E1, E2, E3},
  (
    E0 = (F0 - 10*F2/Dk[2] - 33*F4/Dk[4] - 286*F6/Dk[6]);
    E1 = (70*F2/Dk[2] + 231*F4/Dk[4] + 2002*F6/Dk[6])/9;
    E2 = (F2/Dk[2] - 3*F4/Dk[4] + 7*F6/Dk[6])/9;
    E3 = (5*F2/Dk[2] + 6*F4/Dk[4] - 91*F6/Dk[6])/3;
    Return[{E0, E1, E2, E3}];
  )
];

EtoF::usage = "EtoF[E0, E1, E2, E3] calculates the Slater integral parameters {F0, F2, F4, F6} corresponding to the given Racah parameters {E0, E1, E2, E3}. This is the inverse of the FtoE function.";
```

```
EtoF[E0_, E1_, E2_, E3_] := Module[
  {F0, F2, F4, F6},
  (
    F0 = 1/7      (7 E0 + 9 E1);
    F2 = 75/14    (E1 + 143 E2 + 11 E3);
    F4 = 99/7     (E1 - 130 E2 + 4 E3);
    F6 = 5577/350 (E1 + 35 E2 - 7 E3);
    Return[{F0, F2, F4, F6}];
  )
];

Electrostatic::usage = "Electrostatic[{numE, NKSL, NKSLp}] returns
  the LS reduced matrix element for repulsion matrix element for
  equivalent electrons. See equation 2-79 in Wybourne (1965). The
  option \"Coefficients\" can be set to \"Slater\" or \"Racah\". If
  set to \"Racah\" then E_k parameters and e^k operators are assumed
  , otherwise the Slater integrals F^k and operators f_k. The
  default is \"Slater\".";
Options[Electrostatic] = {"Coefficients" -> "Slater"};
Electrostatic[{numE_, NKSL_, NKSLp_}, OptionsPattern[]] := Module[
  {fsub0, fsub2, fsub4, fsub6,
   esub0, esub1, esub2, esub3,
   fsup0, fsup2, fsup4, fsup6,
   eMatrixVal, orbital},
  (
    orbital = 3;
    Which[
      OptionValue["Coefficients"] == "Slater",
      (
        fsub0 = fsubk[numE, orbital, NKSL, NKSLp, 0];
        fsub2 = fsubk[numE, orbital, NKSL, NKSLp, 2];
        fsub4 = fsubk[numE, orbital, NKSL, NKSLp, 4];
        fsub6 = fsubk[numE, orbital, NKSL, NKSLp, 6];
        eMatrixVal = fsub0*F0 + fsub2*F2 + fsub4*F4 + fsub6*F6;
      ),
      OptionValue["Coefficients"] == "Racah",
      (
        fsup0 = fsupk[numE, orbital, NKSL, NKSLp, 0];
        fsup2 = fsupk[numE, orbital, NKSL, NKSLp, 2];
        fsup4 = fsupk[numE, orbital, NKSL, NKSLp, 4];
        fsup6 = fsupk[numE, orbital, NKSL, NKSLp, 6];
        esub0 = fsup0;
        esub1 = 9/7*fsup0 +   1/42*fsup2 +   1/77*fsup4 +  1/462*
  fsup6;
        esub2 =             143/42*fsup2 - 130/77*fsup4 + 35/462*
  fsup6;
        esub3 =              11/42*fsup2 + 4/77*fsup4   -  7/462*
  fsup6;
        eMatrixVal = esub0*E0 + esub1*E1 + esub2*E2 + esub3*E3;
      )
    ];
    Return[eMatrixVal];
  )
];

GenerateElectrostaticTable::usage = "GenerateElectrostaticTable[
  numEmax] can be used to generate the table for the electrostatic
  interaction from f^1 to f^numEmax. If the option \"Export\" is set
   to True then the resulting data is saved to ./data/
  ElectrostaticTable.m.";
Options[GenerateElectrostaticTable] = {"Export" -> True, "
  Coefficients" -> "Slater"};
GenerateElectrostaticTable[numEmax_Integer:7, OptionsPattern[]] :=
  (
   ElectrostaticTable = Table[
     {numE, SL, SpLp} -> SimplifyFun[Electrostatic[{numE, SL, SpLp},
    "Coefficients" -> OptionValue["Coefficients"]]],
     {numE, 1, numEmax},
     {SL, AllowedNKSLTerms[numE]},
     {SpLp, AllowedNKSLTerms[numE]}
   ];
   ElectrostaticTable = Association[Flatten[ElectrostaticTable]];
   If[OptionValue["Export"],
     Export[FileNameJoin[{moduleDir, "data", "ElectrostaticTable.m"
  }],
     ElectrostaticTable];
```

```
    ];
    Return[ElectrostaticTable];
  );

  (* ###################### Electrostatic ###################### *)
  (* ########################################################### *)

  (* ########################################################### *)
  (* ########################## Bases ########################## *)

  BasisTableGenerator::usage = "BasisTableGenerator[numE] returns an
    association whose keys are triples of the form {numE, J} and whose
     values are lists having the basis elements that correspond to {
    numE, J}.";
  BasisTableGenerator[numE_] := Module[
    {energyStatesTable, allowedJ, J, Jp},
    (
      energyStatesTable = <||>;
      allowedJ = AllowedJ[numE];
      Do[
      (
        energyStatesTable[{numE, J}] = EnergyStates[numE, J];
      ),
      {Jp, allowedJ},
      {J,  allowedJ}];
      Return[energyStatesTable]
    )
  ];

  BasisLSJMJ::usage = "BasisLSJMJ[numE] returns the ordered basis in
    L-S-J-MJ with the total orbital angular momentum L and total spin
    angular momentum S coupled together to form J. The function
    returns a list with each element representing the quantum numbers
    for each basis vector. Each element is of the form {SL (string in
    spectroscopic notation),J, MJ}.
  The option \"AsAssociation\" can be set to True to return the basis
     as an association with the keys corresponding to values of J and
    the values lists with the corresponding {L, S, J, MJ} list. The
    default of this option is False.
  ";
  Options[BasisLSJMJ] = {"AsAssociation" -> False};
  BasisLSJMJ[numE_, OptionsPattern[]] := Module[
    {energyStatesTable, basis, idx1},
    (
      energyStatesTable = BasisTableGenerator[numE];
      basis = Table[
        energyStatesTable[{numE, AllowedJ[numE][[idx1]]}],
        {idx1, 1, Length[AllowedJ[numE]]}];
      basis = Flatten[basis, 1];
      If[OptionValue["AsAssociation"],
        (
          Js    = AllowedJ[numE];
          basis = Table[(J -> Select[basis, #[[2]] == J &]), {J, Js
    }];
          basis = Association[basis];
        )
      ];
      Return[basis]
    )
  ];

  BasisLSJ::usage = "BasisLSJ[numE] returns the level basis LSJ. The
    function returns a list with each element representing the quantum
     numbers for each basis vector. Each element is of the form {SL (
    string in spectroscopic notation), J}.
  The option \"AsAssociation\" can be set to True to return the basis
     as an association with the keys being the allowed J values. The
    default is False.
    ";
  Options[BasisLSJ]={"AsAssociation"->False};
  BasisLSJ[numE_,OptionsPattern[]] := Module[
    {Js, basis},
    (
      Js    = AllowedJ[numE];
      basis = BasisLSJMJ[numE,"AsAssociation"->False];
      basis = DeleteDuplicates[{#[[1]],#[[2]]}& /@ basis];
```

```
    If[OptionValue["AsAssociation"],
      (
        basis = Association @ Table[(J->Select[basis,#[[2]]==J&]),{J,Js}]
      )
    ];
    Return[basis];
  )
];

(* ########################## Bases ########################## *)
(* ########################################################### *)

(* ############################################################ *)
(* ########### Coefficients of Fracional Parentage ########### *)

GenerateCFP::usage = "GenerateCFP[] generates the association for the coefficients of fractional parentage. Result is exported to the file ./data/CFP.m. The coefficients of fractional parentage are taken beyond the half-filled shell using the phase convention determined by the option \"PhaseFunction\". The default is \"NK\" which corresponds to the phase convention of Nielson and Koster. The other option is \"Judd\" which corresponds to the phase convention of Judd.";
Options[GenerateCFP] = {"Export" -> True, "PhaseFunction"-> "NK"};
GenerateCFP[OptionsPattern[]] := (
  CFP = Table[
    {numE, NKSL} -> First[CFPTerms[numE, NKSL]],
    {numE, 1, 7},
    {NKSL, AllowedNKSLTerms[numE]}];
  CFP = Association[CFP];
  (* Go all the way to f14 *)
  CFP = CFPExpander["Export" -> False, "PhaseFunction"->OptionValue["PhaseFunction"]];
  If[OptionValue["Export"],
    Export[FileNameJoin[{moduleDir, "data", "CFPs.m"}], CFP];
  ];
  Return[CFP];
);

JuddCFPPhase::usage = "Phase between conjugate coefficients of fractional parentage according to Velkov's thesis, page 40.";
JuddCFPPhase[parent_, parentS_, parentL_, daughterS_, daughterL_, parentSeniority_, daughterSeniority_] := Module[
  {spin, orbital, expo, phase},
  (
    {spin, orbital} = {1/2, 3};
    expo = (
        (parentS + parentL + daughterS + daughterL) -
        (orbital + spin) +
        1/2 * (parentSeniority + daughterSeniority - 1)
    );
    phase = Phaser[-expo];
    Return[phase];
  )
];

NKCFPPhase::usage = "Phase between conjugate coefficients of fractional parentage according to Nielson and Koster page viii. Note that there is a typo on there the expression for zeta should be (-1)^((v-1)/2) instead of (-1)^(v - 1/2).";
NKCFPPhase[parent_, parentS_, parentL_, daughterS_, daughterL_, parentSeniority_, daughterSeniority_] := Module[
  {spin, orbital, expo, phase},
  (
    {spin, orbital} = {1/2, 3};
    expo = (
        (parentS + parentL + daughterS + daughterL) -
        (orbital + spin)
    );
    phase = Phaser[-expo];
    If[parent == 2*orbital,
        phase = phase * Phaser[(daughterSeniority-1)/2]];
    Return[phase];
  )
];
```

```
919
920 Options[CFPExpander] = {"Export" -> True, "PhaseFunction" -> "NK"};
921 CFPExpander::usage = "Using the coefficients of fractional
      parentage up to f7 this function calculates them up to f14.
922 The coefficients of fractional parentage are taken beyond the half-
      filled shell using the phase convention determined by the option \
      "PhaseFunction\". The default is \"NK\" which corresponds to the
      phase convention of Nielson and Koster. The other option is \"Judd
      \" which corresponds to the phase convention of Judd. The result
      is exported to the file ./data/CFPs_extended.m.";
923 CFPExpander[OptionsPattern[]] := Module[
924   {orbital, halfFilled, fullShell, parentMax, PhaseFun,
925   complementaryCFPs, daughter, conjugateDaughter,
926   conjugateParent, parentTerms, daughterTerms,
927   parentCFPs, daughterSeniority, daughterS, daughterL,
928   parentCFP, parentTerm, parentCFPval,
929   parentS, parentL, parentSeniority, phase, prefactor,
930   newCFPval, key, extendedCFPs, exportFname},
931   (
932     orbital    = 3;
933     halfFilled = 2 * orbital + 1;
934     fullShell  = 2 * halfFilled;
935     parentMax  = 2 * orbital;
936
937     PhaseFun  = <|
938         "Judd" -> JuddCFPPhase,
939         "NK" -> NKCFPPhase|>[OptionValue["PhaseFunction"]];
940     PrintTemporary["Calculating CFPs using the phase system from ",
     PhaseFun];
941     (* Initialize everything with lists to be filled in the next Do
    *)
942     complementaryCFPs =
943         Table[
944         ({numE, term} -> {term}),
945         {numE, halfFilled + 1, fullShell - 1, 1},
946         {term, AllowedNKSLTerms[numE]
947         }];
948     complementaryCFPs = Association[Flatten[complementaryCFPs]];
949     Do[(
950         daughter          = parent + 1;
951         conjugateDaughter = fullShell - parent;
952         conjugateParent   = conjugateDaughter - 1;
953         parentTerms       = AllowedNKSLTerms[parent];
954         daughterTerms     = AllowedNKSLTerms[daughter];
955         Do[
956         (
957             parentCFPs             = Rest[CFP[{daughter,
    daughterTerm}]];
958           daughterSeniority      = Seniority[daughterTerm];
959           {daughterS, daughterL} = FindSL[daughterTerm];
960           Do[
961           (
962               {parentTerm, parentCFPval} = parentCFP;
963               {parentS, parentL}         = FindSL[parentTerm];
964               parentSeniority            = Seniority[parentTerm];
965               phase = PhaseFun[parent, parentS, parentL,
966                                daughterS, daughterL,
967                                parentSeniority, daughterSeniority
    ];
968               prefactor = (daughter * TPO[daughterS, daughterL])
    /
969                           (conjugateDaughter * TPO[parentS,
    parentL]);
970               prefactor = Sqrt[prefactor];
971               newCFPval = phase * prefactor * parentCFPval;
972               key = {conjugateDaughter, parentTerm};
973               complementaryCFPs[key] = Append[complementaryCFPs[
    key], {daughterTerm, newCFPval}]
974           ),
975           {parentCFP, parentCFPs}
976           ]
977       ),
978       {daughterTerm, daughterTerms}
979       ]
980       ),
981     {parent, 1, parentMax}
```

```
982       ];
983
984       complementaryCFPs[{14, "1S"}] = {"1S", {"2F",1}};
985       extendedCFPs         = Join[CFP, complementaryCFPs];
986       If[OptionValue["Export"];,
987       (
988           exportFname = FileNameJoin[{moduleDir, "data", "
      CFPs_extended.m"}];
989           Print["Exporting to ", exportFname];
990           Export[exportFname, extendedCFPs];
991       )
992       ];
993       Return[extendedCFPs];
994   )
995   ];
996
997   GenerateCFPTable::usage = "GenerateCFPTable[] generates the table
        for the coefficients of fractional parentage. If the optional
        parameter \"Export\" is set to True then the resulting data is
        saved to ./data/CFPTable.m.
998   The data being parsed here is the file attachment B1F_ALL.TXT which
         comes from Velkov's thesis.";
999   Options[GenerateCFPTable] = {"Export" -> True};
1000  GenerateCFPTable[OptionsPattern[]] := Module[
1001    {rawText, rawLines, leadChar, configIndex, line, daughter,
1002    lineParts, numberCode, parsedNumber, toAppend, CFPTablefname},
1003    (
1004      CleanWhitespace[string_]      := StringReplace[string,
      RegularExpression["\\s+"]->" "];
1005      AddSpaceBeforeMinus[string_] := StringReplace[string,
      RegularExpression["(?<!\\s)-"]->" -"];
1006      ToIntegerOrString[list_]      := Map[If[StringMatchQ[#,
      NumberString], ToExpression[#], #] &, list];
1007      CFPTable       = ConstantArray[{},7];
1008      CFPTable[[1]] = {{"2F",{"1S",1}}};
1009
1010      (* Cleaning before processing is useful *)
1011      rawText  = Import[FileNameJoin[{moduleDir, "data", "B1F_ALL.TXT
      "}]];
1012      rawLines = StringTrim/@StringSplit[rawText,"\n"];
1013      rawLines = Select[rawLines,#!=""&];
1014      rawLines = CleanWhitespace/@rawLines;
1015      rawLines = AddSpaceBeforeMinus/@rawLines;
1016
1017      Do[(
1018        (* the first character can be used to identify the start of a
       block *)
1019        leadChar=StringTake[line,{1}];
1020        (* ..FN, N is at position 50 in that line *)
1021        If[leadChar=="[",
1022        (
1023          configIndex=ToExpression[StringTake[line,{50}]];
1024          Continue[];
1025        )
1026        ];
1027        (* Identify which daughter term is being listed *)
1028        If[StringContainsQ[line,"[DAUGHTER TERM]"],
1029          daughter=StringSplit[line,"["][[1]];
1030          CFPTable[[configIndex]]=Append[CFPTable[[configIndex]],{
      daughter}];
1031          Continue[];
1032        ];
1033        (* Once we get here we are already parsing a row with
      coefficient data *)
1034        lineParts    = StringSplit[line," "];
1035        parent       = lineParts[[1]];
1036        numberCode   = ToIntegerOrString[lineParts[[3;;]]];
1037        parsedNumber = SquarePrimeToNormal[numberCode];
1038        toAppend     = {parent,parsedNumber};
1039        CFPTable[[configIndex]][[-1]] = Append[CFPTable[[configIndex
      ]][[-1]], toAppend]
1040      ),
1041      {line,rawLines}];
1042      If[OptionValue["Export"],
1043        (
1044        CFPTablefname = FileNameJoin[{moduleDir, "data", "CFPTable.m"
```

```
  }];
1045        Export[CFPTablefname, CFPTable];
1046        )
1047      ];
1048      Return[CFPTable];
1049    )
1050  ];
1051
1052  GenerateCFPAssoc::usage = "GenerateCFPAssoc[export] converts the
      coefficients of fractional parentage into an association in which
      zero values are explicit. If \"Export\" is set to True, the
      association is exported to the file /data/CFPAssoc.m. This
      function requires that the association CFP be defined.";
1053  Options[GenerateCFPAssoc] = {"Export" -> True};
1054  GenerateCFPAssoc[OptionsPattern[]] := (
1055    CFPAssoc = Association[];
1056    Do[
1057      (daughterTerms = AllowedNKSLTerms[numE];
1058      parentTerms    = AllowedNKSLTerms[numE - 1];
1059      Do[
1060        (
1061        cfps = CFP[{numE, daughter}];
1062        cfps = cfps[[2 ;;]];
1063        parents = First /@ cfps;
1064        Do[
1065          (
1066          key = {numE, daughter, parent};
1067          cfp = If[
1068            MemberQ[parents, parent],
1069            (
1070              idx = Position[parents, parent][[1, 1]];
1071              cfps[[idx]][[2]]
1072            ),
1073            0
1074            ];
1075          CFPAssoc[key] = cfp;
1076          ),
1077          {parent, parentTerms}
1078          ]
1079        ),
1080        {daughter, daughterTerms}
1081        ]
1082      ),
1083      {numE, 1, 14}
1084      ];
1085    If[OptionValue["Export"],
1086      (
1087      CFPAssocfname = FileNameJoin[{moduleDir, "data", "CFPAssoc.m"
      }];
1088      Export[CFPAssocfname, CFPAssoc];
1089      )
1090    ];
1091    Return[CFPAssoc];
1092  );
1093
1094  CFPTerms::usage = "CFPTerms[numE] gives all the daughter and parent
       terms, together with the corresponding coefficients of fractional
       parentage, that correspond to the the f^n configuration.
1095  CFPTerms[numE, SL] gives all the daughter and parent terms,
      together with the corresponding coefficients of fractional
      parentage, that are compatible with the given string SL in the f^n
       configuration.
1096  CFPTerms[numE, L, S] gives all the daughter and parent terms,
      together with the corresponding coefficients of fractional
      parentage, that correspond to the given total orbital angular
      momentum L and total spin S n the f^n configuration. L being an
      integer, and S being integer or half-integer.
1097  In all cases the output is in the shape of a list with enclosed
      lists having the format {daughter_term, {parent_term_1, CFP_1}, {
      parent_term_2, CFP_2}, ...}.
1098  Only the one-body coefficients for f-electrons are provided.
1099  In all cases it must be that 1 <= n <= 7.
1100  These are according to the tables from Nielson & Koster.
1101  ";
1102  CFPTerms[numE_] := Part[CFPTable, numE]
1103  CFPTerms[numE_, SL_] := Module[
```

```
    {NKterms, CFPconfig},
    (
      NKterms   = {{}};
      CFPconfig = CFPTable[[numE]];
      Map[
        If[StringFreeQ[First[#], SL],
          Null,
          NKterms = Join[NKterms, {#}, 1]
        ] &,
      CFPconfig
      ];
      NKterms = DeleteCases[NKterms, {}]
    )
  ];
  CFPTerms[numE_, L_, S_] := Module[
  {NKterms, SL, CFPconfig},
  (
    SL = StringJoin[ToString[2 S + 1], PrintL[L]];
    NKterms = {{}};
    CFPconfig = Part[CFPTable, numE];
    Map[
      If[StringFreeQ[First[#], SL],
        Null,
        NKterms = Join[NKterms, {#}, 1]
      ]&,
    CFPconfig
    ];
    NKterms = DeleteCases[NKterms, {}]
  )
  ];

  (* ############ Coefficients of Fracional Parentage ############ *)
  (* ############################################################## *)

  (* ############################################################## *)
  (* ######################## Spin Orbit ########################## *)

  SpinOrbit::usage = "SpinOrbit[numE, SL, SpLp, J] returns the LSJ
    reduced matrix element ζ <SL, J|L.S|SpLp, J>. These are given as a
     function of ζ. This function requires that the association
    ReducedV1kTable be defined.
  See equations 2-106 and 2-109 in Wybourne (1965). Equivalently see
    eqn. 12.43 in TASS.";
  SpinOrbit[numE_, SL_, SpLp_, J_] := Module[
    {S, L, Sp, Lp, orbital, sign, prefactor, val},
    (
      orbital   = 3;
      {S, L}    = FindSL[SL];
      {Sp, Lp}  = FindSL[SpLp];
      prefactor = Sqrt[orbital * (orbital+1) * (2*orbital+1)] *
                  SixJay[{L, Lp, 1}, {Sp, S, J}];
      sign      = Phaser[J + L + Sp];
      val       = sign * prefactor * ζ * ReducedV1kTable[{numE, SL,
    SpLp, 1}];
      Return[val];
    )
  ];

  GenerateSpinOrbitTable::usage = "GenerateSpinOrbitTable[nmax]
    computes the matrix elements for the spin-orbit interaction for f^
    n configurations up to n = nmax. The function returns an
    association whose keys are lists of the form {n, SL, SpLp, J}. If
    export is set to True, then the result is exported to the data
    subfolder for the folder in which this package is in. It requires
    ReducedV1kTable to be defined.";
  Options[GenerateSpinOrbitTable] = {"Export" -> True};
  GenerateSpinOrbitTable[nmax_Integer:7, OptionsPattern[]] := Module[
    {numE, J, SL, SpLp, exportFname},
    (
      SpinOrbitTable =
        Table[
          {numE, SL, SpLp, J} -> SpinOrbit[numE, SL, SpLp, J],
        {numE, 1, nmax},
        {J, MinJ[numE], MaxJ[numE]},
        {SL,   Map[First, AllowedNKSLforJTerms[numE, J]]},
        {SpLp, Map[First, AllowedNKSLforJTerms[numE, J]]}
```

```
        ];
      SpinOrbitTable = Association[SpinOrbitTable];

      exportFname = FileNameJoin[{moduleDir, "data", "SpinOrbitTable.m"}];
      If[OptionValue["Export"],
        (
          Print["Exporting to file "<>ToString[exportFname]];
          Export[exportFname, SpinOrbitTable];
        )
      ];
      Return[SpinOrbitTable];
    )
  ];

  (* ###################### Spin Orbit ########################### *)
  (* ############################################################ *)

  (* ############################################################ *)
  (* ################## Three Body Operators ################### *)

  ParseJudd1984::usage = "This function parses the data from tables 1 and 2 of Judd from Judd, BR, and MA Suskin. \"Complete Set of Orthogonal Scalar Operators for the Configuration f^3\". JOSA B 1, no. 2 (1984): 261-65.";
  Options[ParseJudd1984] = {"Export" -> False};
  ParseJudd1984[OptionsPattern[]] := (
    ParseJuddTab1[str_] := (
      strR = ToString[str];
      strR = StringReplace[strR, ".5" -> "^(1/2)"];
      num = ToExpression[strR];
      sign = Sign[num];
      num = sign*Simplify[Sqrt[num^2]];
      If[Round[num] == num, num = Round[num]];
      Return[num]);

    (* Parse table 1 from Judd 1984 *)
    judd1984Fname1 = FileNameJoin[{moduleDir, "data", "Judd1984-1.csv"}];
    data = Import[judd1984Fname1, "CSV", "Numeric" -> False];
    headers = data[[1]];
    data = data[[2 ;;]];
    data = Transpose[data];
    \[Psi] = Select[data[[1]], # != "" &];
    \[Psi]p = Select[data[[2]], # != "" &];
    matrixKeys = Transpose[{\[Psi], \[Psi]p}];
    data = data[[3 ;;]];
    cols = Table[ParseJuddTab1 /@ Select[col, # != "" &], {col, data}];
    cols = Select[cols, Length[#] == 21 &];
    tab1 = Prepend[Prepend[cols, \[Psi]p], \[Psi]];
    tab1 = Transpose[Prepend[Transpose[tab1], headers]];

    (* Parse table 2 from Judd 1984 *)
    judd1984Fname2 = FileNameJoin[{moduleDir, "data", "Judd1984-2.csv"}];
    data = Import[judd1984Fname2, "CSV", "Numeric" -> False];
    headers = data[[1]];
    data = data[[2 ;;]];
    data = Transpose[data];
    {operatorLabels, WUlabels, multiFactorSymbols, multiFactorValues} = data[[;; 4]];
    multiFactorValues = ParseJuddTab1 /@ multiFactorValues;
    multiFactorValues = AssociationThread[multiFactorSymbols -> multiFactorValues];

    (*scale values of table 1 given the values in table 2*)
    oppyS = {};
    normalTable =
      Table[header = col[[1]];
        If[StringContainsQ[header, " "],
          (
            multiplierSymbol = StringSplit[header, " "][[1]];
            multiplierValue = multiFactorValues[multiplierSymbol];
            operatorSymbol = StringSplit[header, " "][[2]];
            oppyS = Append[oppyS, operatorSymbol];
```

```
1236            ),
1237            (
1238              multiplierValue = 1;
1239              operatorSymbol = header;
1240            )
1241          ];
1242          normalValues = 1/multiplierValue*col[[2 ;;]];
1243          Join[{operatorSymbol}, normalValues], {col, tab1[[3 ;;]]}
1244        ];
1245
1246      (*Create an association for the reduced matrix elements in the f
        ^3 config*)
1247      juddOperators = Association[];
1248      Do[(
1249        col      = normalTable[[colIndex]];
1250        opLabel  = col[[1]];
1251        opValues = col[[2 ;;]];
1252        opMatrix = AssociationThread[matrixKeys -> opValues];
1253        Do[(
1254          opMatrix[Reverse[mKey]] = opMatrix[mKey]
1255          ),
1256        {mKey, matrixKeys}
1257        ];
1258        juddOperators[{3, opLabel}] = opMatrix),
1259        {colIndex, 1, Length[normalTable]}
1260      ];
1261
1262      (* special case of t2 in f3 *)
1263      (* this is the same as getting the reduced matrix elements from
        Judd 1966 *)
1264      numE = 3;
1265      e3Op       = juddOperators[{3, "e_{3}"}];
1266      t2prime    = juddOperators[{3, "t_{2}^{'}"}];
1267      prefactor = 1/(70 Sqrt[2]);
1268      t2Op = (# -> (t2prime[#] + prefactor*e3Op[#])) & /@ Keys[t2prime
        ];
1269      t2Op = Association[t2Op];
1270      juddOperators[{3, "t_{2}"}] = t2Op;
1271
1272      (*Special case of t11 in f3*)
1273      t11 = juddOperators[{3, "t_{11}"}];
1274      eβprimeOp = juddOperators[{3, "e_{\\beta}^{'}"}];
1275      t11primeOp = (# -> (t11[#] + Sqrt[3/385] eβprimeOp[#])) & /@ Keys
        [t11];
1276      t11primeOp = Association[t11primeOp];
1277      juddOperators[{3, "t_{11}^{'}"}] = t11primeOp;
1278      If[OptionValue["Export"],
1279        (
1280          (*export them*)
1281          PrintTemporary["Exporting ..."];
1282          exportFname = FileNameJoin[{moduleDir, "data", "juddOperators
            .m"}];
1283          Export[exportFname, juddOperators];
1284        )
1285      ];
1286      Return[juddOperators];
1287    );
1288
1289    GenerateThreeBodyTables::usage = "This function generates the
        reduced matrix elements for the three body operators using the
        coefficients of fractional parentage, including those beyond f^7."
        ;
1290    Options[GenerateThreeBodyTables] = {"Export" -> False};
1291    GenerateThreeBodyTables[OptionsPattern[]] := (
1292      tiKeys        = (StringReplace[ToString[#], {"T" -> "t_{", "p" ->
        "}^{'"}] <> "}") & /@ TSymbols;
1293      TSymbolsAssoc = AssociationThread[tiKeys -> TSymbols];
1294      juddOperators = ParseJudd1984[];
1295      (* op3MatrixElement[SL, SpLp, opSymbol] returns the value for the
        reduced matrix element of the operator opSymbol for the terms {SL
        , SpLp} in the f^3 configuration. *)
1296      op3MatrixElement[SL_, SpLp_, opSymbol_] := (
1297        jOP = juddOperators[{3, opSymbol}];
1298        key = {SL, SpLp};
1299        val = If[MemberQ[Keys[jOP], key],
1300          jOP[key],
```

```
1301          0];
1302        Return[val];
1303      );
1304      (* ti: This is the implementation of formula (2) in Judd & Suskin
           1984. It computes the reduced matrix elements of ti in f^n by
          using the reduced matrix elements in f^3 and the coefficients of
          fractional parentage. If the option \"Fast\" is set to True then
          the values for n>7 are simply computed as the negatives of the
          values in the complementary configuration; this except for t2 and
          t11 which are treated as special cases. *)
1305      Options[ti] = {"Fast" -> True};
1306      ti[nE_, SL_, SpLp_, tiKey_, opOrder_ : 3, OptionsPattern[]] :=
          Module[
1307        {nn, S, L, Sp, Lp,
1308        cfpSL, cfpSpLp,
1309        parentSL, parentSpLp,
1310        tnk, tnks},
1311        (
1312          {S, L}   = FindSL[SL];
1313          {Sp, Lp} = FindSL[SpLp];
1314          fast     = OptionValue["Fast"];
1315          numH     = 14 - nE;
1316          If[fast && Not[MemberQ[{"t_{2}","t_{11}"},tiKey]] && nE > 7,
1317            Return[-tktable[{numH, SL, SpLp, tiKey}]]
1318          ];
1319          If[(S == Sp && L == Lp),
1320          (
1321            cfpSL   = CFP[{nE, SL}];
1322            cfpSpLp = CFP[{nE, SpLp}];
1323            tnks = Table[(
1324                parentSL   = cfpSL[[nn, 1]];
1325                parentSpLp = cfpSpLp[[mm, 1]];
1326                cfpSL[[nn, 2]] * cfpSpLp[[mm, 2]] *
1327                tktable[{nE - 1, parentSL, parentSpLp, tiKey}]
1328                ),
1329                {nn, 2, Length[cfpSL]},
1330                {mm, 2, Length[cfpSpLp]}
1331                ];
1332            tnk = Total[Flatten[tnks]];
1333            ),
1334          tnk = 0;
1335          ];
1336          Return[ nE / (nE - opOrder) * tnk];
1337        )
1338      ];
1339      (* Calculate the reduced matrix elements of t^i for n up to 14 *)
1340      tktable = <||>;
1341      Do[(
1342        Do[(
1343          tkValue = Which[numE <= 2,
1344            (*Initialize n=1,2 with zeros*)
1345            0,
1346            numE == 3,
1347            (* Grab matrix elem in f^3 from Judd 1984 *)
1348            SimplifyFun[op3MatrixElement[SL, SpLp, opKey]],
1349            True,
1350            SimplifyFun[ti[numE, SL, SpLp, opKey, If[opKey == "e_{3}",
          2, 3]]]
1351            ];
1352          tktable[{numE, SL, SpLp, opKey}] = tkValue;
1353          ),
1354        {SL, AllowedNKSLTerms[numE]},
1355        {SpLp, AllowedNKSLTerms[numE]},
1356        {opKey, Append[tiKeys, "e_{3}"]}
1357        ];
1358        PrintTemporary[StringJoin["\[ScriptF]", ToString[numE], "
          configuration complete"]];
1359        ),
1360        {numE, 1, 14}
1361      ];
1362
1363      (* Now use those reduced matrix elements to determine their sum
          as weighted by their corresponding strengths Ti *)
1364      ThreeBodyTable = <||>;
1365      Do[
1366        Do[
```

```
      (
        ThreeBodyTable[{numE, SL, SpLp}] = (
          Sum[(
            If[tiKey == "t_{2}", t2Switch, 1] *
            tktable[{numE, SL, SpLp, tiKey}] *
            TSymbolsAssoc[tiKey] +
            If[tiKey == "t_{2}", 1 - t2Switch, 0] *
            (-tktable[{14 - numE, SL, SpLp, tiKey}]) *
            TSymbolsAssoc[tiKey]
            ),
          {tiKey, tiKeys}
          ]
        );
      ),
      {SL, AllowedNKSLTerms[numE]},
      {SpLp, AllowedNKSLTerms[numE]}
      ];
    PrintTemporary[StringJoin["\[ScriptF]", ToString[numE], " matrix
    complete"]];,
    {numE, 1, 7}
    ];

    ThreeBodyTables = Table[(
      terms = AllowedNKSLTerms[numE];
      singleThreeBodyTable =
        Table[
          {SL, SLp} -> ThreeBodyTable[{numE, SL, SLp}],
          {SL, terms},
          {SLp, terms}
        ];
      singleThreeBodyTable  = Flatten[singleThreeBodyTable];
      singleThreeBodyTables = Table[(
          notNullPosition = Position[TSymbols, notNullSymbol][[1,
    1]];
          reps = ConstantArray[0, Length[TSymbols]];
          reps[[notNullPosition]] = 1;
          rep = AssociationThread[TSymbols -> reps];
          notNullSymbol -> Association[(singleThreeBodyTable /. rep)]
          ),
        {notNullSymbol, TSymbols}
        ];
      singleThreeBodyTables = Association[singleThreeBodyTables];
      numE -> singleThreeBodyTables),
      {numE, 1, 7}
  ];

  ThreeBodyTables = Association[ThreeBodyTables];
  If[OptionValue["Export"],
    (
      threeBodyTablefname = FileNameJoin[{moduleDir, "data", "
    ThreeBodyTable.m"}];
      Export[threeBodyTablefname, ThreeBodyTable];
      threeBodyTablesfname = FileNameJoin[{moduleDir, "data", "
    ThreeBodyTables.m"}];
      Export[threeBodyTablesfname, ThreeBodyTables];
    )
   ];
  Return[{ThreeBodyTable, ThreeBodyTables}];
  );

  ScalarOperatorProduct::usage = "ScalarOperatorProduct[op1, op2,
    numE] calculated the innerproduct between the two scalar operators
     op1 and op2.";
  ScalarOperatorProduct[op1_, op2_, numE_] := Module[
    {terms, S, L, factor, term1, term2},
    (
      terms = AllowedNKSLTerms[numE];
      Simplify[
        Sum[(
          {S, L} = FindSL[term1];
          factor = TPO[S, L];
          factor * op1[{term1, term2}] * op2[{term2, term1}]
          ),
        {term1, terms},
        {term2, terms}
        ]
```

```
      ]
    )
];

(* ################## Three Body Operators ###################### *)
(* ############################################################## *)

(* ############################################################## *)
(* ################### Reduced SOO and ECSO ##################### *)

ReducedT11inf2::usage = "ReducedT11inf2[SL, SpLp] returns the
  reduced matrix element of the scalar component of the double
  tensor T11 for the given SL terms SL, SpLp.
Data used here for m0, m2, m4 is from Table II of Judd, BR, HM
  Crosswhite, and Hannah Crosswhite. Intra-Atomic Magnetic
  Interactions for f Electrons. Physical Review 169, no. 1 (1968):
  130.
";
ReducedT11inf2[SL_, SpLp_] := Module[
  {T11inf2},
  (
    T11inf2 = <|
      {"1S", "3P"} -> 6 M0 + 2 M2 + 10/11 M4,
      {"3P", "3P"} -> -36 M0 - 72 M2 - 900/11 M4,
      {"3P", "1D"} -> -Sqrt[(2/15)] (27 M0 + 14 M2 + 115/11 M4),
      {"1D", "3F"} -> Sqrt[2/5] (23 M0 + 6 M2 - 195/11 M4),
      {"3F", "3F"} -> 2 Sqrt[14] (-15 M0 - M2 + 10/11 M4),
      {"3F", "1G"} -> Sqrt[11] (-6 M0 + 64/33 M2 - 1240/363 M4),
      {"1G", "3H"} -> Sqrt[2/5] (39 M0 - 728/33 M2 - 3175/363 M4),
      {"3H", "3H"} -> 8/Sqrt[55] (-132 M0 + 23 M2 + 130/11 M4),
      {"3H", "1I"} -> Sqrt[26] (-5 M0 - 30/11 M2 - 375/1573 M4)
      |>;
    Which[
      MemberQ[Keys[T11inf2],{SL,SpLp}],
        Return[T11inf2[{SL,SpLp}]],
      MemberQ[Keys[T11inf2],{SpLp,SL}],
        Return[T11inf2[{SpLp,SL}]],
      True,
        Return[0]
      ]
  )
];

Reducedt11inf2::usage = "Reducedt11inf2[SL, SpLp] returns the
  reduced matrix element in f^2 of the double tensor operator t11
  for the corresponding given terms {SL, SpLp}.
Values given here are those from Table VII of \"Judd, BR, HM
  Crosswhite, and Hannah Crosswhite. \"Intra-Atomic Magnetic
  Interactions for f Electrons.\" Physical Review 169, no. 1 (1968):
   130.\"
";
Reducedt11inf2[SL_, SpLp_] := Module[
  {t11inf2},
  (
    t11inf2 = <|
      {"1S", "3P"} -> -2 P0 - 105 P2 - 231 P4 - 429 P6,
      {"3P", "3P"} -> -P0 - 45 P2 - 33 P4 + 1287 P6,
      {"3P", "1D"} -> Sqrt[15/2] (P0 + 32 P2 - 33 P4 - 286 P6),
      {"1D", "3F"} -> Sqrt[10] (-P0 - 9/2 P2 + 66 P4 - 429/2 P6),
      {"3F", "3F"} -> Sqrt[14] (-P0 + 10 P2 + 33 P4 + 286 P6),
      {"3F", "1G"} -> Sqrt[11] (P0 - 20 P2 + 32 P4 - 104 P6),
      {"1G", "3H"} -> Sqrt[10] (-P0 + 55/2 P2 - 23 P4 - 65/2 P6),
      {"3H", "3H"} -> Sqrt[55] (-P0 + 25 P2 + 51 P4 + 13 P6),
      {"3H", "1I"} -> Sqrt[13/2] (P0 - 21 P4 - 6 P6)
      |>;
    Which[
      MemberQ[Keys[t11inf2],{SL,SpLp}],
        Return[t11inf2[{SL,SpLp}]],
      MemberQ[Keys[t11inf2],{SpLp,SL}],
        Return[t11inf2[{SpLp,SL}]],
      True,
        Return[0]
    ]
  )
];
```

```
ReducedSOOandECSOinf2::usage = "ReducedSOOandECSOinf2[SL, SpLp]
  returns the reduced matrix element corresponding to the operator (
  T11 + t11 - a13 * z13 / 6) for the terms {SL, SpLp}. This
  combination of operators corresponds to the spin-other-orbit plus
  ECSO interaction.
The T11 operator corresponds to the spin-other-orbit interaction,
  and the t11 operator (associated with electrostatically-correlated
   spin-orbit) originates from configuration interaction analysis.
  To their sum a factor proportional to the operator z13 is
  subtracted since its effect is redundant to the spin-orbit
  interaction. The factor of 1/6 is not on Judd's 1968 paper, but it
   is on \"Chen, Xueyuan, Guokui Liu, Jean Margerie, and Michael F
  Reid. \"A Few Mistakes in Widely Used Data Files for Fn
  Configurations Calculations.\" Journal of Luminescence 128, no. 3
  (2008): 421-27\".
The values for the reduced matrix elements of z13 are obtained from
   Table IX of the same paper. The value for a13 is from table VIII.
Rigurously speaking the Pk parameters here are subscripted. The
  conversion to superscripted parameters is performed elsewhere with
   the Prescaling replacement rules.
";
ReducedSOOandECSOinf2[SL_, SpLp_]  := Module[
  {a13, z13, z13inf2, matElement, redSOOandECSOinf2},
  (
    a13 = (-33 M0 + 3 M2 + 15/11 M4 -
          6 P0 + 3/2 (35 P2 + 77 P4 + 143 P6));
    z13inf2 = <|
        {"1S","3P"} -> 2,
        {"3P","3P"} -> 1,
        {"3P","1D"} -> -Sqrt[(15/2)],
        {"1D","3F"} -> Sqrt[10],
        {"3F","3F"} -> Sqrt[14],
        {"3F","1G"} -> -Sqrt[11],
        {"1G","3H"} -> Sqrt[10],
        {"3H","3H"} -> Sqrt[55],
        {"3H","1I"} -> -Sqrt[(13/2)]
        |>;
    matElement = Which[
      MemberQ[Keys[z13inf2],{SL,SpLp}],
        z13inf2[{SL,SpLp}],
      MemberQ[Keys[z13inf2],{SpLp,SL}],
        z13inf2[{SpLp,SL}],
      True,
        0
    ];
    redSOOandECSOinf2 = (
        ReducedT11inf2[SL, SpLp] +
        Reducedt11inf2[SL, SpLp] -
        a13 / 6 * matElement
    );
    redSOOandECSOinf2 = SimplifyFun[redSOOandECSOinf2];
    Return[redSOOandECSOinf2];
  )
];

ReducedSOOandECSOinfn::usage = "ReducedSOOandECSOinfn[numE, SL,
  SpLp] calculates the reduced matrix elements of the (spin-other-
  orbit + ECSO) operator for the f^numE configuration corresponding
  to the terms SL and SpLp. This is done recursively, starting from
  tabulated values for f^2 from \"Judd, BR, HM Crosswhite, and
  Hannah Crosswhite. \"Intra-Atomic Magnetic Interactions for f
  Electrons.\" Physical Review 169, no. 1 (1968): 130.\", and by
  using equation (4) of that same paper.
";
ReducedSOOandECSOinfn[numE_, SL_, SpLp_] := Module[
  {spin, orbital, t, S, L, Sp, Lp,
  idx1, idx2, cfpSL, cfpSpLp, parentSL,
  Sb, Lb, Sbp, Lbp, parentSpLp, funval},
  (
    {spin, orbital} = {1/2, 3};
    {S, L}   = FindSL[SL];
    {Sp, Lp} = FindSL[SpLp];
    t = 1;
    cfpSL    = CFP[{numE, SL}];
    cfpSpLp  = CFP[{numE, SpLp}];
    funval   = Sum[
```

```
        (
          parentSL = cfpSL[[idx2, 1]];
          parentSpLp = cfpSpLp[[idx1, 1]];
          {Sb, Lb}   = FindSL[parentSL];
          {Sbp, Lbp} = FindSL[parentSpLp];
          phase = Phaser[Sb + Lb + spin + orbital + Sp + Lp];
          (
            phase *
            cfpSpLp[[idx1, 2]] * cfpSL[[idx2, 2]] *
            SixJay[{S, t, Sp}, {Sbp, spin, Sb}] *
            SixJay[{L, t, Lp}, {Lbp, orbital, Lb}] *
            SOOandECSOLSTable[{numE - 1, parentSL, parentSpLp}]
          )
        ),
      {idx1, 2, Length[cfpSpLp]},
      {idx2, 2, Length[cfpSL]}
      ];
      funval *= numE / (numE - 2) * Sqrt[TPO[S, Sp, L, Lp]];
      Return[funval];
    )
  ];

  GenerateSOOandECSOLSTable::usage = "GenerateSOOandECSOLSTable[nmax]
     generates the LS reduced matrix elements of the spin-other-orbit
    + ECSO for the f^n configurations up to n=nmax. The values for n=1
     and n=2 are taken from \"Judd, BR, HM Crosswhite, and Hannah
    Crosswhite. \"Intra-Atomic Magnetic Interactions for f Electrons.\
    " Physical Review 169, no. 1 (1968): 130.\", and the values for n
    >2 are calculated recursively using equation (4) of that same
    paper. The values are then exported to a file \"
    ReducedSOOandECSOLSTable.m\" in the data folder of this module.
    The values are also returned as an association.";
  Options[GenerateSOOandECSOLSTable] = {"Progress" -> True, "Export"
    -> True};
  GenerateSOOandECSOLSTable[nmax_Integer, OptionsPattern[]] := (
    If[And[OptionValue["Progress"], frontEndAvailable],
      (
        numItersai = Association[Table[numE->Length[AllowedNKSLTerms[
    numE]]^2, {numE, 1, nmax}]];
        counters   = Association[Table[numE->0, {numE, 1, nmax}]];
        totalIters = Total[Values[numItersai[[1;;nmax]]]];
        template1  = StringTemplate["Iteration `numiter` of `
    totaliter`"];
        template2  = StringTemplate["`remtime` min remaining"];
    template3 = StringTemplate["Iteration speed = `speed` ms/it"];
        template4  = StringTemplate["Time elapsed = `runtime` min"];
        progBar = PrintTemporary[
          Dynamic[
            Pane[
              Grid[{
                    {Superscript["f", numE]},
                    {template1[<|"numiter"->numiter, "totaliter"->
    totalIters|>]},
                    {template4[<|"runtime"->Round[QuantityMagnitude[
    UnitConvert[(Now-startTime), "min"]], 0.1]|>]},
                    {template2[<|"remtime"->Round[QuantityMagnitude[
    UnitConvert[(Now-startTime)/(numiter)*(totalIters-numiter), "min"
    ]], 0.1]|>]},
                    {template3[<|"speed"->Round[QuantityMagnitude[Now
    -startTime, "ms"]/(numiter), 0.01]|>]}, {ProgressIndicator[Dynamic
    [numiter], {1, totalIters}]}
                  },
                  Frame->All
              ],
              Full,
              Alignment->Center
            ]
          ]
        ];
      )
    ];
    SOOandECSOLSTable = <||>;
    numiter   = 1;
    startTime = Now;
    Do[
      (
```

```
        numiter+= 1;
        SOOandECSOLSTable[{numE, SL, SpLp}] = Which[
          numE==1,
          0,
          numE==2,
          SimplifyFun[ReducedSOOandECSOinf2[SL, SpLp]],
          True,
          SimplifyFun[ReducedSOOandECSOinfn[numE,  SL, SpLp]]
        ];
      ),
    {numE, 1, nmax},
    {SL, AllowedNKSLTerms[numE]},
    {SpLp, AllowedNKSLTerms[numE]}
    ];
    If[And[OptionValue["Progress"], frontEndAvailable],
      NotebookDelete[progBar]];
    If[OptionValue["Export"],
      (fname = FileNameJoin[{moduleDir, "data", "
  ReducedSOOandECSOLSTable.m"}];
      Export[fname, SOOandECSOLSTable];
      )
    ];
    Return[SOOandECSOLSTable];
  );

  (* ################## Reduced SOO and ECSO ################## *)
  (* ######################################################### *)

  (* ######################################################### *)
  (* ###################### Spin-Spin ######################## *)

  ReducedT22inf2::usage = "ReducedT22inf2[SL, SpLp] returns the
    reduced matrix element of the scalar component of the double
    tensor T22 for the terms SL, SpLp in f^2.
  Data used here for m0, m2, m4 is from Table I of Judd, BR, HM
    Crosswhite, and Hannah Crosswhite. Intra-Atomic Magnetic
    Interactions for f Electrons. Physical Review 169, no. 1 (1968):
    130.
  ";
  ReducedT22inf2[SL_, SpLp_] := Module[
    {statePosition, PsiPsipStates, m0, m2, m4, Tkk2m},
    (
      T22inf2 = <|
      {"3P", "3P"} -> -12 M0 - 24 M2 - 300/11 M4,
      {"3P", "3F"} -> 8/Sqrt[3] (3 M0 + M2 - 100/11 M4),
      {"3F", "3F"} -> 4/3 Sqrt[14] (-M0 + 8 M2 - 200/11 M4),
      {"3F", "3H"} -> 8/3 Sqrt[11/2] (2 M0 - 23/11 M2 - 325/121 M4),
      {"3H", "3H"} -> 4/3 Sqrt[143] (M0 - 34/11 M2 - (1325/1573) M4)
      |>;
      Which[
        MemberQ[Keys[T22inf2],{SL,SpLp}],
          Return[T22inf2[{SL,SpLp}]],
        MemberQ[Keys[T22inf2],{SpLp,SL}],
          Return[T22inf2[{SpLp,SL}]],
        True,
          Return[0]
      ]
    )
  ];

  ReducedT22infn::usage = "ReducedT22infn[n, SL, SpLp] calculates the
     reduced matrix element of the T22 operator for the f^n
    configuration corresponding to the terms SL and SpLp. This is the
    operator corresponding to the inter-electron between spin.
  It does this by using equation (4) of \"Judd, BR, HM Crosswhite,
    and Hannah Crosswhite. \"Intra-Atomic Magnetic Interactions for f
    Electrons.\" Physical Review 169, no. 1 (1968): 130.\"
  ";
  ReducedT22infn[numE_, SL_, SpLp_] := Module[
    {spin, orbital, t, idx1, idx2, S, L,
    Sp, Lp, cfpSL, cfpSpLp, parentSL,
    parentSpLp, Sb, Lb, Tnkk, phase, Sbp, Lbp},
    (
      {spin, orbital} = {1/2, 3};
      {S, L}   = FindSL[SL];
      {Sp, Lp} = FindSL[SpLp];
```

```
      t = 2;
      cfpSL    = CFP[{numE, SL}];
      cfpSpLp  = CFP[{numE, SpLp}];
      Tnkk = Sum[(
        parentSL   = cfpSL[[idx2, 1]];
        parentSpLp = cfpSpLp[[idx1, 1]];
        {Sb, Lb}   = FindSL[parentSL];
        {Sbp, Lbp} = FindSL[parentSpLp];
        phase = Phaser[Sb + Lb + spin + orbital + Sp + Lp];
        (
          phase *
          cfpSpLp[[idx1, 2]] * cfpSL[[idx2, 2]] *
          SixJay[{S, t, Sp}, {Sbp, spin, Sb}] *
          SixJay[{L, t, Lp}, {Lbp, orbital, Lb}] *
          T22Table[{numE - 1, parentSL, parentSpLp}]
        )
      ),
      {idx1, 2, Length[cfpSpLp]},
      {idx2, 2, Length[cfpSL]}
      ];
      Tnkk *= numE / (numE - 2) * Sqrt[TPO[S,Sp,L,Lp]];
      Return[Tnkk];
    )
  ];

  GenerateT22Table::usage = "GenerateT22Table[nmax] generates the LS
    reduced matrix elements for the double tensor operator T22 in f^n
    up to n=nmax. If the option \"Export\" is set to true then the
    resulting association is saved to the data folder. The values for
    n=1 and n=2 are taken from \"Judd, BR, HM Crosswhite, and Hannah
    Crosswhite. \"Intra-Atomic Magnetic Interactions for f Electrons.\
    " Physical Review 169, no. 1 (1968): 130.\", and the values for n
    >2 are calculated recursively using equation (4) of that same
    paper.
  This is an intermediate step to the calculation of the reduced
    matrix elements of the spin-spin operator.";
  Options[GenerateT22Table] = {"Export" -> True, "Progress" -> True};
  GenerateT22Table[nmax_Integer, OptionsPattern[]] := (
    If[And[OptionValue["Progress"], frontEndAvailable],
      (
        numItersai = Association[Table[numE->Length[AllowedNKSLTerms[
    numE]]^2, {numE, 1, nmax}]];
        counters = Association[Table[numE->0, {numE, 1, nmax}]];
        totalIters = Total[Values[numItersai[[1;;nmax]]]];
        template1 = StringTemplate["Iteration `numiter` of `totaliter
    `"];
        template2 = StringTemplate["`remtime` min remaining"];
    template3 = StringTemplate["Iteration speed = `speed` ms/it"];
        template4 = StringTemplate["Time elapsed = `runtime` min"];
        progBar = PrintTemporary[
          Dynamic[
            Pane[
              Grid[{{Superscript["f", numE]},
                    {template1[<|"numiter"->numiter, "totaliter"->
    totalIters|>]},
                    {template4[<|"runtime"->Round[QuantityMagnitude[
    UnitConvert[(Now-startTime), "min"]], 0.1]|>]},
                    {template2[<|"remtime"->Round[QuantityMagnitude[
    UnitConvert[(Now-startTime)/(numiter)*(totalIters-numiter), "min"
    ]], 0.1]|>]},
                    {template3[<|"speed"->Round[QuantityMagnitude[Now
    -startTime, "ms"]/(numiter), 0.01]|>]},
                    {ProgressIndicator[Dynamic[numiter], {1,
    totalIters}]}},
                    Frame->All],
                    Full,
                    Alignment->Center]
                ]
              ];
      )
    ];
    T22Table = <||>;
    startTime = Now;
    numiter = 1;
    Do[
      (
```

```
1736          numiter+= 1;
1737          T22Table[{numE, SL, SpLp}] = Which[
1738            numE==1,
1739            0,
1740            numE==2,
1741            SimplifyFun[ReducedT22inf2[SL, SpLp]],
1742            True,
1743            SimplifyFun[ReducedT22infn[numE,  SL, SpLp]]
1744          ];
1745        ),
1746      {numE, 1, nmax},
1747      {SL,   AllowedNKSLTerms[numE]},
1748      {SpLp, AllowedNKSLTerms[numE]}
1749      ];
1750      If[And[OptionValue["Progress"],frontEndAvailable],
1751        NotebookDelete[progBar]
1752      ];
1753      If[OptionValue["Export"],
1754        (
1755          fname = FileNameJoin[{moduleDir, "data", "ReducedT22Table.m"
        }];
1756          Export[fname, T22Table];
1757        )
1758      ];
1759      Return[T22Table];
1760    );
1761
1762    SpinSpin::usage = "SpinSpin[n, SL, SpLp, J] returns the matrix
        element <|SL,J|spin-spin|SpLp,J|> for the spin-spin operator
        within the configuration f^n. This matrix element is independent
        of MJ. This is obtained by querying the relevant reduced matrix
        element from the association T22Table, putting in the adequate
        phase, and 6-j symbol.
1763    This is calculated according to equation (3) in \"Judd, BR, HM
        Crosswhite, and Hannah Crosswhite. \"Intra-Atomic Magnetic
        Interactions for f Electrons.\" Physical Review 169, no. 1 (1968):
         130.\"
1764    \".
1765    ";
1766    SpinSpin[numE_, SL_, SpLp_, J_] := Module[
1767      {S, L, Sp, Lp, α, val},
1768      (
1769        α = 2;
1770        {S, L} = FindSL[SL];
1771        {Sp, Lp} = FindSL[SpLp];
1772        val = (
1773                Phaser[Sp + L + J] *
1774                SixJay[{Sp, Lp, J}, {L, S, α}] *
1775                T22Table[{numE, SL, SpLp}]
1776              );
1777        Return[val]
1778      )
1779    ];
1780
1781    GenerateSpinSpinTable::usage = "GenerateSpinSpinTable[nmax]
        generates the reduced matrix elements in the |LSJ> basis for the (
        spin-other-orbit + electrostatically-correlated-spin-orbit)
        operator. It returns an association where the keys are of the form
         {numE, SL, SpLp, J}. If the option \"Export\" is set to True then
         the resulting object is saved to the data folder. Since this is a
         scalar operator, there is no MJ dependence. This dependence only
        comes into play when the crystal field contribution is taken into
        account.";
1782    Options[GenerateSpinSpinTable] = {"Export"->False};
1783    GenerateSpinSpinTable[nmax_, OptionsPattern[]] :=
1784      (
1785        SpinSpinTable = <||>;
1786        PrintTemporary[Dynamic[numE]];
1787        Do[
1788          SpinSpinTable[{numE, SL, SpLp, J}] = (SpinSpin[numE, SL, SpLp
      , J]);,
1789          {numE, 1, nmax},
1790          {J, MinJ[numE], MaxJ[numE]},
1791          {SL,   First /@ AllowedNKSLforJTerms[numE, J]},
1792          {SpLp, First /@ AllowedNKSLforJTerms[numE, J]}
1793          ];
```

```
      If[OptionValue["Export"],
      (fname = FileNameJoin[{moduleDir, "data", "SpinSpinTable.m"}];
        Export[fname, SpinSpinTable];
        )
      ];
      Return[SpinSpinTable];
    );

(* ###################### Spin-Spin ######################### *)
(* ############################################################ *)

(*
  ######################################################################
   *)
(* ## Spin-Other-Orbit and Electrostatically-Correlated-Spin-Orbit
  ## *)

SOOandECSO::usage = "SOOandECSO[n, SL, SpLp, J] returns the matrix
  element <|SL,J|spin-spin|SpLp,J|> for the combined effects of the
  spin-other-orbit interaction and the electrostatically-correlated-
  spin-orbit (which originates from configuration interaction
  effects) within the configuration f^n. This matrix element is
  independent of MJ. This is obtained by querying the relevant
  reduced matrix element by querying the association
  SOOandECSOLSTable and putting in the adequate phase and 6-j symbol
  . The SOOandECSOLSTable puts together the reduced matrix elements
  from three operators.
This is calculated according to equation (3) in \"Judd, BR, HM
  Crosswhite, and Hannah Crosswhite. \"Intra-Atomic Magnetic
  Interactions for f Electrons.\" Physical Review 169, no. 1 (1968):
   130.\".
";
SOOandECSO[numE_, SL_, SpLp_, J_] := Module[
  {S, Sp, L, Lp, α, val},
  (
    α = 1;
    {S, L}   = FindSL[SL];
    {Sp, Lp} = FindSL[SpLp];
    val = (
            Phaser[Sp + L + J] *
            SixJay[{Sp, Lp, J}, {L, S, α}] *
            SOOandECSOLSTable[{numE, SL, SpLp}]
          );
    Return[val];
  )
];

Prescaling = {P2 -> P2/225, P4 -> P4/1089, P6 -> 25 * P6 / 184041};

GenerateSOOandECSOTable::usage = "GenerateSOOandECSOTable[nmax]
  generates the reduced matrix elements in the |LSJ> basis for the (
  spin-other-orbit + electrostatically-correlated-spin-orbit)
  operator. It returns an association where the keys are of the form
   {n, SL, SpLp, J}. If the option \"Export\" is set to True then
  the resulting object is saved to the data folder. Since this is a
  scalar operator, there is no MJ dependence. This dependence only
  comes into play when the crystal field contribution is taken into
  account.";
Options[GenerateSOOandECSOTable] = {"Export"->False};
GenerateSOOandECSOTable[nmax_, OptionsPattern[]] := (
  SOOandECSOTable = <||>;
  Do[
    SOOandECSOTable[{numE, SL, SpLp, J}] = (SOOandECSO[numE, SL,
  SpLp, J] /. Prescaling);,
  {numE, 1, nmax},
  {J, MinJ[numE], MaxJ[numE]},
  {SL,   First /@ AllowedNKSLforJTerms[numE, J]},
  {SpLp, First /@ AllowedNKSLforJTerms[numE, J]}
  ];
  If[OptionValue["Export"],
  (
    fname = FileNameJoin[{moduleDir, "data", "SOOandECSOTable.m"}];
    Export[fname, SOOandECSOTable];
  )
  ];
  Return[SOOandECSOTable];
```

```
);

(* ## Spin-Other-Orbit and Electrostatically-Correlated-Spin-Orbit ## *)
(* ###################################################################### *)

(* ############################################################ *)
(* ################## Magnetic Interactions ################## *)

MagneticInteractions::usage = "MagneticInteractions[{numE, SL, SLp, J}] returns the matrix element of the magnetic interaction between the terms SL and SLp in the f^numE configuration for the given value of J. The interaction is given by the sum of the spin-spin, the spin-other-orbit, and the electrostatically-correlated-spin-orbit interactions.
The part corresponding to the spin-spin interaction is provided by SpinSpin[{numE, SL, SLp, J}].
The part corresponding to SOO and ECSO is provided by the function SOOandECSO[{numE, SL, SLp, J}].
The option \"ChenDeltas\" can be used to include or exclude the Chen deltas from the calculation. The default is to exclude them. If this option is used, then the chenDeltas association needs to be loaded into the session with LoadChen[].";
Options[MagneticInteractions] = {"ChenDeltas" -> False};
MagneticInteractions[{numE_, SL_, SLp_, J_}, OptionsPattern[]] := Module[
  {key, ss, sooandecso, total,
  S, L, Sp, Lp, phase, sixjay,
  M0v, M2v, M4v,
  P2v, P4v, P6v},
  (
    key        = {numE, SL, SLp, J};
    ss         = \[Sigma]SS * SpinSpinTable[key];
    sooandecso = SOOandECSOTable[key];
    total = ss + sooandecso;
    total = SimplifyFun[total];
    If[
      Not[OptionValue["ChenDeltas"]],
      Return[total]
    ];
    (* In the type A errors the wrong values are different *)
    If[MemberQ[Keys[chenDeltas["A"]], {numE, SL, SLp}],
      (
        {S, L}   = FindSL[SL];
        {Sp, Lp} = FindSL[SLp];
        phase    = Phaser[Sp + L + J];
        sixjay   = SixJay[{Sp, Lp, J}, {L, S, 1}];
        {M0v, M2v, M4v, P2v, P4v, P6v} = chenDeltas["A"][{numE, SL, SLp}]["wrong"];
        total    = (
                     phase * sixjay *
                     (
                       M0v*M0 + M2v*M2 + M4v*M4 +
                       P2v*P2 + P4v*P4 + P6v*P6
                     )
                   );
        total    = wChErrA * total + (1 - wChErrA) * (ss + sooandecso)
      )
    ];
    (* In the type B errors the wrong values are zeros all around *)
    If[MemberQ[chenDeltas["B"], {numE, SL, SLp}],
      (
        total  = (1 - wChErrB) * (ss + sooandecso)
      )
    ];
    Return[total];
  )
];

(* ################## Magnetic Interactions ################## *)
(* ############################################################ *)
```

```
(* ############################################################ *)
(* ##################### Free-Ion Energies ##################### *)

GenerateFreeIonTable::usage="GenerateFreeIonTable[] generates an
  association for free-ion energies in terms of Slater integrals Fk
  and spin-orbit parameter ζ. It returns an association where the
  keys are of the form {nE, SL, SpLp}. If the option \"Export\" is
  set to True then the resulting object is saved to the data folder.
   The free-ion Hamiltonian is the sum of the electrostatic and spin
  -orbit interactions. The electrostatic interaction is given by the
   function Electrostatic[{numE, SL, SpLp}] and the spin-orbit
  interaction is given by the function SpinOrbitTable[{numE, SL,
  SpLp}]. The values for the electrostatic interaction are taken
  from the data file ElectrostaticTable.m and the values for the
  spin-orbit interaction are taken from the data file SpinOrbitTable
  .m. The values for the free-ion Hamiltonian are then exported to a
   file \"FreeIonTable.m\" in the data folder of this module. The
  values are also returned as an association.";
Options[GenerateFreeIonTable] = {"Export" -> False};
GenerateFreeIonTable[OptionsPattern[]] := Module[
  {terms, numEH, zetaSign, fname, FreeIonTable},
  (
    If[Not[ValueQ[ElectrostaticTable]],
      LoadElectrostatic[]
      ];
    If[Not[ValueQ[SpinOrbitTable]],
      LoadSpinOrbit[]
    ];
    If[Not[ValueQ[ReducedUkTable]],
      LoadUk[]
    ];
    FreeIonTable = <||>;
    Do[
      (
        terms = AllowedNKSLJTerms[nE];
        numEH = Min[nE, 14 - nE];
        zetaSign = If[nE > 7, -1, 1];
        Do[
          FreeIonTable[{nE,term[[1]],term[[2]]}] = (
            Electrostatic[{numEH, term[[1]], term[[1]]}] +
              zetaSign * SpinOrbitTable[{numEH, term[[1]], term
  [[1]], term[[2]]}]
              ),
          {term, terms}];
      ),
      {nE, 1, 14}
    ];
    If[OptionValue["Export"],
      (
        fname = FileNameJoin[{moduleDir, "data", "FreeIonTable.m"
  }];
        Export[fname, FreeIonTable];
      )
    ];
    Return[FreeIonTable];
  )
];

LoadFreeIon::usage = "LoadFreeIon[] loads the free-ion energies
  from the data folder. The values are stored in the association
  FreeIonTable.";
LoadFreeIon[] := (
  If[ValueQ[FreeIonTable],
    Return[]
  ];
  PrintTemporary["Loading the association of free-ion energies ..."
  ];
  FreeIonTableFname = FileNameJoin[{moduleDir, "data", "
  FreeIonTable.m"}];
  FreeIonTable = If[!FileExistsQ[FreeIonTableFname],
    (
      PrintTemporary[">> FreeIonTable.m not found, generating ..."
  ];
      GenerateFreeIonTable["Export" -> True]
    ),
      Import[FreeIonTableFname]
```

```
    ];
);

(* ##################### Free-Ion Energies ##################### *)
(* ############################################################## *)

(* ############################################################## *)
(* ###################### Crystal Field ######################### *)

Cqk::usage = "Cqk[numE, q, k, NKSL, J, M, NKSLp, Jp, Mp]. In
  Wybourne (1965) see equations 6-3, 6-4, and 6-5. Also in TASS see
  equation 11.53.";
Cqk[numE_, q_, k_, NKSL_, J_, M_, NKSLp_, Jp_, Mp_] := Module[
  {S, Sp, L, Lp, orbital, val},
  (
    orbital = 3;
    {S, L}   = FindSL[NKSL];
    {Sp, Lp} = FindSL[NKSLp];
    f1  = ThreeJay[{J, -M}, {k, q}, {Jp, Mp}];
    val =
      If[f1==0,
        0,
        (
          f2 = SixJay[{L, J, S}, {Jp, Lp, k}] ;
          If[f2==0,
            0,
            (
              f3 = ReducedUkTable[{numE, orbital, NKSL, NKSLp, k}];
              If[f3==0,
                0,
                (
                  (
                    Phaser[J - M + S + Lp + J + k] *
                    Sqrt[TPO[J, Jp]] *
                    f1 *
                    f2 *
                    f3 *
                    Ck[orbital, k]
                  )
                )
              ]
            )
          ]
        )
      ];
    Return[val];
  )
];

Bqk::usage = "Real part of the Bqk coefficients.";
Bqk[q_, 2] := {B02/2, B12, B22}[[q + 1]];
Bqk[q_, 4] := {B04/2, B14, B24, B34, B44}[[q + 1]];
Bqk[q_, 6] := {B06/2, B16, B26, B36, B46, B56, B66}[[q + 1]];

Sqk::usage = "Imaginary part of the Bqk coefficients.";
Sqk[q_, 2] := {0, S12, S22}[[q + 1]];
Sqk[q_, 4] := {0, S14, S24, S34, S44}[[q + 1]];
Sqk[q_, 6] := {0, S16, S26, S36, S46, S56, S66}[[q + 1]];

CrystalField::usage = "CrystalField[n, NKSL, J, M, NKSLp, Jp, Mp]
  gives the general expression for the matrix element of the crystal
   field Hamiltonian parametrized with Bqk and Sqk coefficients as a
   sum over spherical harmonics Cqk.
Sometimes this expression only includes Bqk coefficients, see for
  example eqn 6-2 in Wybourne (1965), but one may also split the
  coefficient into real and imaginary parts as is done here, in an
  expression that is patently Hermitian.";
CrystalField[numE_, NKSL_, J_, M_, NKSLp_, Jp_, Mp_] := (
  Sum[
    (
      cqk  = Cqk[numE,  q, k, NKSL, J, M, NKSLp, Jp, Mp];
      cmqk = Cqk[numE, -q, k, NKSL, J, M, NKSLp, Jp, Mp];
      Bqk[q, k]   * (cqk + (-1)^q * cmqk) +
      I*Sqk[q, k] * (cqk - (-1)^q * cmqk)
      ),
  {k, {2, 4, 6}},
```

```
    {q, 0, k}
    ]
  )

  TotalCFIters::usage = "TotalIters[i, j] returns total number of
    function evaluations for calculating all the matrix elements for
    the \!\(\*SuperscriptBox[\(f\), \(i\)]\) to the \!\(\*
    SuperscriptBox[\(f\), \(j\)]\) configurations.";
  TotalCFIters[i_, j_] := (
    numIters = {196, 8281, 132496, 1002001, 4008004, 9018009,
    11778624};
    Return[Total[numIters[[i ;; j]]]];
    )

  GenerateCrystalFieldTable::usage = "GenerateCrystalFieldTable[{
    numEs}] computes the matrix values for the crystal field
    interaction for f^n configurations the given list of numE in
    numEs. The function calculates the association CrystalFieldTable
    with keys of the form {numE, NKSL, J, M, NKSLp, Jp, Mp}. If the
    option \"Export\" is set to True, then the result is exported to
    the data subfolder for the folder in which this package is in. If
    the option \"Progress\" is set to True then an interactive
    progress indicator is shown. If \"Compress\" is set to true the
    exported values are compressed when exporting.";
  Options[GenerateCrystalFieldTable] = {"Export" -> False, "Progress"
     -> True, "Compress" -> True};
  GenerateCrystalFieldTable[numEs_List:{1,2,3,4,5,6,7},
    OptionsPattern[]] := (
    ExportFun =
    If[OptionValue["Compress"],
      ExportMZip,
      Export
    ];
    numiter = 1;
    template1 = StringTemplate["Iteration `numiter` of `totaliter`"];
    template2 = StringTemplate["`remtime` min remaining"];
    template3 = StringTemplate["Iteration speed = `speed` ms/it"];
    template4 = StringTemplate["Time elapsed = `runtime` min"];
    totalIter = Total[TotalCFIters[#, #] & /@ numEs];
    freebies = 0;
    startTime = Now;
    If[And[OptionValue["Progress"], frontEndAvailable],
      progBar = PrintTemporary[
        Dynamic[
          Pane[
            Grid[
              {
                {Superscript["f", numE]},
                {template1[<|"numiter" -> numiter, "totaliter" ->
  totalIter|>]},
                {template4[<|"runtime" -> Round[QuantityMagnitude[
  UnitConvert[(Now - startTime), "min"]], 0.1]|>]},
                {template2[<|"remtime" -> Round[QuantityMagnitude[
  UnitConvert[(Now - startTime)/(numiter - freebies) * (totalIter -
  numiter), "min"]], 0.1]|>]},
                {template3[<|"speed" -> Round[QuantityMagnitude[Now -
   startTime, "ms"]/(numiter-freebies), 0.01]|>]},
                {ProgressIndicator[Dynamic[numiter], {1, totalIter}]}
              },
            Frame -> All
            ],
          Full,
          Alignment -> Center
          ]
        ]
      ];
    ];
    Do[
      (
        exportFname = FileNameJoin[{moduleDir, "data", "
  CrystalFieldTable_f"<>ToString[numE]<>".m"}];
        If[FileExistsQ[exportFname],
          Print["File exists, skipping ..."];
          numiter+=  TotalCFIters[numE, numE];
          freebies+= TotalCFIters[numE, numE];
          Continue[];
```

```
        ];
        CrystalFieldTable = <||>;
        Do[
          (
            numiter+= 1;
            CrystalFieldTable[{numE, NKSL, J, M, NKSLp, Jp, Mp}] =
  CrystalField[numE, NKSL, J, M, NKSLp, Jp, Mp];
          ),
        {J, MinJ[numE], MaxJ[numE]},
        {Jp, MinJ[numE], MaxJ[numE]},
        {M, AllowedMforJ[J]},
        {Mp, AllowedMforJ[Jp]},
        {NKSL , First /@ AllowedNKSLforJTerms[numE, J]},
        {NKSLp, First /@ AllowedNKSLforJTerms[numE, Jp]}
        ];
        If[And[OptionValue["Progress"],frontEndAvailable],
          NotebookDelete[progBar]
        ];
        If[OptionValue["Export"],
          (
            Print["Exporting to file "<>ToString[exportFname]];
            ExportFun[exportFname, CrystalFieldTable];
          )
        ];
      ),
    {numE, numEs}
    ]
  )

  Options[ParseBenelli2015] = {"Export"->False};
  ParseBenelli2015[OptionsPattern[]] := Module[
    {fname, crystalSym,
    crystalSymmetries, parseFun,
    chars, qk, groupName, family,
    groupNum, params},
  (
    fname      = FileNameJoin[{moduleDir,"data","
   benelli_and_gatteschi_table3p3.csv"}];
    crystalSym = Import[fname][[2;;33]];
    crystalSymmetries = <||>;
    parseFun[txt_] := (
      chars = Characters[txt];
      qk    = chars[[-2;;]];
      If[chars[[1]]=="R",
      (
        Return[{ToExpression@StringJoin[{"B",qk[[1]],qk[[2]]}]}]
      ),
      (
        If[qk[[1]]=="0",
          Return[{ToExpression@StringJoin[{"B",qk[[1]],qk[[2]]}]}]
        ];
        Return[{
          ToExpression@StringJoin[{"B",qk[[1]],qk[[2]]}],
          ToExpression@StringJoin[{"S",qk[[1]],qk[[2]]}]
        }]
      )]
    );
    Do[
    (
      groupNum  = Round@ToExpression@row[[1]];
      groupName = row[[2]];
      family    = row[[3]];
      params    = Select[row[[4;;]],#=!=""&];
      params    = parseFun/@params;
      params    = <|"BqkSqk"->Sort@Flatten[params],
        "aliases"->{groupNum},
        "constraints"->{}|>;
      If[MemberQ[{"T","Th","O","Td","Oh"},groupName],
        params["constraints"] = {
            {B44 ->  Sqrt[5/14] B04, B46 -> -Sqrt[7/2] B06},
            {B44 -> -Sqrt[5/14] B04, B46 ->  Sqrt[7/2] B06}
            }
      ];
      If[StringContainsQ[groupName,","],
      (
        {alias1, alias2}          = StringSplit[groupName,","];
```

```
        crystalSymmetries[alias1] = params;
        crystalSymmetries[alias1]["aliases"] = {groupNum, alias2};
        crystalSymmetries[alias2] = params;
        crystalSymmetries[alias2]["aliases"] = {groupNum, alias1};
      ),
      (
      crystalSymmetries[groupName] = params;
      )
      ]
    ),
    {row,crystalSym}];
    crystalSymmetries["source"] = "Benelli and Gatteschi, 2015,
    Introduction to Molecular Magnetism, table 3.3.";
    If[OptionValue["Export"],
      Export[FileNameJoin[{moduleDir,"data","
    crystalFieldFunctionalForms.m"}],crystalSymmetries];
    ];
    Return[crystalSymmetries];
  )
  ]

  CrystalFieldForm::usage = "CrystalFieldForm[symmetryGroup] returns
    an association that describes the crystal field parameters that
    are necessary to desribe a crystal field for the given symmetry
    group.

  The symmetry group must be given as a string in Schoenflies
    notation and must be one of C1, Ci, S2, Cs, C1h, C2, C2h, C2v, D2,
     D2h, S4, C4, C4h, D2d, C4v, D4, D4h, C3, S6, C3h, C3v, D3, D3d,
    D3h, C6, C6h, C6v, D6, D6h, T, Th, Td, O, Oh.

  The returned association has three keys:
    \"BqkSqk\" whose values is a list with the nonzero Bqk and Sqk
    parameters;
    \"constraints\" whose value is either an empty list, or a lists
    of replacements rules that are constraints on the Bqk and Sqk
    parameters;
    \"simplifier\" whose value is an association that can be used to
    set to zero the crystal field parameters that are zero for the
    given symmetry group;
    \"aliases\" whose value is a list with the integer by which the
    point group is also known for and an alternate Schoenflies symbol
    if it exists.

  This uses data from table 3.3 in Benelli and Gatteschi, 2015.";
  CrystalFieldForm[symmetryGroupString_] := (
    If[Not@ValueQ[crystalFieldFunctionalForms],
      crystalFieldFunctionalForms = Import[FileNameJoin[{moduleDir, "
    data", "crystalFieldFunctionalForms.m"}]];
    ];
    cfForm = crystalFieldFunctionalForms[symmetryGroupString];
    simplifier = Association[(# -> 0) &/@ Complement[cfSymbols,
    cfForm["BqkSqk"]]];
    Return[Join[cfForm, <|"simplifier"->simplifier|>]];
  )

  (* ###################### Crystal Field ######################### *)
  (* ############################################################## *)

  (* ############################################################## *)
  (* #### Configuration-Interaction via Casimir Operators ###### *)

  CasimirSO3::usage = "CasimirSO3[SL, SpLp] returns LS reduced matrix
     element of the configuration interaction term corresponding to
    the Casimir operator of R3.";
  CasimirSO3[{SL_, SpLp_}] := (
    {S, L} = FindSL[SL];
    If[SL == SpLp,
      α * L * (L + 1),
      0
    ]
  )

  GG2U::usage = "GG2U is an association whose keys are labels for the
     irreducible representations of group G2 and whose values are the
    eigenvalues of the corresponding Casimir operator.
```

```
Reference: Wybourne, \"Spectroscopic Properties of Rare Earths\",
  table 2-6.";
GG2U = Association[{
    "00" -> 0,
    "10" -> 6/12 ,
    "11" -> 12/12,
    "20" -> 14/12,
    "21" -> 21/12,
    "22" -> 30/12,
    "30" -> 24/12,
    "31" -> 32/12,
    "40" -> 36/12}
  ];

CasimirG2::usage = "CasimirG2[SL, SpLp] returns LS reduced matrix
  element of the configuration interaction term corresponding to the
   Casimir operator of G2.";
CasimirG2[{SL_, SpLp_}] := (
  Ulabel = FindNKLSTerm[SL][[1]][[4]];
  If[SL==SpLp,
    β * GG2U[Ulabel],
    0
  ]
)

GSO7W::usage = "GSO7W is an association whose keys are labels for
  the irreducible representations of group R7 and whose values are
  the eigenvalues of the corresponding Casimir operator.
Reference: Wybourne, \"Spectroscopic Properties of Rare Earths\",
  table 2-7.";
GSO7W := Association[
  {
    "000" -> 0,
    "100" -> 3/5,
    "110" -> 5/5,
    "111" -> 6/5,
    "200" -> 7/5,
    "210" -> 9/5,
    "211" -> 10/5,
    "220" -> 12/5,
    "221" -> 13/5,
    "222" -> 15/5
  }
];

CasimirSO7::usage = "CasimirSO7[SL, SpLp] returns the LS reduced
  matrix element of the configuration interaction term corresponding
   to the Casimir operator of R7.";
CasimirSO7[{SL_, SpLp_}] := (
  Wlabel = FindNKLSTerm[SL][[1]][[3]];
  If[SL==SpLp,
    γ * GSO7W[Wlabel],
    0
  ]
)

ElectrostaticConfigInteraction::usage = "
  ElectrostaticConfigInteraction[{SL, SpLp}] returns the matrix
  element for configuration interaction as approximated by the
  Casimir operators of the groups R3, G2, and R7. SL and SpLp are
  strings that represent terms under LS coupling.";
ElectrostaticConfigInteraction[{SL_, SpLp_}] := Module[
  {S, L, val},
  (
    {S, L} = FindSL[SL];
    val = (
      If[SL == SpLp,
        CasimirSO3[{SL, SL}] +
        CasimirSO7[{SL, SL}] +
        CasimirG2[{SL, SL}],
        0
      ]
      );
    ElectrostaticConfigInteraction[{S, L}] = val;
    Return[val];
  )
```

```
];

(* #### Configuration-Interaction via Casimir Operators ###### *)
(* ############################################################ *)

(* ############################################################ *)
(* ###################### Block assembly ###################### *)

JJBlockMatrix::usage = "For given J, J' in the f^n configuration
  JJBlockMatrix[numE, J, J'] determines all the SL S'L' terms that
  may contribute to them and using those it provides the matrix
  elements <J, LS | H | J', LS'>. H having contributions from the
  following interactions: Coulomb, spin-orbit, spin-other-orbit,
  electrostatically-correlated-spin-orbit, spin-spin, three-body
  interactions, and crystal-field.";
Options[JJBlockMatrix] = {"Sparse"->True, "ChenDeltas"->False};
JJBlockMatrix[numE_, J_, Jp_, CFTable_, OptionsPattern[]] := Module
  [
   {NKSLJMs, NKSLJMps, NKSLJM, NKSLJMp,
   SLterm, SpLpterm,
   MJ, MJp,
   subKron, matValue, eMatrix},
   (
     NKSLJMs  = AllowedNKSLJMforJTerms[numE, J];
     NKSLJMps = AllowedNKSLJMforJTerms[numE, Jp];
     eMatrix =
       Table[
         (*Condition for a scalar matrix op*)
         SLterm   = NKSLJM[[1]];
         SpLpterm = NKSLJMp[[1]];
         MJ       = NKSLJM[[3]];
         MJp      = NKSLJMp[[3]];
         subKron  = (
             KroneckerDelta[J, Jp] *
             KroneckerDelta[MJ, MJp]
                   );
         matValue =
           If[subKron==0,
             0,
               (
                 ElectrostaticTable[{numE, SLterm, SpLpterm}] +
                 ElectrostaticConfigInteraction[{SLterm, SpLpterm}]
  +
                 SpinOrbitTable[{numE, SLterm, SpLpterm, J}] +
                 MagneticInteractions[{numE, SLterm, SpLpterm, J},
                   "ChenDeltas" -> OptionValue["ChenDeltas"]] +
                 ThreeBodyTable[{numE, SLterm, SpLpterm}]
               )
           ];
         matValue += CFTable[{numE, SLterm, J, MJ, SpLpterm, Jp, MJp
  }];
         matValue,
       {NKSLJMp, NKSLJMps},
       {NKSLJM , NKSLJMs}
       ];
    If[OptionValue["Sparse"],
      eMatrix = SparseArray[eMatrix]
    ];
    Return[eMatrix]
  )
  ];

EnergyStates::usage = "Alias for AllowedNKSLJMforJTerms. At some
  point may be used to redefine states used in basis.";
EnergyStates[numE_, J_]:= AllowedNKSLJMforJTerms[numE, J];

JJBlockMatrixFileName::usage = "JJBlockMatrixFileName[numE] gives
  the filename for the energy matrix table for an atom with numE f-
  electrons. The function admits an optional parameter \"
  FilenameAppendix\" which can be used to modify the filename.";
Options[JJBlockMatrixFileName] = {"FilenameAppendix" -> ""};
JJBlockMatrixFileName[numE_Integer, OptionsPattern[]] := (
   fileApp = OptionValue["FilenameAppendix"];
   fname = FileNameJoin[{moduleDir,
       "hams",
       StringJoin[{"f", ToString[numE], "_JJBlockMatrixTable",
```

```
    fileApp ,".m"}]}];
    Return[fname];
  );

  TabulateJJBlockMatrixTable::usage = "TabulateJJBlockMatrixTable[
    numE, I] returns a list with three elements {JJBlockMatrixTable,
    EnergyStatesTable, AllowedM}. JJBlockMatrixTable is an association
     with keys equal to lists of the form {numE, J, Jp}.
    EnergyStatesTable is an association with keys equal to lists of
    the form {numE, J}. AllowedM is another association with keys
    equal to lists of the form {numE, J} and values equal to lists
    equal to the corresponding values of MJ. It's unnecessary (and it
    won't work in this implementation) to give numE > 7 given the
    equivalency between electron and hole configurations.";
  Options[TabulateJJBlockMatrixTable] = {"Sparse"->True, "ChenDeltas"
    ->False};
  TabulateJJBlockMatrixTable[numE_, CFTable_, OptionsPattern[]] := (
    JJBlockMatrixTable = <||>;
    totalIterations = Length[AllowedJ[numE]]^2;
    template1 = StringTemplate["Iteration `numiter` of `totaliter`"];
    template2 = StringTemplate["`remtime` min remaining"];
    template4 = StringTemplate["Time elapsed = `runtime` min"];
    numiter   = 0;
    startTime = Now;
    If[$FrontEnd =!= Null,
      (
        temp = PrintTemporary[
          Dynamic[
            Grid[
              {
                {template1[<|"numiter"->numiter, "totaliter"->
    totalIterations|>]},
                {template2[<|"remtime"->Round[QuantityMagnitude[
    UnitConvert[(Now-startTime)/(Max[1,numiter])*(totalIterations-
    numiter), "min"]], 0.1]|>]},
                {template4[<|"runtime"->Round[QuantityMagnitude[
    UnitConvert[(Now-startTime), "min"]], 0.1]|>]},
                {ProgressIndicator[numiter, {1, totalIterations}]}
              }
            ]
        ]
        ];
      )
    ];
    Do[
      (
        JJBlockMatrixTable[{numE, J, Jp}] = JJBlockMatrix[numE, J, Jp
    , CFTable, "Sparse"->OptionValue["Sparse"], "ChenDeltas" ->
    OptionValue["ChenDeltas"]];
        numiter += 1;
      ),
    {Jp, AllowedJ[numE]},
    {J, AllowedJ[numE]}
    ];
    If[$FrontEnd =!= Null,
      NotebookDelete[temp]
    ];
    Return[JJBlockMatrixTable];
  );

  TabulateManyJJBlockMatrixTables::usage = "
    TabulateManyJJBlockMatrixTables[{n1, n2, ...}] calculates the
    tables of matrix elements for the requested f^n_i configurations.
    The function does not return the matrices themselves. It instead
    returns an association whose keys are numE and whose values are
    the filenames where the output of TabulateJJBlockMatrixTables was
    saved to.The output consists of an association whose keys are of
    the form {n, J, Jp} and whose values are rectangular arrays given
    the values of <|LSJMJa|H|L'S'J'MJ'a'|>.";
  Options[TabulateManyJJBlockMatrixTables] = {"Overwrite"->False, "
    Sparse"->True, "ChenDeltas"->False, "FilenameAppendix"-> "", "
    Compressed" -> False};
  TabulateManyJJBlockMatrixTables[ns_, OptionsPattern[]] := (
    overwrite = OptionValue["Overwrite"];
    fNames = <||>;
    fileApp = OptionValue["FilenameAppendix"];
```

```
    ExportFun = If[OptionValue["Compressed"], ExportMZip, Export];
    Do[
      (
        CFdataFilename = FileNameJoin[{moduleDir, "data", "
    CrystalFieldTable_f"<>ToString[numE]<>".zip"}];
        PrintTemporary["Importing CrystalFieldTable from ",
    CFdataFilename, " ..."];
        CrystalFieldTable = ImportMZip[CFdataFilename];

        PrintTemporary["#------- numE = ", numE, " -------#"];
        exportFname = JJBlockMatrixFileName[numE, "FilenameAppendix"
    -> fileApp];
        fNames[numE] = exportFname;
        If[FileExistsQ[exportFname] && Not[overwrite],
          Continue[]
        ];
        JJBlockMatrixTable = TabulateJJBlockMatrixTable[numE,
    CrystalFieldTable, "Sparse"->OptionValue["Sparse"], "ChenDeltas"
    -> OptionValue["ChenDeltas"]];
        If[FileExistsQ[exportFname]&&overwrite,
          DeleteFile[exportFname]
        ];
        ExportFun[exportFname, JJBlockMatrixTable];

        ClearAll[CrystalFieldTable];
      ),
    {numE, ns}
    ];
    Return[fNames];
  );

  HamMatrixAssembly::usage = "HamMatrixAssembly[numE] returns the
    Hamiltonian matrix for the f^n_i configuration. The matrix is
    returned as a SparseArray.
  The function admits an optional parameter \"FilenameAppendix\"
    which can be used to modify the filename to which the resulting
    array is exported to.
  It also admits an optional parameter \"IncludeZeeman\" which can be
     used to include the Zeeman interaction. The default is False
  The option \"Set t2Switch\" can be used to toggle on or off setting
     the t2 selector automatically or not, the default is True, which
    replaces the parameter according to numE.
  The option \"ReturnInBlocks\" can be used to return the matrix in
    block or flattened form. The default is to return it in flattened
    form.";
  Options[HamMatrixAssembly] = {
        "FilenameAppendix"->"",
        "IncludeZeeman"->False,
        "Set t2Switch"->True,
        "ReturnInBlocks"->False};
  HamMatrixAssembly[nf_, OptionsPattern[]] := Module[
    {numE, ii, jj, howManyJs, Js, blockHam},
    (
      (*######################################*)
      ImportFun = ImportMZip;
      (*######################################*)
      (*hole-particle equivalence enforcement*)
      numE = nf;
      allVars = {E0, E1, E2, E3, ζ, F0, F2, F4, F6, M0, M2, M4, T2,
    T2p,
        T3, T4, T6, T7, T8, P0, P2, P4, P6, gs,
        α, β, γ, B02, B04, B06, B12, B14, B16,
        B22, B24, B26, B34, B36, B44, B46, B56, B66, S12, S14, S16,
    S22,
        S24, S26, S34, S36, S44, S46, S56, S66, T11p, T12, T14, T15,
    T16,
        T17, T18, T19, Bx, By, Bz};
      params0 = AssociationThread[allVars, allVars];
      If[nf > 7,
        (
          numE = 14 - nf;
          params = HoleElectronConjugation[params0];
          If[OptionValue["Set t2Switch"], params[t2Switch] = 0];
        ),
        params = params0;
        If[OptionValue["Set t2Switch"], params[t2Switch] = 1];
```

```
2447        ];
2448        (* Load symbolic expressions for LS,J,J' energy sub-matrices.
    *)
2449        emFname = JJBlockMatrixFileName[numE, "FilenameAppendix" ->
    OptionValue["FilenameAppendix"]];
2450        JJBlockMatrixTable = ImportFun[emFname];
2451        (*Patch together the entire matrix representation using J,J'
    blocks.*)
2452        PrintTemporary["Patching JJ blocks ..."];
2453        Js        = AllowedJ[numE];
2454        howManyJs = Length[Js];
2455        blockHam  = ConstantArray[0, {howManyJs, howManyJs}];
2456        Do[
2457          blockHam[[jj, ii]] = JJBlockMatrixTable[{numE, Js[[ii]], Js[[
    jj]]}];,
2458        {ii, 1, howManyJs},
2459        {jj, 1, howManyJs}
2460        ];
2461
2462        (* Once the block form is created flatten it *)
2463        If[Not[OptionValue["ReturnInBlocks"]],
2464          (blockHam = ArrayFlatten[blockHam];
2465          blockHam  = ReplaceInSparseArray[blockHam, params];
2466          ),
2467          (blockHam  = Map[ReplaceInSparseArray[#, params]&,blockHam
    ,{2}];)
2468        ];
2469
2470        If[OptionValue["IncludeZeeman"],
2471          (
2472            PrintTemporary["Including Zeeman terms ..."];
2473            {magx, magy, magz} = MagDipoleMatrixAssembly[numE, "
    ReturnInBlocks" -> OptionValue["ReturnInBlocks"]];
2474            blockHam += - teslaToKayser * (Bx * magx + By * magy + Bz *
     magz);
2475          )
2476        ];
2477        Return[blockHam];
2478      )
2479    ];
2480
2481    SimplerSymbolicHamMatrix::usage = "SimplerSymbolicHamMatrix[numE,
      simplifier] is a simple addition to HamMatrixAssembly that applies
       a given simplification to the full Hamiltonian. simplifier is a
      list of replacement rules. If the option \"Export\" is set to True
      , then the function also exports the resulting sparse array to the
       ./hams/ folder. The option \"PrependToFilename\" can be used to
      append a string to the filename to which the function may export
      to. The option \"Return\" can be used to choose whether the
      function returns the matrix or not. The option \"Overwrite\" can
      be used to overwrite the file if it already exists, if this
      options is set to False then this function simply reloads a file
      that it assumed to be present already in the ./hams folder. The
      option \"IncludeZeeman\" can be used to toggle the inclusion of
      the Zeeman interaction with an external magnetic field.";
2482    Options[SimplerSymbolicHamMatrix] = {
2483      "Export"->True,
2484      "PrependToFilename"->"",
2485      "EorF"->"F",
2486      "Overwrite" -> False,
2487      "Return" -> True,
2488      "Set t2Switch" -> False,
2489      "IncludeZeeman" -> False};
2490    SimplerSymbolicHamMatrix[numE_Integer, simplifier_List,
      OptionsPattern[]] := Module[
2491      {thisHam,fname, fnamemx},
2492      (
2493        If[Not[ValueQ[ElectrostaticTable]],
2494          LoadElectrostatic[]
2495          ];
2496        If[Not[ValueQ[SOOandECSOTable]],
2497          LoadSOOandECSO[]
2498        ];
2499        If[Not[ValueQ[SpinOrbitTable]],
2500          LoadSpinOrbit[]
2501        ];
```

```
2502      If[Not[ValueQ[SpinSpinTable]],
2503        LoadSpinSpin[]
2504      ];
2505      If[Not[ValueQ[ThreeBodyTable]],
2506        LoadThreeBody[]
2507      ];
2508
2509      fname   = FileNameJoin[{moduleDir, "hams",
2510        OptionValue["PrependToFilename"]<>"SymbolicMatrix-f"<>
    ToString[numE]<>".m"}];
2511      fnamemx = FileNameJoin[{moduleDir,"hams",
2512        OptionValue["PrependToFilename"]<> "SymbolicMatrix-f" <>
    ToString[numE] <> ".mx"}];
2513      If[Or[FileExistsQ[fname], FileExistsQ[fnamemx]]
2514        && Not[OptionValue["Overwrite"]],
2515        (
2516          If[OptionValue["Return"],
2517            (
2518              Which[
2519                FileExistsQ[fnamemx],
2520                (
2521                  Print["File ", fnamemx, " already exists, and
    option \"Overwrite\" is set to False, loading file ..."];
2522                  thisHam = Import[fnamemx];
2523                  Return[thisHam];
2524                ),
2525                FileExistsQ[fname],
2526                (
2527                  Print["File ", fname, " already exists, and option
    \"Overwrite\" is set to False, loading file ..."];
2528                  thisHam = Import[fname];
2529                  Print["Exporting to file ", fnamemx, " for quicker
    loading."];
2530                  Export[fnamemx, thisHam];
2531                  Return[thisHam];
2532                )
2533              ]
2534            ),
2535            (
2536              Print["File ", fname, " already exists, skipping ..."];
2537              Return[Null];
2538            )
2539          ]
2540        )
2541      ];
2542
2543      thisHam = HamMatrixAssembly[numE, "Set t2Switch" -> OptionValue
    ["Set t2Switch"], "IncludeZeeman" -> OptionValue["IncludeZeeman"
    ]];
2544      If[Length[simplifier] > 0,
2545        thisHam = ReplaceInSparseArray[thisHam, simplifier];
2546      ];
2547      (* This removes zero entries from being included in the sparse
    array *)
2548      thisHam = SparseArray[thisHam];
2549      If[OptionValue["Export"],
2550      (
2551        Print["Exporting to file ", fname, " and to ", fnamemx];
2552        Export[fname,   thisHam];
2553        Export[fnamemx, thisHam];
2554      )
2555      ];
2556      If[OptionValue["Return"],
2557        Return[thisHam],
2558        Return[Null]
2559      ];
2560    )
2561  ];
2562
2563  ScalarLSJMFromLS::usage = "ScalarLSJMFromLS[numE,
      LSReducedMatrixElements]. Given the LS-reduced matrix elements
      LSReducedMatrixElements of a scalar operator, this function
      returns the corresponding LSJM representation. This is returned as
       a SparseArray.";
2564  ScalarLSJMFromLS[numE_, LSReducedMatrixElements_] := Module[
2565    {jjBlocktable, NKSLJMs, NKSLJMps, J, Jp, eMatrix, SLterm,
```

```
    SpLpterm,
    MJ, MJp, subKron, matValue, Js, howManyJs, blockHam, ii, jj},
    (
    SparseDiagonalArray[diagonalElements_] := SparseArray[
      Table[{i, i} -> diagonalElements[[i]],
        {i, 1, Length[diagonalElements]}]
      ];
    SparseZeroArray[width_, height_] := (
      SparseArray[
        Join[
        Table[{1, i} -> 0, {i, 1, width}],
        Table[{i, 1} -> 0, {i, 1, height}]
        ]
        ]
      );
    jjBlockTable = <||>;
    Do[
      NKSLJMs  = AllowedNKSLJMforJTerms[numE, J];
      NKSLJMps = AllowedNKSLJMforJTerms[numE, Jp];
      If[J != Jp,
        jjBlockTable[{numE, J, Jp}] = SparseZeroArray[Length[NKSLJMs
    ], Length[NKSLJMps]];
      Continue[];
      ];
      eMatrix = Table[
        (* Condition for a scalar matrix op *)
        SLterm = NKSLJM[[1]];
        SpLpterm = NKSLJMp[[1]];
        MJ = NKSLJM[[3]];
        MJp = NKSLJMp[[3]];
        subKron = (KroneckerDelta[MJ, MJp]);
        matValue = If[subKron == 0,
        0,
          (
            Which[MemberQ[Keys[LSReducedMatrixElements], {numE,
    SLterm, SpLpterm}],
              LSReducedMatrixElements[{numE, SLterm, SpLpterm}],
              MemberQ[Keys[LSReducedMatrixElements], {numE, SpLpterm,
     SLterm}],
              LSReducedMatrixElements[{numE, SpLpterm, SLterm}],
              True,
              0
            ]
          )
        ];
        matValue,
        {NKSLJMp, NKSLJMps},
        {NKSLJM, NKSLJMs}
        ];
      jjBlockTable[{numE, J, Jp}] = SparseArray[eMatrix],
      {J, AllowedJ[numE]},
      {Jp, AllowedJ[numE]}
      ];

    Js = AllowedJ[numE];
    howManyJs = Length[Js];
    blockHam = ConstantArray[0, {howManyJs, howManyJs}];
    Do[blockHam[[jj, ii]] = jjBlockTable[{numE, Js[[ii]], Js[[jj
    ]]}];,
      {ii, 1, howManyJs},
      {jj, 1, howManyJs}];
    blockHam = ArrayFlatten[blockHam];
    blockHam = SparseArray[blockHam];
    Return[blockHam];
    )
    ];

  (* ###################### Block assembly ###################### *)
  (* ############################################################ *)

  (* ############################################################ *)
  (* ##################### Level Description ##################### *)

  FreeHam::usage = "FreeHam[JJBlocks, numE] given the JJ blocks of
    the Hamiltonian for f^n, this function returns a list with all the
     scalar-simplified versions of the blocks.";
```

```
FreeHam[JJBlocks_List, numE_Integer] := Module[
  {Js, basisJ, pivot, freeHam, idx, J,
  thisJbasis, shrunkBasisPositions, theBlock},
  (
    Js       = AllowedJ[numE];
    basisJ   = BasisLSJMJ[numE, "AsAssociation" -> True];
    pivot    = If[OddQ[numE], 1/2, 0];
    freeHam = Table[(
      J          = Js[[idx]];
      theBlock   = JJBlocks[[idx]];
      thisJbasis = basisJ[J];
      (* find the basis vectors that end with pivot *)
      shrunkBasisPositions = Flatten[Position[thisJbasis, {_ ..., pivot}]];
      (* take only those rows and columns *)
      theBlock[[shrunkBasisPositions, shrunkBasisPositions]]
    ),
    {idx, 1, Length[Js]}
    ];
    Return[freeHam];
  )
];

ListRepeater::usage = "ListRepeater[list, reps] repeats each element of list reps times.";
ListRepeater[list_List, repeats_Integer] := (
  Flatten[ConstantArray[#, repeats] & /@ list]
);

ListLever::usage = "ListLever[vecs, multiplicity] takes a list of vectors and returns all interleaved shifted versions of them.";
ListLever[vecs_, multiplicity_] := Module[
{uppityVecs, uppityVec},
(
  uppityVecs = Table[(
    uppityVec = PadRight[{#}, multiplicity] & /@ vec;
    uppityVec = Permutations /@ uppityVec;
    uppityVec = Transpose[uppityVec];
    uppityVec = Flatten /@ uppityVec
    ),
  {vec, vecs}
  ];
  Return[Flatten[uppityVecs, 1]];
)
];

EigenLever::usage = "EigenLever[eigenSys, multiplicity] takes a list eigenSys of the form {eigenvalues, eigenvectors} and returns the eigenvalues repeated multiplicity times and the eigenvectors interleaved and shifted accordingly.";
EigenLever[eigenSys_, multiplicity_] := Module[
  {eigenVals, eigenVecs,
  leveledEigenVecs, leveledEigenVals},
  (
    {eigenVals, eigenVecs} = eigenSys;
    leveledEigenVals       = ListRepeater[eigenVals, multiplicity];
    leveledEigenVecs       = ListLever[eigenVecs, multiplicity];
    Return[{Flatten[leveledEigenVals], leveledEigenVecs}]
  )
];


LevelSimplerSymbolicHamMatrix::usage = "
  LevelSimplerSymbolicHamMatrix[numE] is a variation of
  HamMatrixAssembly that returns the diagonal JJ Hamiltonian blocks
  applying a simplifier and with simplifications adequate for the
  level description. The keys of the given association correspond to
   the different values of J that are possible for f^numE, the
  values are sparse array that are meant to be interpreted in the
  basis provided by BasisLSJ.
The option \"Simplifier\" is a list of symbols that are set to zero
  . At a minimum this has to include the crystal field parameters.
  By default this includes everything except the Slater parameters
  Fk and the spin orbit coupling ζ.
The option \"Export\" controls whether the resulting association is
   saved to disk, the default is True and the resulting file is
```

```
    saved to the ./hams/ folder. A hash is appended to the filename
    that corresponds to the simplifier used in the resulting
    expression. If the option \"Overwrite\" is set to False then these
     files may be used to quickly retrieve a previously computed case.
     The file is saved both in .m and .mx format.
2694  The option \"PrependToFilename\" can be used to append a string to
    the filename to which the function may export to.
2695  The option \"Return\" can be used to choose whether the function
    returns the matrix or not.
2696  The option \"Overwrite\" can be used to overwrite the file if it
    already exists.";
2697  Options[LevelSimplerSymbolicHamMatrix] = {
2698    "Export" -> True,
2699    "PrependToFilename" -> "",
2700    "Overwrite" -> False,
2701    "Return" -> True,
2702    "Simplifier" -> Join[
2703      {F0,\[Sigma]SS},
2704      cfSymbols,
2705      TSymbols,
2706      casimirSymbols,
2707      pseudoMagneticSymbols,
2708      marvinSymbols,
2709      DeleteCases[magneticSymbols,ζ]
2710    ]
2711  };
2712  LevelSimplerSymbolicHamMatrix[numE_Integer, OptionsPattern[]] :=
    Module[
2713    {thisHamAssoc, Js, fname,
2714    fnamemx, hash, simplifier},
2715    (
2716      simplifier = (#->0)&/@Sort[OptionValue["Simplifier"]];
2717      hash       = Hash[simplifier];
2718      If[Not[ValueQ[ElectrostaticTable]],LoadElectrostatic[]];
2719      If[Not[ValueQ[SOOandECSOTable]],LoadSOOandECSO[]];
2720      If[Not[ValueQ[SpinOrbitTable]],LoadSpinOrbit[]];
2721      If[Not[ValueQ[SpinSpinTable]],LoadSpinSpin[]];
2722      If[Not[ValueQ[ThreeBodyTable]],LoadThreeBody[]];
2723      fname    = FileNameJoin[{moduleDir,"hams",OptionValue["
    PrependToFilename"]<>"Level-SymbolicMatrix-f"<>ToString[numE]<>"-"
    <>ToString[hash]<>".m"}];
2724      fnamemx = FileNameJoin[{moduleDir,"hams",OptionValue["
    PrependToFilename"]<>"Level-SymbolicMatrix-f"<>ToString[numE]<>"-"
    <>ToString[hash]<>".mx"}];
2725      If[Or[FileExistsQ[fname],FileExistsQ[fnamemx]]&&Not[OptionValue
    ["Overwrite"]],
2726      (
2727        If[OptionValue["Return"],
2728        (
2729          Which[FileExistsQ[fnamemx],
2730          (
2731            Print["File ",fnamemx," already exists, and option \"
    Overwrite\" is set to False, loading file ..."];
2732            thisHamAssoc=Import[fnamemx];
2733            Return[thisHamAssoc];
2734          ),
2735          FileExistsQ[fname],
2736          (
2737            Print["File ",fname," already exists, and option \"
    Overwrite\" is set to False, loading file ..."];
2738            thisHamAssoc=Import[fname];
2739            Print["Exporting to file ",fnamemx," for quicker loading.
    "];
2740            Export[fnamemx,thisHamAssoc];
2741            Return[thisHamAssoc];
2742          )
2743          ]
2744        ),
2745        (
2746          Print["File ",fname," already exists, skipping ..."];
2747          Return[Null];
2748        )
2749        ]
2750      )
2751      ];
2752      Js           = AllowedJ[numE];
```

```
2753        thisHamAssoc = HamMatrixAssembly[numE,
2754          "Set t2Switch"->True,
2755          "IncludeZeeman"->False,
2756          "ReturnInBlocks"->True
2757        ];
2758        thisHamAssoc = Diagonal[thisHamAssoc];
2759        thisHamAssoc = Map[SparseArray[ReplaceInSparseArray[#,
      simplifier]]&,thisHamAssoc,{1}];
2760        thisHamAssoc = FreeHam[thisHamAssoc,numE];
2761        thisHamAssoc = AssociationThread[Js->thisHamAssoc];
2762        If[OptionValue["Export"],
2763          (
2764            Print["Exporting to file ",fname," and to ",fnamemx];
2765            Export[fname,thisHamAssoc];
2766            Export[fnamemx,thisHamAssoc];
2767          )
2768        ];
2769        If[OptionValue["Return"],
2770          Return[thisHamAssoc],
2771          Return[Null]
2772        ];
2773      )
2774    ];
2775
2776    LevelSolver::usage = "LevelSolver[numE, params] puts together (or
       retrieves from disk) the symbolic level Hamiltonian for the f^numE
        configuration and solves it for the given params returning the
       resultant energies and eigenstates.
2777    If the option \"Return as states\" is set to False, then the
       function returns an association whose keys are values for J in f^
       numE, and whose values are lists with two elements. The first
       element being equal to the ordered basis for the corresponding
       subpsace, given as a list of lists of the form {LS string, J}. The
        second element being another list of two elements, the first
       element being equal to the energies and the second being equal to
       the corresponding normalized eigenvectors. The energies given have
        been subtracted the energy of the ground state.
2778    If the option \"Return as states\" is set to True, then the
       function returns a list with three elements. The first element is
       the global level basis for the f^numE configuration, given as a
       list of lists of the form {LS string, J}. The second element are
       the mayor LSJ components in the returned eigenstates. The third
       element is a list of lists with three elements, in each list the
       first element being equal to the energy, the second being equal to
        the value of J, and the third being equal to the corresponding
       normalized eigenvector (given as a row). The energies given have
       been subtracted the energy of the ground state, and the states
       have been sorted in order of increasing energy.
2779    The following options are admitted:
2780      - \"Overwrite Hamiltonian\", if set to True the function will
       overwrite the symbolic Hamiltonian. Default is False.
2781      - \"Return as states\", see description above. Default is True.
2782      - \"Simplifier\", this is a list with symbols that are set to
       zero for defining the parameters kept in the level  description.
2783    ";
2784    Options[LevelSolver] = {
2785      "Overwrite Hamiltonian" -> False,
2786      "Return as states" -> True,
2787      "Simplifier" -> Join[
2788        cfSymbols,
2789        TSymbols,
2790        casimirSymbols,
2791        pseudoMagneticSymbols,
2792        marvinSymbols,
2793        DeleteCases[magneticSymbols,ζ]
2794      ],
2795      "PrintFun" -> PrintTemporary
2796    };
2797    LevelSolver[numE_Integer, params0_Association, OptionsPattern[]] :=
        Module[
2798      {ln, simplifier, simpleHam, basis,
2799      numHam, eigensys, startTime, endTime,
2800      diagonalTime, params=params0, globalBasis,
2801      eigenVectors, eigenEnergies, eigenJs,
2802      states, groundEnergy, allEnergies, PrintFun},
2803      (
```

```
    ln          = theLanthanides[[numE]];
    basis       = BasisLSJ[numE, "AsAssociation"->True];
    simplifier = OptionValue["Simplifier"];
    PrintFun    = OptionValue["PrintFun"];
    PrintFun["> LevelSolver for ",ln," with ",numE," f-electrons."];
    PrintFun["> Loading the symbolic level Hamiltonian ..."];
    simpleHam  = LevelSimplerSymbolicHamMatrix[numE,
      "Simplifier" -> simplifier,
      "Overwrite"  -> OptionValue["Overwrite Hamiltonian"]
    ];
    (* Everything that is not given is set to zero *)
    PrintFun["> Setting to zero every parameter not given ..."];
    params     = ParamPad[params, "PrintFun" -> PrintFun];
    PrintFun[params];
    (* Create the numeric hamiltonian *)
    PrintFun["> Replacing parameters in the J-blocks of the Hamiltonian to produce numeric arrays ..."];
    numHam     = N /@ Map[ReplaceInSparseArray[#, params]&, simpleHam];
    Clear[simpleHam];
    (* Eigensolver *)
    PrintFun["> Diagonalizing the numerical Hamiltonian within each separate J-subspace ..."];
    startTime     = Now;
    eigensys      = Eigensystem /@ numHam;
    endTime       = Now;
    diagonalTime  = QuantityMagnitude[endTime-startTime,"Seconds"];
    allEnergies   = Flatten[First/@Values[eigensys]];
    groundEnergy  = Min[allEnergies];
    eigensys      = Map[Chop[{#[[1]]-groundEnergy,#[[2]]}]&,eigensys];
    eigensys      = Association@KeyValueMap[#1->{basis[#1],#2} &, eigensys];
    PrintFun[">> Diagonalization took ",diagonalTime," seconds."];
    If[OptionValue["Return as states"],
      (
        PrintFun["> Padding the eigenvectors to correspond to the level basis ..."];
        eigenVectors  = SparseArray @ BlockDiagonalMatrix[Values[#[[2, 2]] & /@ eigensys]];
        globalBasis   = Flatten[Values[basis], 1];
        eigenEnergies = Flatten[Values[#[[2, 1]] & /@ eigensys]];
        eigenJs       = Flatten[KeyValueMap[ConstantArray[#1, Length[#2[[2, 2]]]] &, eigensys]];
        states        = Transpose[{eigenEnergies, eigenJs, eigenVectors}];
        states        = SortBy[states, First];
        eigenVectors  = Last /@ states;
        LSJmultiplets = (RemoveTrailingDigits[#[[1]]] <> ToString[InputForm[#[[2]]]]) & /@ globalBasis;
        majorComponentIndices = Ordering[Abs[#]][[-1]] & /@ eigenVectors;
        levelLabels           = LSJmultiplets[[majorComponentIndices]];
        Return[{globalBasis, levelLabels, states}];
      ),
      Return[{basis, eigensys}]
    ];
  )
];


(* ################### Level Description ################### *)
(* ########################################################## *)

(* ########################################################## *)
(* ################### Optical Operators ################### *)

magOp = <||>;

JJBlockMagDip::usage = "JJBlockMagDip[numE, J, Jp] returns an array
   for the LSJM matrix elements of the magnetic dipole operator
  between states with given J and Jp. The option \"Sparse\" can be
  used to return a sparse matrix. The default is to return a sparse
  matrix.
```

```
2863  See eqn 15.7 in TASS.
2864  Here it is provided in atomic units in which the Bohr magneton is
        1/2.
2865  \[Mu] = -(1/2) (L + gs S)
2866  We are using the Racah convention for the reduced matrix elements
        in the Wigner-Eckart theorem. See TASS eqn 11.15.
2867  ";
2868  Options[JJBlockMagDip]={"Sparse"->True};
2869  JJBlockMagDip[numE_, braJ_, ketJ_, OptionsPattern[]] := Module[
2870    {braSLJs, ketSLJs,
2871    braSLJ,   ketSLJ,
2872    braSL,    ketSL,
2873    braS,     braL,
2874    ketS,     ketL,
2875    braMJ,    ketMJ,
2876    matValue, magMatrix,
2877    summand1, summand2,
2878    threejays},
2879    (
2880      braSLJs  = AllowedNKSLJMforJTerms[numE,braJ];
2881      ketSLJs  = AllowedNKSLJMforJTerms[numE,ketJ];
2882      magMatrix  = Table[
2883        braSL     = braSLJ[[1]];
2884        ketSL     = ketSLJ[[1]];
2885        {braS, braL}   = FindSL[braSL];
2886        {ketS, ketL}   = FindSL[ketSL];
2887        braMJ       = braSLJ[[3]];
2888        ketMJ       = ketSLJ[[3]];
2889        summand1    = If[Or[braJ  != ketJ,
2890                            braSL != ketSL],
2891          0,
2892          Sqrt[braJ*(braJ+1)*TPO[braJ]]
2893        ];
2894        (* looking at the string includes checking L=L', S=S', and \
    alpha=\alpha'*)
2895        summand2 = If[braSL!= ketSL,
2896          0,
2897          (gs-1) *
2898            Phaser[braS+braL+ketJ+1] *
2899              Sqrt[TPO[braJ]*TPO[ketJ]] *
2900                SixJay[{braJ,1,ketJ},{braS,braL,braS}] *
2901                  Sqrt[braS(braS+1)TPO[braS]]
2902        ];
2903        matValue = summand1 + summand2;
2904        (* We are using the Racah convention for red matrix elements
    in Wigner-Eckart *)
2905        threejays = (ThreeJay[{braJ, -braMJ}, {1, #}, {ketJ, ketMJ}]
    &) /@ {-1,0,1};
2906        threejays *= Phaser[braJ-braMJ];
2907        matValue  = - 1/2 * threejays * matValue;
2908        matValue,
2909      {braSLJ, braSLJs},
2910      {ketSLJ, ketSLJs}
2911      ];
2912      If[OptionValue["Sparse"],
2913        magMatrix = SparseArray[magMatrix]
2914      ];
2915      Return[magMatrix];
2916    )
2917  ];
2918
2919  Options[TabulateJJBlockMagDipTable]={"Sparse"->True};
2920  TabulateJJBlockMagDipTable[numE_,OptionsPattern[]] := (
2921    JJBlockMagDipTable=<||>;
2922    Js=AllowedJ[numE];
2923    Do[
2924      (
2925        JJBlockMagDipTable[{numE,braJ,ketJ}]=
2926          JJBlockMagDip[numE,braJ,ketJ,"Sparse"->OptionValue["Sparse"
    ]]
2927      ),
2928    {braJ, Js},
2929    {ketJ, Js}
2930    ];
2931    Return[JJBlockMagDipTable]
2932  );
```

```
2933
2934  TabulateManyJJBlockMagDipTables::usage = "
        TabulateManyJJBlockMagDipTables[{n1, n2, ...}] calculates the
        tables of matrix elements for the requested f^n_i configurations.
        The function does not return the matrices themselves. It instead
        returns an association whose keys are numE and whose values are
        the filenames where the output of TabulateManyJJBlockMagDipTables
        was saved to. The output consists of an association whose keys are
         of the form {n, J, Jp} and whose values are rectangular arrays
        given the values of <|LSJMJa|H_dip|L'S'J'MJ'a'|>.";
2935  Options[TabulateManyJJBlockMagDipTables]={"FilenameAppendix"->"","
        Overwrite"->False,"Compressed"->True};
2936  TabulateManyJJBlockMagDipTables[ns_,OptionsPattern[]] := (
2937    fnames=<||>;
2938    Do[
2939    (
2940      ExportFun=If[OptionValue["Compressed"],ExportMZip,Export];
2941      PrintTemporary["#------- numE = ",numE," -------#"];
2942      appendTo     = (OptionValue["FilenameAppendix"]<>"-magDip");
2943      exportFname  = JJBlockMatrixFileName[numE,"FilenameAppendix"->
      appendTo];
2944      fnames[numE] = exportFname;
2945      If[FileExistsQ[exportFname]&&Not[OptionValue["Overwrite"]],
2946        Continue[]
2947      ];
2948      JJBlockMatrixTable = TabulateJJBlockMagDipTable[numE];
2949      If[FileExistsQ[exportFname]&&OptionValue["Overwrite"],
2950        DeleteFile[exportFname]
2951      ];
2952      ExportFun[exportFname,  JJBlockMatrixTable];
2953    ),
2954    {numE,ns}
2955    ];
2956    Return[fnames];
2957  );
2958
2959  MagDipoleMatrixAssembly::usage = "MagDipoleMatrixAssembly[numE]
        returns the matrix representation of the operator - 1/2 (L + gs S)
         in the f^numE configuration. The function returns a list with
        three elements corresponding to the x,y,z components of this
        operator. The option \"FilenameAppendix\" can be used to append a
        string to the filename from which the function imports from in
        order to patch together the array. For numE beyond 7 the function
        returns the same as for the complementary configuration. The
        option \"ReturnInBlocks\" can be used to return the matrices in
        blocks. The default is to return the matrices in flattened form
        and as sparse array.";
2960  Options[MagDipoleMatrixAssembly]={
2961    "FilenameAppendix"->"",
2962    "ReturnInBlocks"->False};
2963  MagDipoleMatrixAssembly[nf_Integer, OptionsPattern[]] := Module[
2964    {ImportFun, numE, appendTo,
2965    emFname, JJBlockMagDipTable,
2966    Js, howManyJs, blockOp,
2967    rowIdx, colIdx},
2968    (
2969      ImportFun = ImportMZip;
2970      numE      = nf;
2971      numH      = 14 - numE;
2972      numE      = Min[numE,numH];
2973
2974      appendTo  = (OptionValue["FilenameAppendix"]<>"-magDip");
2975      emFname   = JJBlockMatrixFileName[numE,"FilenameAppendix"->
      appendTo];
2976      JJBlockMagDipTable = ImportFun[emFname];
2977
2978      Js        = AllowedJ[numE];
2979      howManyJs = Length[Js];
2980      blockOp   = ConstantArray[0,{howManyJs,howManyJs}];
2981      Do[
2982        blockOp[[rowIdx,colIdx]] = JJBlockMagDipTable[{numE,Js[[
      rowIdx]],Js[[colIdx]]}],
2983        {rowIdx,1,howManyJs},
2984        {colIdx,1,howManyJs}
2985      ];
2986      If[OptionValue["ReturnInBlocks"],
```

```
        (
          opMinus = Map[#[[1]]&, blockOp, {4}];
          opZero  = Map[#[[2]]&, blockOp, {4}];
          opPlus  = Map[#[[3]]&, blockOp, {4}];
          opX =   (opMinus - opPlus)/Sqrt[2];
          opY = I (opPlus + opMinus)/Sqrt[2];
          opZ = opZero;
        ),
          blockOp = ArrayFlatten[blockOp];
          opMinus = blockOp[[;; , ;; , 1]];
          opZero  = blockOp[[;; , ;; , 2]];
          opPlus  = blockOp[[;; , ;; , 3]];
          opX =   (opMinus - opPlus)/Sqrt[2];
          opY = I (opPlus + opMinus)/Sqrt[2];
          opZ = opZero;
      ];
      Return[{opX, opY, opZ}];
    )
  ];

  MagDipLineStrength::usage = "MagDipLineStrength[theEigensys, numE]
    takes the eigensystem of an ion and the number numE of f-electrons
     that correspond to it and calculates the line strength array Stot
    .
  The option \"Units\" can be set to either \"SI\" (so that the units
     of the returned array are (A m^2)^2) or to \"Hartree\".
  The option \"States\" can be used to limit the states for which the
     line strength is calculated. The default, All, calculates the
    line strength for all states. A second option for this is to
    provide an index labelling a specific state, in which case only
    the line strengths between that state and all the others are
    computed.
  The returned array should be interpreted in the eigenbasis of the
    Hamiltonian. As such the element Stot[[i,i]] corresponds to the
    line strength states between states |i> and |j>.";
  Options[MagDipLineStrength]={"Reload MagOp" -> False, "Units"->"SI"
    , "States" -> All};
  MagDipLineStrength[theEigensys_List, numE0_Integer, OptionsPattern
    []] := Module[
    {numE, allEigenvecs, Sx, Sy, Sz, Stot, factor},
    (
      numE = Min[14-numE0, numE0];
      (*If not loaded then load it, *)
      If[Or[
          Not[MemberQ[Keys[magOp], numE]],
          OptionValue["Reload MagOp"]],
      (
        magOp[numE] = ReplaceInSparseArray[#, {gs->2}]& /@
    MagDipoleMatrixAssembly[numE];
      )
      ];
      allEigenvecs = Transpose[Last /@ theEigensys];
      Which[OptionValue["States"] === All,
        (
          {Sx, Sy, Sz} = (ConjugateTranspose[allEigenvecs].#.
    allEigenvecs) & /@ magOp[numE];
          Stot         = Abs[Sx]^2+Abs[Sy]^2+Abs[Sz]^2;
        ),
        IntegerQ[OptionValue["States"]],
        (
          singleState  = theEigensys[[OptionValue["States"],2]];
          {Sx, Sy, Sz} = (ConjugateTranspose[allEigenvecs].#.
    singleState) & /@ magOp[numE];
          Stot         = Abs[Sx]^2+Abs[Sy]^2+Abs[Sz]^2;
        )
      ];
      Which[
        OptionValue["Units"] == "SI",
          Return[4 \[Mu]B^2 * Stot],
        OptionValue["Units"] == "Hartree",
          Return[Stot],
        True,
        (
          Print["Invalid option for \"Units\". Options are \"SI\" and
     \"Hartree\"."];
          Abort[];
```

```
        )
      ];
    )
];

MagDipoleRates::usage = "MagDipoleRates[eigenSys, numE] calculates
  the magnetic dipole transition rate array for the provided
  eigensystem. The option \"Units\" can be set to \"SI\" or to \"
  Hartree\". If the option \"Natural Radiative Lifetimes\" is set to
   true then the reciprocal of the rate is returned instead.
  eigenSys is a list of lists with two elements, in each list the
  first element is the energy and the second one the corresponding
  eigenvector.
Based on table 7.3 of Thorne 1999, using g2=1.
The energy unit assumed in eigenSys is kayser.
The returned array should be interpreted in the eigenbasis of the
  Hamiltonian. As such the element AMD[[i,i]] corresponds to the
  transition rate (or the radiative lifetime, depending on options)
  between eigenstates |i> and |j>.
By default this assumes that the refractive index is unity, this
  may be changed by setting the option \"RefractiveIndex\" to the
  desired value.
The option \"Lifetime\" can be used to return the reciprocal of the
   transition rates. The default is to return the transition rates."
  ;
Options[MagDipoleRates]={"Units"->"SI", "Lifetime"->False, "
  RefractiveIndex"->1};
MagDipoleRates[eigenSys_List, numE0_Integer,OptionsPattern[]] :=
  Module[
   {AMD, Stot, eigenEnergies,
   transitionWaveLengthsInMeters, nRefractive},
   (
     nRefractive   = OptionValue["RefractiveIndex"];
     numE          = Min[14-numE0, numE0];
     Stot          = MagDipLineStrength[eigenSys, numE, "Units" ->
  OptionValue["Units"]];
     eigenEnergies = Chop[First/@eigenSys];
     energyDiffs   = Outer[Subtract, eigenEnergies, eigenEnergies];
     energyDiffs   = ReplaceDiagonal[energyDiffs, Indeterminate];
     (* Energies assumed in kayser.*)
     transitionWaveLengthsInMeters = 0.01/energyDiffs;

     unitFactor    = Which[
     OptionValue["Units"]=="Hartree",
     (
       (* The bohrRadius factor in SI needed to convert the
  wavelengths which are assumed in m*)
       16 \[Pi]^3 (\[Mu]0Hartree /(3 hPlanckFine)) * bohrRadius^3
     ),
     OptionValue["Units"]=="SI",
     (
       16 \[Pi]^3 \[Mu]0/(3 hPlanck)
     ),
     True,
     (
       Print["Invalid option for \"Units\". Options are \"SI\" and \
  "Hartree\"."];
       Abort[];
     )
     ];
     AMD = unitFactor / transitionWaveLengthsInMeters^3 * Stot *
  nRefractive^3;
     Which[OptionValue["Lifetime"],
       Return[1/AMD],
       True,
       Return[AMD]
     ]
   )
];

GroundMagDipoleOscillatorStrength::usage = "
  GroundMagDipoleOscillatorStrength[eigenSys, numE] calculates the
  magnetic diople oscillator strengths between the ground state and
  the excited states as given by eigenSys.
Based on equation 8 of Carnall 1965, removing the 2J+1 factor since
   this degeneracy has been removed by the crystal field.
```

```
3098  eigenSys is a list of lists with two elements, in each list the
        first element is the energy and the second one the corresponding
        eigenvector.
3099  The energy unit assumed in eigenSys is Kayser.
3100  The oscillator strengths are dimensionless.
3101  The returned array should be interpreted in the eigenbasis of the
        Hamiltonian. As such the element fMDGS[[i]] corresponds to the
        oscillator strength between ground state and eigenstate |i>.
3102  By default this assumes that the refractive index is unity, this
        may be changed by setting the option \"RefractiveIndex\" to the
        desired value.";
3103  Options[GroundMagDipoleOscillatorStrength]={"RefractiveIndex"->1};
3104  GroundMagDipoleOscillatorStrength[eigenSys_List, numE_Integer,
        OptionsPattern[]] := Module[
3105    {eigenEnergies, SMDGS, GSEnergy, energyDiffs,
3106    transitionWaveLengthsInMeters, unitFactor, nRefractive},
3107    (
3108      eigenEnergies    = First/@eigenSys;
3109      nRefractive      = OptionValue["RefractiveIndex"];
3110      SMDGS            = MagDipLineStrength[eigenSys,numE, "Units"->"
        SI", "States"->1];
3111      GSEnergy         = eigenSys[[1,1]];
3112      energyDiffs      = eigenEnergies-GSEnergy;
3113      energyDiffs[[1]] = Indeterminate;
3114      transitionWaveLengthsInMeters = 0.01/energyDiffs;
3115      unitFactor       = (8\[Pi]^2 me)/(3 hPlanck eCharge^2 cLight);
3116      fMDGS            = unitFactor / transitionWaveLengthsInMeters *
       SMDGS * nRefractive;
3117      Return[fMDGS];
3118    )
3119  ];
3120
3121  (* ##################### Optical Operators ##################### *)
3122  (* ############################################################ *)
3123
3124  (* ############################################################ *)
3125  (* ################### Printers and Labels ################### *)
3126
3127  PrintL::usage = "PrintL[L] give the string representation of a
        given angular momentum.";
3128  PrintL[L_] := If[StringQ[L], L, StringTake[specAlphabet, {L + 1}]]
3129
3130  FindSL::usage = "FindSL[LS] gives the spin and orbital angular
        momentum that corresponds to the provided string LS.";
3131  FindSL[SL_] := (
3132    FindSL[SL] =
3133    If[StringQ[SL],
3134      {
3135        (ToExpression[StringTake[SL, 1]]-1)/2,
3136        StringPosition[specAlphabet, StringTake[SL, {2}]][[1, 1]]-1
3137      },
3138      SL
3139    ]
3140  );
3141
3142  PrintSLJ::usage = "Given a list with three elements {S, L, J} this
        function returns a symbol where the spin multiplicity is presented
       as a superscript, the orbital angular momentum as its
        corresponding spectroscopic letter, and J as a subscript. Function
       does not check to see if the given J is compatible with the given
       S and L.";
3143  PrintSLJ[SLJ_] := (
3144    RowBox[{
3145      SuperscriptBox[" ", 2 SLJ[[1]] + 1],
3146      SubscriptBox[PrintL[SLJ[[2]]], SLJ[[3]]]
3147      }
3148      ] // DisplayForm
3149    );
3150
3151  PrintSLJM::usage = "Given a list with four elements {S, L, J, MJ}
        this function returns a symbol where the spin multiplicity is
        presented as a superscript, the orbital angular momentum as its
        corresponding spectroscopic letter, and {J, MJ} as a subscript. No
       attempt is made to guarantee that the given input is consistent."
        ;
3152  PrintSLJM[SLJM_] := (
```

```
3153      RowBox[{
3154        SuperscriptBox[" ", 2 SLJM[[1]] + 1],
3155        SubscriptBox[PrintL[SLJM[[2]]], {SLJM[[3]], SLJM[[4]]}]
3156        }
3157        ] // DisplayForm
3158      );
3159
3160    (* ################### Printers and Labels ################### *)
3161    (* ############################################################ *)
3162
3163    (* ############################################################ *)
3164    (* ###################### Term management ###################### *)
3165
3166    AllowedSLTerms::usage = "AllowedSLTerms[numE] returns a list with
        the allowed terms in the f^numE configuration, the terms are given
         as lists in the format {S, L}. This list may have redundancies
        which are compatible with the degeneracies that might correspond
        to the given case.";
3167    AllowedSLTerms[numE_] := Map[FindSL[First[#]] &, CFPTerms[Min[numE,
        14-numE]]];
3168
3169    AllowedNKSLTerms::usage = "AllowedNKSLTerms[numE] returns a list
        with the allowed terms in the f^numE configuration, the terms are
        given as strings in spectroscopic notation. The integers in the
        last positions are used to distinguish cases with degeneracy.";
3170    AllowedNKSLTerms[numE_] := Map[First, CFPTerms[Min[numE, 14-numE
        ]]];
3171    AllowedNKSLTerms[0]  = {"1S"};
3172    AllowedNKSLTerms[14] = {"1S"};
3173
3174    MaxJ::usage = "MaxJ[numE] gives the maximum J = S+L that
        corresponds to the configuration f^numE.";
3175    MaxJ[numE_] := Max[Map[Total, AllowedSLTerms[Min[numE, 14-numE]]]];
3176
3177    MinJ::usage = "MinJ[numE] gives the minimum J = S+L that
        corresponds to the configuration f^numE.";
3178    MinJ[numE_] := Min[Map[Abs[Part[#, 1] - Part[#, 2]] &,
        AllowedSLTerms[Min[numE, 14-numE]]]]
3179
3180    AllowedSLJTerms::usage = "AllowedSLJTerms[numE] returns a list with
         the allowed {S, L, J} terms in the f^n configuration, the terms
        are given as lists in the format {S, L, J}. This list may have
        repeated elements which account for possible degeneracies of the
        related term.";
3181    AllowedSLJTerms[numE_] := Module[
3182      {idx1, allowedSL, allowedSLJ},
3183      (
3184        allowedSL = AllowedSLTerms[numE];
3185        allowedSLJ = {};
3186        For[
3187          idx1 = 1,
3188          idx1 <= Length[allowedSL],
3189          termSL = allowedSL[[idx1]];
3190          termsSLJ =
3191            Table[
3192              {termSL[[1]], termSL[[2]], J},
3193            {J,Abs[termSL[[1]] - termSL[[2]]], Total[termSL]}
3194            ];
3195          allowedSLJ = Join[allowedSLJ, termsSLJ];
3196          idx1++
3197        ];
3198        SortBy[allowedSLJ, Last]
3199      )
3200    ];
3201
3202    AllowedNKSLJTerms::usage = "AllowedNKSLJTerms[numE] returns a list
        with the allowed {SL, J} terms in the f^n configuration, the terms
         are given as lists in the format {SL, J} where SL is a string in
        spectroscopic notation.";
3203    AllowedNKSLJTerms[numE_] := Module[
3204      {allowedSL, allowedNKSL, allowedSLJ, nn},
3205      (
3206        allowedNKSL = AllowedNKSLTerms[numE];
3207        allowedSL = AllowedSLTerms[numE];
3208        allowedSLJ = {};
3209        For[
```

```
3210        nn = 1,
3211        nn <= Length[allowedSL],
3212        (
3213          termSL = allowedSL[[nn]];
3214          termNKSL = allowedNKSL[[nn]];
3215          termsSLJ =
3216            Table[{termNKSL, J},
3217            {J, Abs[termSL[[1]] - termSL[[2]]], Total[termSL]}
3218            ];
3219          allowedSLJ = Join[allowedSLJ, termsSLJ];
3220          nn++
3221        )
3222      ];
3223      SortBy[allowedSLJ, Last]
3224    )
3225  ];
3226
3227  AllowedNKSLforJTerms::usage = "AllowedNKSLforJTerms[numE, J] gives
       the terms that correspond to the given total angular momentum J in
        the f^n configuration. The result is a list whose elements are
       lists of length 2, the first element being the SL term in
       spectroscopic notation, and the second element being J.";
3228  AllowedNKSLforJTerms[numE_, J_] := Module[
3229    {allowedSL, allowedNKSL, allowedSLJ,
3230    nn, termSL, termNKSL, termsSLJ},
3231    (
3232      allowedNKSL = AllowedNKSLTerms[numE];
3233      allowedSL = AllowedSLTerms[numE];
3234      allowedSLJ = {};
3235      For[
3236        nn = 1,
3237        nn <= Length[allowedSL],
3238        (
3239          termSL = allowedSL[[nn]];
3240          termNKSL = allowedNKSL[[nn]];
3241          termsSLJ = If[Abs[termSL[[1]] - termSL[[2]]] <= J <= Total[
       termSL],
3242            {{termNKSL, J}},
3243            {}
3244            ];
3245          allowedSLJ = Join[allowedSLJ, termsSLJ];
3246          nn++
3247        )
3248      ];
3249      Return[allowedSLJ]
3250    )
3251  ];
3252
3253  AllowedSLJMTerms::usage = "AllowedSLJMTerms[numE] returns a list
       with all the states that correspond to the configuration f^n. A
       list is returned whose elements are lists of the form {S, L, J, MJ
       }.";
3254  AllowedSLJMTerms[numE_] := Module[
3255    {allowedSLJ, allowedSLJM,
3256    termSLJ, termsSLJM, nn},
3257    (
3258    allowedSLJ = AllowedSLJTerms[numE];
3259    allowedSLJM = {};
3260    For[
3261      nn = 1,
3262      nn <= Length[allowedSLJ],
3263      nn++,
3264      (
3265        termSLJ = allowedSLJ[[nn]];
3266        termsSLJM =
3267          Table[{termSLJ[[1]], termSLJ[[2]], termSLJ[[3]], M},
3268          {M, - termSLJ[[3]], termSLJ[[3]]}
3269          ];
3270        allowedSLJM = Join[allowedSLJM, termsSLJM];
3271      )
3272    ];
3273    Return[SortBy[allowedSLJM, Last]];
3274    )
3275  ];
3276
3277  AllowedNKSLJMforJMTerms::usage = "AllowedNKSLJMforJMTerms[numE, J,
```

```
    MJ] returns a list with all the terms that contain states of the f
    ^n configuration that have a total angular momentum J, and a
    projection along the z-axis MJ. The returned list has elements of
    the form {SL (string in spectroscopic notation), J, MJ}.";
3278  AllowedNKSLJMforJMTerms[numE_, J_, MJ_] := Module[
3279    {allowedSL, allowedNKSL,
3280    allowedSLJM, nn},
3281    (
3282      allowedNKSL = AllowedNKSLTerms[numE];
3283      allowedSL   = AllowedSLTerms[numE];
3284      allowedSLJM = {};
3285      For[
3286        nn = 1,
3287        nn <= Length[allowedSL],
3288        termSL = allowedSL[[nn]];
3289        termNKSL = allowedNKSL[[nn]];
3290        termsSLJ = If[(Abs[termSL[[1]] - termSL[[2]]]
3291                      <= J
3292                      <= Total[termSL]
3293                      && (Abs[MJ] <= J)
3294                      ),
3295                      {{termNKSL, J, MJ}},
3296                      {}];
3297        allowedSLJM = Join[allowedSLJM, termsSLJ];
3298        nn++
3299      ];
3300      Return[allowedSLJM];
3301    )
3302  ];
3303
3304  AllowedNKSLJMforJTerms::usage = "AllowedNKSLJMforJTerms[numE, J]
    returns a list with all the states that have a total angular
    momentum J. The returned list has elements of the form {{SL (
    string in spectroscopic notation), J}, MJ}, and if the option \"
    Flat\" is set to True then the returned list has element of the
    form {SL (string in spectroscopic notation), J, MJ}.";
3305  AllowedNKSLJMforJTerms[numE_, J_] := Module[
3306    {MJs, labelsAndMomenta, termsWithJ},
3307    (
3308      MJs = AllowedMforJ[J];
3309      (* Pair LS labels and their {S,L} momenta *)
3310      labelsAndMomenta = ({#, FindSL[#]}) & /@ AllowedNKSLTerms[numE
    ];
3311      (* A given term will contain J if |L-S|<=J<=L+S *)
3312      ContainsJ[{SL_String, {S_, L_}}] := (Abs[S - L] <= J <= (S + L)
    );
3313      (* Keep just the terms that satisfy this condition *)
3314      termsWithJ = Select[labelsAndMomenta, ContainsJ];
3315      (* We don't want to keep the {S,L} *)
3316      termsWithJ = {#[[1]], J} & /@ termsWithJ;
3317      (* This is just a quick way of including up all the MJ values
    *)
3318      Return[Flatten /@ Tuples[{termsWithJ, MJs}]]
3319    )
3320  ];
3321
3322  AllowedMforJ::usage = "AllowedMforJ[J] is shorthand for Range[-J, J
    , 1].";
3323  AllowedMforJ[J_] := Range[-J, J, 1];
3324
3325  AllowedJ::usage = "AllowedJ[numE] returns the total angular momenta
     J that appear in the f^numE configuration.";
3326  AllowedJ[numE_] := Table[J, {J, MinJ[numE], MaxJ[numE]}];
3327
3328  Seniority::usage = "Seniority[LS] returns the seniority of the
    given term.";
3329  Seniority[LS_] := FindNKLSTerm[LS][[1, 2]];
3330
3331  FindNKLSTerm::usage = "Given the string LS FindNKLSTerm[SL] returns
     all the terms that are compatible with it. This is only for f^n
    configurations. The provided terms might belong to more than one
    configuration. The function returns a list with elements of the
    form {LS, seniority, W, U}.";
3332  FindNKLSTerm[SL_] := Module[
3333    {NKterms, n},
3334    (
```

```
3335      n = 7;
3336      NKterms = {{}};
3337      Map[
3338        If[! StringFreeQ[First[#], SL],
3339          If[ToExpression[Part[#, 2]] <= n,
3340            NKterms = Join[NKterms, {#}, 1]
3341          ]
3342        ] &,
3343      fnTermLabels
3344      ];
3345      NKterms = DeleteCases[NKterms, {}];
3346      NKterms
3347    )
3348  ];
3349
3350  ParseTermLabels::usage = "ParseTermLabels[] parses the labels for
       the terms in the f^n configurations based on the labels for the f6
        and f7 configurations. The function returns a list whose elements
        are of the form {LS, seniority, W, U}.";
3351  Options[ParseTermLabels] = {"Export" -> True};
3352  ParseTermLabels[OptionsPattern[]] := Module[
3353    {labelsTextData, fNtextLabels, nielsonKosterLabels,
3354    seniorities, RacahW, RacahU},
3355    (
3356      labelsTextData = FileNameJoin[{moduleDir, "data", "
       NielsonKosterLabels_f6_f7.txt"}];
3357      fNtextLabels   = Import[labelsTextData];
3358      nielsonKosterLabels = Partition[StringSplit[fNtextLabels], 3];
3359      termLabels = Map[Part[#, {1}] &, nielsonKosterLabels];
3360      seniorities = Map[ToExpression[Part[# , {2}]] &,
       nielsonKosterLabels];
3361      racahW =
3362        Map[
3363          StringTake[
3364            Flatten[StringCases[Part[# , {3}],
3365              "(" ~~ DigitCharacter ~~ DigitCharacter ~~
       DigitCharacter ~~ ")"]],
3366            {2, 4}
3367          ] &,
3368        nielsonKosterLabels];
3369      racahU =
3370        Map[
3371          StringTake[
3372            Flatten[StringCases[Part[# , {3}],
3373              "(" ~~ DigitCharacter ~~ DigitCharacter ~~ ")"]],
3374            {2, 3}
3375          ] &,
3376        nielsonKosterLabels];
3377      fnTermLabels = Join[termLabels, seniorities, racahW, racahU,
       2];
3378      fnTermLabels = Sort[fnTermLabels];
3379      If[OptionValue["Export"],
3380        (
3381          broadFname = FileNameJoin[{moduleDir,"data","fnTerms.m"}];
3382          Export[broadFname, fnTermLabels];
3383        )
3384      ];
3385      Return[fnTermLabels];
3386    )
3387  ];
3388
3389  (* ###################### Term management ###################### *)
3390  (* ############################################################ *)
3391
3392  LoadLaF3Parameters::usage = "LoadLaF3Parameters[ln] takes a string
       with the symbol the element of a trivalent lanthanide ion and
       returns model parameters for it. It is based on the data for LaF3.
        If the option \"Free Ion\" is set to True then the function sets
       all crystal field parameters to zero. Through the option \"gs\" it
        allows modyfing the electronic gyromagnetic ratio. For
       completeness this function also computes the E parameters using
       the F parameters quoted on Carnall.";
3393  Options[LoadLaF3Parameters] = {
3394      "Free Ion"->False,
3395      "gs"->2.002319304386,
3396      "With Uncertainties"->False
```

```
    };
LoadLaF3Parameters[Ln_String, OptionsPattern[]] := Module[
  {params, uncertain,
  uncertainKeys, uncertainRules},
  (
    If[Not[ValueQ[Carnall]],
      LoadCarnall[];
    ];
    params = Association[Carnall["data"][Ln]];
    (*If a free ion then all the parameters from the crystal field
  are set to zero*)
    If[OptionValue["Free Ion"],
      Do[params[cfSymbol] = 0, {cfSymbol, cfSymbols}]
    ];
    params[F0] = 0;
    params[M2] = 0.56 * params[M0]; (*See Carnall 1989,Table I,
  caption,probably fixed based on HF values*)
    params[M4] = 0.31 * params[M0]; (*See Carnall 1989,Table I,
  caption,probably fixed based on HF values*)
    params[P0] = 0;
    params[P4] = 0.5 * params[P2];  (*See Carnall 1989,Table I,
  caption,probably fixed based on HF values*)
    params[P6] = 0.1 * params[P2];  (*See Carnall 1989,Table I,
  caption,probably fixed based on HF values*)
    params[gs] = OptionValue["gs"];
    {params[E0], params[E1], params[E2], params[E3]} = FtoE[params[
  F0], params[F2], params[F4], params[F6]];
    params[E0] = 0;
    If[
      Not[OptionValue["With Uncertainties"]],
      Return[params],
      (
        uncertain     = Association[Carnall["annotations"][Ln]];
        uncertainKeys = Keys[uncertain];
        uncertain     = If[# == "Not allowed to vary in fitting."
  || # == "Interpolated",
            0., #] & /@ uncertain;
        paramKeys = Keys[params];
        uncertainVals = Sort[Intersection[paramKeys, uncertainKeys
  ]] /. Association[uncertain];
        uncertainRules = MapThread[Rule, {Sort[uncertainKeys],
  uncertainVals}];
        Which[
          MemberQ[{"Ce", "Yb"}, Ln],
          (
            subsetL = {F0};
            subsetR = {0};
          ),
          True,
          (
          subsetL = {F0, M2, M4, P0, P4, P6, E0, E1, E2, E3};
          subsetR = {0, M0*0.65, M0*0.31, 0, P2*0.5, P2*0.1,
            0,
            Sqrt[(196 F2^2)/164025 + (49 F4^2)/88209 + (122500 F6
  ^2)/134165889],
            Sqrt[F2^2/4100625 + F4^2/10673289 + (30625 F6^2)
  /2743558264161],
            Sqrt[F2^2/18225 + (4 F4^2)/1185921 + (30625 F6^2)
  /1803785841]};
          )
        ];
        uncertainRules = Join[uncertainRules, MapThread[Rule, {
  subsetL,subsetR /. uncertainRules}]];
        uncertainRules = Association[uncertainRules];
        Which[
          Ln == "Eu",
          (
            uncertainRules[F4] = 12.121;
            uncertainRules[F6] = 15.872;
          ),
          Ln == "Gd",
          (
            uncertainRules[F4] = 12.07;
          ),
          Ln == "Tb",
          (
```

```
3460              uncertainRules[F4] = 41.006;
3461            )
3462          ];
3463          If[MemberQ[{"Eu","Gd","Tb"},Ln],
3464            (
3465              uncertainRules[E1] = Sqrt[(196 F2^2)/164025 + (49 F4^2)
    /88209 + (122500 F6^2)/134165889] /. uncertainRules;
3466              uncertainRules[E2] = Sqrt[F2^2/4100625 + F4^2/10673289
    + (30625 F6^2)/2743558264161] /. uncertainRules;
3467              uncertainRules[E3] = Sqrt[F2^2/18225 + (4 F4^2)/1185921
     + (30625 F6^2)/1803785841] /. uncertainRules;
3468            )
3469          ];
3470          uncertainKeys = First /@ Normal[uncertainRules];
3471          fullParams = Association[MapThread[Rule, {uncertainKeys,
    MapThread[Around, {uncertainKeys /. params, uncertainKeys /.
    uncertainRules}]}]];
3472          Return[Join[params, fullParams]]
3473        )
3474        ];
3475     )
3476   ];
3477
3478   LoadLiYF4Parameters::usage="LoadLiYF4Parameters[ln] takes a string
      with the symbol the element of a trivalent lanthanide ion and
      returns model parameters for it. It return the data for LiYF4 from
       Cheng et al.";
3479   LoadLiYF4Parameters[ln_, OptionsPattern[]]:=(
3480     If[!ValueQ[paramsLiYF4],
3481       paramsChengLiYF4 = Import[FileNameJoin[{moduleDir,"data","
    chengLiYF4.m"}]];
3482     ];
3483     Return[paramsChengLiYF4[ln]];
3484   )
3485
3486   HoleElectronConjugation::usage = "HoleElectronConjugation[params]
      takes the parameters (as an association) that define a
      configuration and converts them so that they may be interpreted as
       corresponding to a complentary hole configuration. Some of this
      can be simply done by changing the sign of the model parameters.
      In the case of the effective three body interaction the
      relationship is more complex and is controlled by the value of the
       isE variable.";
3487   HoleElectronConjugation[params_] := Module[
3488     {newparams = params},
3489     (
3490       flipSignsOf = Join[{ζ} , cfSymbols, TSymbols];
3491       flipped = Table[
3492         (
3493           flipper -> - newparams[flipper]
3494         ),
3495         {flipper, flipSignsOf}
3496         ];
3497       nonflipped = Table[
3498         (
3499           flipper -> newparams[flipper]
3500         ),
3501         {flipper, Complement[Keys[newparams], flipSignsOf]}
3502         ];
3503       flippedParams = Association[Join[nonflipped, flipped]];
3504       flippedParams = Select[flippedParams, FreeQ[#, Missing]&];
3505       Return[flippedParams];
3506     )
3507   ];
3508
3509   IonSolver::usage = "IonSolver[numE, params, host] puts together (or
       retrieves from disk) the symbolic Hamiltonian for the f^numE
      configuration and solves it for the given params.
3510   params is an Association with keys equal to parameter symbols and
      values their numerical values. The function will replace the
      symbols in the symbolic Hamiltonian with their numerical values
      and then diagonalize the resulting matrix. Any parameter that is
      not defined in the params Association is assumed to be zero.
3511   host is an optional string that may be used to prepend the filename
       of the symbolic Hamiltonian that is saved to disk. The default is
       \"Ln\".
```

```
3512  The function returns the eigensystem as a list of lists where in
        each list the first element is the energy and the second element
        the corresponding eigenvector.
3513  Tha ordered basis in which this eigenvector is to be interpreted is
         the one corresponding to BasisLSJMJ[numE].
3514  The function admits the following options:
3515  \"Include Spin-Spin\" (bool) : If True then the spin-spin
        interaction is included as a contribution to the m_k operators.
        The default is True.
3516  \"Overwrite Hamiltonian\" (bool) : If True then the function will
        overwrite the symbolic Hamiltonian that is saved to disk to
        expedite calculations. The default is False. The symbolic
        Hamiltonian is saved to disk to the ./hams/ folder preceded by the
         string host.
3517  \"Zeroes\" (list) : A list with symbols assumed to be zero.
3518  ";
3519  Options[IonSolver] = {
3520    "Include Spin-Spin" -> True,
3521    "Overwrite Hamiltonian" -> False,
3522    "Zeroes" -> {}
3523  };
3524  IonSolver[numE_Integer, params0_Association, host_String:"Ln",
        OptionsPattern[]] := Module[
3525    {ln, simplifier, simpleHam, numHam, eigensys,
3526    startTime, endTime, diagonalTime,
3527    params=params0, zeroSymbols},
3528    (
3529      ln = theLanthanides[[numE]];
3530
3531      (* This could be done when replacing values, but this produces
        smaller saved arrays. *)
3532      simplifier = (#-> 0) & /@ OptionValue["Zeroes"];
3533      simpleHam = SimplerSymbolicHamMatrix[numE,
3534        simplifier,
3535        "PrependToFilename" -> host,
3536        "Overwrite" -> OptionValue["Overwrite Hamiltonian"]
3537      ];
3538
3539      (* Note that we don't have to flip signs of parameters for fn
        beyond f7 since the matrix produced
3540      by SimplerSymbolicHamMatrix has already accounted for this. *)
3541
3542      (* Everything that is not given is set to zero *)
3543      params = ParamPad[params];
3544      PrintFun[params];
3545
3546      (* Enforce the override to the spin-spin contribution to the
        magnetic interactions *)
3547      params[\[Sigma]SS] = If[OptionValue["Include Spin-Spin"], 1,
        0];
3548
3549      (* Create the numeric hamiltonian *)
3550      numHam = ReplaceInSparseArray[simpleHam, params];
3551      Clear[simpleHam];
3552
3553      (* Eigensolver *)
3554      PrintFun["> Diagonalizing the numerical Hamiltonian ..."];
3555      startTime = Now;
3556      eigensys  = Eigensystem[numHam];
3557      endTime   = Now;
3558      diagonalTime = QuantityMagnitude[endTime - startTime, "Seconds"
        ];
3559      PrintFun[">> Diagonalization took ", diagonalTime, " seconds."
        ];
3560      eigensys = Chop[eigensys];
3561      eigensys = Transpose[eigensys];
3562
3563      (* Shift the baseline energy *)
3564      eigensys = ShiftedLevels[eigensys];
3565      (* Sort according to energy *)
3566      eigensys = SortBy[eigensys, First];
3567      Return[eigensys];
3568    )
3569  ];
3570
3571  ShiftedLevels::usage = "ShiftedLevels[eigenSys] takes a list of
```

```
    levels of the form
{{energy_1, coeff_vector_1}, {energy_2, coeff_vector_2},...}} and
    returns the same input except that now to every energy the minimum
     of all of them has been subtracted.";
ShiftedLevels[originalLevels_] := Module[
  {groundEnergy, shifted},
  (
    groundEnergy = Sort[originalLevels][[1,1]];
    shifted      = Map[{#[[1]] - groundEnergy, #[[2]]} &,
  originalLevels];
    Return[shifted];
  )
];


(* ############################################################ *)
(* ############## Optical Transitions for Levels ############## *)

JuddOfeltUkSquared::usage = "JuddOfeltUkSquared[numE, params]
  calculates the matrix elements of the Uk operator in the level
  basis. These are calculated according to equation (7) in Carnall
  1965.
The function returns a list with the following elements:
  - basis : A list with the allowed {SL, J} terms in the f^numE
  configuration. Equal to BasisLSJ[numE].
  - eigenSys : A list with the eigensystem of the Hamiltonian for
  the f^n configuration.
  - levelLabels : A list with the labels of the major components of
   the level eigenstates.
  - LevelUkSquared : An association with the squared matrix
  elements of the Uk operators in the level eigenbasis. The keys
  being {2, 4, 6} corresponding to the rank of the Uk operator. The
  basis in which the matrix elements are given is the one
  corresponding to the level eigenstates given in eigenSys and whose
   major SLJ components are given in levelLabels. The matrix is
  symmetric and given as a SymmetrizedArray.
  The function admits the following options:
  \"PrintFun\" : A function that will be used to print the progress
   of the calculations. The default is PrintTemporary.";
Options[JuddOfeltUkSquared] = {"PrintFun" -> PrintTemporary};
JuddOfeltUkSquared[numE_, params_, OptionsPattern[]] := Module[
  {eigenChanger, numEH, basis, eigenSys,
  Js, Ukmat, LevelUkSquared, kRank,
  S, L, Sp, Lp, J, Jp, phase,
  braTerm, ketTerm, levelLabels,
  eigenVecs, majorComponentIndices},
  (
    If[Not[ValueQ[ReducedUkTable]],
      LoadUk[]
    ];
    numEH = Min[numE, 14-numE];
    PrintFun = OptionValue["PrintFun"];
    PrintFun["> Calculating the levels for the given parameters ...
  "];
    {basis, eigenSys} = LevelSolver[numE, params];
    (* The change of basis matrix to the eigenstate basis *)
    eigenChanger = Transpose[Last /@ eigenSys];
    PrintFun["Calculating the matrix elements of Uk in the physical
   coupling basis ..."];
    LevelUkSquared = <||>;
    Do[(
      Ukmat = Table[(
          {S, L}   = FindSL[braTerm[[1]]];
          J        = braTerm[[2]];
          Jp       = ketTerm[[2]];
          {Sp, Lp} = FindSL[ketTerm[[1]]];
          phase    = Phaser[S + Lp + J + kRank];
          Simplify @ (
            phase *
            Sqrt[TPO[J]*TPO[Jp]] *
            SixJay[{J, Jp, kRank}, {Lp, L, S}] *
            ReducedUkTable[{numEH, 3, braTerm[[1]], ketTerm[[1]],
  kRank}]
            )
          ),
        {braTerm, basis},
```

```
3628            {ketTerm, basis}
3629          ];
3630          Ukmat = (Transpose[eigenChanger] . Ukmat . eigenChanger)^2;
3631          Ukmat = Chop@Ukmat;
3632          LevelUkSquared[kRank] = SymmetrizedArray[Ukmat, Dimensions[
    eigenChanger], Symmetric[{1, 2}]];
3633          ),
3634          {kRank, {2, 4, 6}}
3635        ];
3636        LSJmultiplets = (RemoveTrailingDigits[#[[1]]] <> ToString[
    InputForm[#[[2]]]]) & /@ basis;
3637        eigenVecs = Last /@ eigenSys;
3638        majorComponentIndices = Ordering[Abs[#]][[-1]] & /@ eigenVecs;
3639        levelLabels = LSJmultiplets[[majorComponentIndices]];
3640        Return[{basis, eigenSys, levelLabels, LevelUkSquared}];
3641      )
3642    ];
3643
3644    LevelElecDipoleOscillatorStrength::usage = "
      LevelElecDipoleOscillatorStrength[numE, levelParams,
      juddOfeltParams] uses Judd-Ofelt theory to estimate the forced
      electric dipole oscillator strengths ions whose level description
      is determined by levelParams.
3645  The third parameter juddOfeltParams is an asssociation with keys
      equal to the three Judd-Ofelt intensity parameters {\[CapitalOmega
      ]2, \[CapitalOmega]4, \[CapitalOmega]6} and corresponding values
      in cm^2.
3646  The local field correction implemented here corresponds to the one
      given by the virtual cavity model of Lorentz.
3647  The function returns a list with the following elements:
3648    - basis : A list with the allowed {SL, J} terms in the f^numE
      configuration. Equal to BasisLSJ[numE].
3649    - eigenSys : A list with the eigensystem of the Hamiltonian for
      the f^n configuration in the level description.
3650    - levelLabels : A list with the labels of the major components of
       the calculated levels.
3651    - oStrengthArray : A square array whose elements represent the
      oscillator strengths between levels such that the element
      oStrengthArray[[i,j]] is the oscillator strength between the
      levels |Subscript[\[Psi], i]> and |Subscript[\[Psi], j]>. In this
      array, the elements below the diagonal represent emission
      oscillator strengths, and elements above the diagonal represent
      absorption oscillator strengths.
3652  The function admits the following three options:
3653    \"PrintFun\" : A function that will be used to print the progress
       of the calculations. The default is PrintTemporary.
3654    \"RefractiveIndex\" : The refractive index of the medium where
      the transitions are taking place. This may be a number or a
      function. If a number then the oscillator strengths are calculated
       for assuming a wavelength-independent refractive index. If a
      function then the refractive indices are calculated accordingly to
       the wavelength of each transition (the function must admit a
      single argument equal to the wavelength in nm). The default is 1.
3655    \"LocalFieldCorrection\" : The local field correction to be used.
       The default is \"VirtualCavity\". The options are: \"
      VirtualCavity\" and \"EmptyCavity\".
3656  The equation implemented here is the one given in eqn. 29 from the
      review article of Hehlen (2013). See that same article for a
      discussion on the local field correction.
3657  ";
3658  Options[LevelElecDipoleOscillatorStrength]={
3659    "PrintFun"        -> PrintTemporary,
3660    "RefractiveIndex" -> 1,
3661    "LocalFieldCorrection" -> "VirtualCavity"
3662  };
3663  LevelElecDipoleOscillatorStrength[numE_, levelParams_Association,
      juddOfeltParams_Association, OptionsPattern[]] := Module[
3664    {PrintFun, basis, eigenSys, levelLabels,
3665    LevelUkSquared, eigenEnergies, energyDiffs,
3666    oStrengthArray, nRef, \[Chi], nRefs,
3667    \[Chi]OverN, groundLevel, const,
3668    transitionFrequencies, wavelengthsInNM,
3669    fieldCorrectionType},
3670    (
3671      PrintFun = OptionValue["PrintFun"];
3672      nRef     = OptionValue["RefractiveIndex"];
```

```
3673      PrintFun["Calculating the Uk^2 matrix elements for the given
    parameters ..."];
3674      {basis, eigenSys, levelLabels, LevelUkSquared} =
    JuddOfeltUkSquared[numE, levelParams, "PrintFun"->PrintFun];
3675      eigenEnergies = First/@eigenSys;
3676      const         = (8\[Pi]^2)/3 me/hPlanck;
3677      energyDiffs   = Transpose@Outer[Subtract,eigenEnergies,
    eigenEnergies];
3678      (* since energies are assumed in Kayser, speed of light needs
    to be in cm/s, so that the frequencies are in 1/s *)
3679      transitionFrequencies = energyDiffs*cLight*100;
3680      (* grab the J for each level *)
3681      levelJs        = #[[2]] & /@ eigenSys;
3682      oStrengthArray = (
3683        juddOfeltParams[\[CapitalOmega]2]*LevelUkSquared[2]+
3684        juddOfeltParams[\[CapitalOmega]4]*LevelUkSquared[4]+
3685        juddOfeltParams[\[CapitalOmega]6]*LevelUkSquared[6]
3686      );
3687      oStrengthArray = Abs@(const * transitionFrequencies *
    oStrengthArray);
3688      (* it is necessary to divide each oscillator strength by the
    degeneracy of the initial level *)
3689      oStrengthArray = MapIndexed[1/(2 levelJs[[#2[[1]]]]+1) #1 &,
    oStrengthArray,{2}];
3690      (* including the effects of the refractive index *)
3691      fieldCorrectionType = OptionValue["LocalFieldCorrection"];
3692      Which[
3693        nRef === 1,
3694          True,
3695        NumberQ[nRef],
3696        (
3697          \[Chi] = Which[
3698            fieldCorrectionType == "VirtualCavity",
3699            (
3700              ( (nRef^2 + 2) / 3 )^2
3701            ),
3702            fieldCorrectionType == "EmptyCavity",
3703            (
3704              ( 3 * nRef^2 / ( 2 * nRef^2 + 1 ) )^2
3705            )
3706          ];
3707          \[Chi]OverN    = \[Chi] / nRef;
3708          oStrengthArray = \[Chi]OverN * oStrengthArray;
3709          (* the refractive index participates differently in
    absorption and in emission *)
3710          aFunction      = If[#2[[1]]>#2[[2]], #1 * nRef^2, #1]&;
3711          oStrengthArray = MapIndexed[aFunction, oStrengthArray,
    {2}];
3712        ),
3713        True,
3714        (
3715          wavelengthsInNM = Abs[1 / energyDiffs] * 10^7;
3716          nRefs           = Map[nRef, wavelengthsInNM];
3717          Print["Calculating the oscillator strengths for the given
    refractive index ..."];
3718          \[Chi] = Which[
3719            fieldCorrectionType == "VirtualCavity",
3720            (
3721              ( (nRefs^2 + 2) / 3 )^2
3722            ),
3723            fieldCorrectionType == "EmptyCavity",
3724            (
3725              ( 3 * nRefs^2 / ( 2*nRefs^2 + 1 ) )^2
3726            )
3727          ];
3728          \[Chi]OverN     = \[Chi] / nRefs;
3729          oStrengthArray  = \[Chi]OverN * oStrengthArray
3730        )
3731      ];
3732      Return[{basis, eigenSys, levelLabels, oStrengthArray}];
3733    )
3734  ];
3735
3736  LevelJJBlockMagDipole::usage = "LevelJJBlockMagDipole[numE, J, Jp]
      returns an array of the LSJ reduced matrix elements of the
      magnetic dipole operator between states with given J and Jp. The
```

```
    option \"Sparse\" can be used to return a sparse matrix. The
    default is to return a sparse matrix.";
3737  Options[LevelJJBlockMagDipole] = {"Sparse"->True};
3738  LevelJJBlockMagDipole[numE_, braJ_, ketJ_, OptionsPattern[]] :=
    Module[
3739    {
3740      braSLJs, ketSLJs,
3741      braSLJ, ketSLJ,
3742      braSL, ketSL,
3743      braS, braL,
3744      ketS, ketL,
3745      matValue, magMatrix,
3746      summand1, summand2
3747    },
3748  (
3749    braSLJs     = AllowedNKSLforJTerms[numE,braJ];
3750    ketSLJs     = AllowedNKSLforJTerms[numE,ketJ];
3751    magMatrix   = Table[
3752      (
3753        braSL       = braSLJ[[1]];
3754        ketSL       = ketSLJ[[1]];
3755        {braS,braL} = FindSL[braSL];
3756        {ketS,ketL} = FindSL[ketSL];
3757        summand1    = If[Or[braJ!=ketJ,braSL!=ketSL],
3758          0,
3759          Sqrt[braJ*(braJ+1)*TPO[braJ]
3760          ]
3761        ];
3762        (*looking at the string includes checking L=L',S=S',and\alpha
    =\alpha'*)
3763        summand2    = If[braSL!=ketSL,
3764          0,
3765          (gs-1)*
3766          Phaser[braS+braL+ketJ+1]*
3767          Sqrt[TPO[braJ]*TPO[ketJ]]*
3768          SixJay[{braJ,1,ketJ},{braS,braL,braS}]*
3769          Sqrt[braS(braS+1)TPO[braS]]
3770        ];
3771        matValue = summand1 + summand2;
3772        matValue = -1/2 * matValue;
3773        matValue
3774      ),
3775      {braSLJ,braSLJs},
3776      {ketSLJ,ketSLJs}
3777    ];
3778    If[OptionValue["Sparse"],
3779      magMatrix = SparseArray[magMatrix]];
3780    Return[magMatrix];
3781  )
3782  ];
3783
3784  LevelMagDipoleMatrixAssembly::usage = "LevelMagDipoleMatrixAssembly
    [numE] puts together an array with the reduced matrix elements of
    the magnetic dipole operator in the level basis for the f^numE
    configuration. The function admits the two following options:
3785    \"Flattened\": If True then the returned matrix is flattened. The
     default is True.
3786    \"gs\": The electronic gyromagnetic ratio. The default is 2.";
3787  Options[LevelMagDipoleMatrixAssembly] = {
3788    "Flattened" -> True,
3789    gs -> 2
3790  };
3791  LevelMagDipoleMatrixAssembly[numE_, OptionsPattern[]] := Module[
3792    {Js, magDip, braJ, ketJ},
3793    (
3794      Js       = AllowedJ[numE];
3795      magDip   = Table[
3796        ReplaceInSparseArray[LevelJJBlockMagDipole[numE, braJ, ketJ],
    {gs -> OptionValue[gs]}],
3797        {braJ,Js},
3798        {ketJ,Js}
3799      ];
3800      If[OptionValue["Flattened"],
3801        magDip = ArrayFlatten[magDip];
3802      ];
3803      Return[magDip];
```

```
    )
];

LevelMagDipoleLineStrength::usage = "LevelMagDipoleLineStrength[
  eigenSys, numE] calculates the magnetic dipole line strengths for
  an ion whose level description is determined by levelParams. The
  function returns a square array whose elements represent the
  magnetic dipole line strengths between the levels given in
  eigenSys such that the element magDipoleLineStrength[[i,j]] is the
   line strength between the levels |Subscript[\[Psi], i]> and |
  Subscript[\[Psi], j]>. Eigensys must be such that it consists of a
   lists of lists where in each list the last element corresponds to
   the eigenvector of a level (given as a row) in the standard basis
   for levels of the f^numE configuration.
The function admits the following options:
  \"Units\" : The units in which the line strengths are given. The
  default is \"SI\". The options are \"SI\" and \"Hartree\". If \"SI
  \" then the unit of the line strength is (A m^2)^2 = (J/T)^2. If \
  "Hartree\" then the line strength is given in units of 2 \[Mu]B.";
Options[LevelMagDipoleLineStrength] = {
  "Units"->"SI"
  };
LevelMagDipoleLineStrength[theEigensys_List, numE0_Integer,
  OptionsPattern[]] := Module[
  {numE, levelMagOp, allEigenvecs, magDipoleLineStrength, units},
  (
    numE          = Min[14-numE0,numE0];
    levelMagOp    = LevelMagDipoleMatrixAssembly[numE];
    allEigenvecs  = Transpose[Last/@theEigensys];
    units         = OptionValue["Units"];
    magDipoleLineStrength          = Transpose[allEigenvecs].
  levelMagOp.allEigenvecs;
    magDipoleLineStrength          = Abs[magDipoleLineStrength]^2;
    Which[
      units=="SI",
        Return[4 \[Mu]B^2 * magDipoleLineStrength],
      units=="Hartree",
        Return[magDipoleLineStrength]
    ];
  )
];

LevelMagDipoleOscillatorStrength::usage = "
  LevelMagDipoleOscillatorStrength[eigenSys, numE] calculates the
  magnetic dipole oscillator strengths for an ion whose level
  description is determined by levelParams. The refractive index of
  the medium is relevant, but here it is assumed to be 1, this can
  be changed through the option \"RefractiveIndex\". eigenSys must
  consist of a lists of lists with three elements: the first element
   being the energy of the level, the second element being the J of
  the level, and the third element being the eigenvector of the
  level.
   The function returns a list with the following elements:
     - basis : A list with the allowed {SL, J} terms in the f^numE
  configuration. Equal to BasisLSJ[numE].
     - eigenSys : A list with the eigensystem of the Hamiltonian for
   the f^n configuration in the level description.
     - levelLabels : A list with the labels of the major components
  of the calculated levels.
     - magDipoleOstrength : A square array whose elements represent
  the magnetic dipole oscillator strengths between the levels given
  in eigenSys such that the element magDipoleOstrength[[i,j]] is the
   oscillator strength between the levels |Subscript[\[Psi], i]> and
   |Subscript[\[Psi], j]>. In this array the elements below the
  diagonal represent emission oscillator strengths, and elements
  above the diagonal represent absorption oscillator strengths. The
  emission oscillator strengths are negative. The oscillator
  strength is a dimensionless quantity.
   The function admits the following option:
     \"RefractiveIndex\" : The refractive index of the medium where
  the transitions are taking place. This may be a number or a
  function. If a number then the oscillator strengths are calculated
   assuming a wavelength-independent refractive index as given. If a
   function then the refractive indices are calculated accordingly
  to the vaccum wavelength of each transition (the function must
  admit a single argument equal to the wavelength in nm). The
```

```
    default is 1.
3839    For reference see equation (27.8) in Rudzikas (2007). The
    expression for the line strenght is the simplest when using atomic
     units, (27.8) is missing a factor of α^2.";
3840  Options[LevelMagDipoleOscillatorStrength]={
3841    "RefractiveIndex" -> 1
3842  };
3843  LevelMagDipoleOscillatorStrength[eigenSys_, numE_, OptionsPattern
    []] := Module[
3844    {eigenEnergies, eigenVecs, levelJs,
3845    energyDiffs, magDipoleOstrength, nRef,
3846    wavelengthsInNM, nRefs, degenDivisor},
3847    (
3848      basis          = BasisLSJ[numE];
3849      eigenEnergies  = First/@eigenSys;
3850      nRef           = OptionValue["RefractiveIndex"];
3851      eigenVecs      = Last/@eigenSys;
3852      levelJs        = #[[2]]&/@eigenSys;
3853      energyDiffs    = -Outer[Subtract,eigenEnergies,eigenEnergies];
3854      energyDiffs   *= kayserToHartree;
3855      magDipoleOstrength = LevelMagDipoleLineStrength[eigenSys, numE,
     "Units"->"Hartree"];
3856      magDipoleOstrength = 2/3 * αFine^2 * energyDiffs *
    magDipoleOstrength;
3857      degenDivisor       = #1 / ( 2 * levelJs[[#2[[1]]]] + 1 ) &;
3858      magDipoleOstrength = MapIndexed[degenDivisor,
    magDipoleOstrength, {2}];
3859      Which[nRef===1,
3860        True,
3861        NumberQ[nRef],
3862          (
3863            magDipoleOstrength = nRef * magDipoleOstrength;
3864          ),
3865        True,
3866          (
3867            wavelengthsInNM    = Abs[kayserToHartree / energyDiffs] *
     10^7;
3868            nRefs              = Map[nRef, wavelengthsInNM];
3869            magDipoleOstrength = nRefs * magDipoleOstrength;
3870          )
3871      ];
3872      Return[{basis, eigenSys, magDipoleOstrength}];
3873    )
3874  ];
3875
3876  LevelMagDipoleSpontaneousDecayRates::usage = "
    LevelMagDipoleSpontaneousDecayRates[eigenSys, numE] calculates the
     spontaneous emission rates for the magnetic dipole transitions
    between the levels given in eigenSys. The function returns a
    square array whose elements represent the spontaneous emission
    rates between the levels given in eigenSys such that the element
    [[i,j]] of the returned array is the rate of spontaneous emission
    from the level |Subscript[\[Psi], i]> to the level |Subscript[\[
    Psi], j]>. In this array the elements below the diagonal represent
     emission rates, and elements above the diagonal are identically
    zero.
3877  The function admits two optional arguments:
3878    + \"Units\" : The units in which the rates are given. The default
     is \"SI\". The options are \"SI\" and \"Hartree\". If \"SI\" then
     the rates are given in s^-1. If \"Hartree\" then the rates are
    given in the atomic unit of frequency.
3879    + \"RefractiveIndex\" : The refractive index of the medium where
    the transitions are taking place. This may be a number or a
    function. If a number then the rates are calculated assuming a
    wavelength-independent refractive index as given. If a function
    then the refractive indices are calculated accordingly to the
    vaccum wavelength of each transition (the function must admit a
    single argument equal to the wavelength in nm). The default is 1."
    ;
3880  Options[LevelMagDipoleSpontaneousDecayRates] = {
3881    "Units" -> "SI",
3882    "RefractiveIndex" -> 1};
3883  LevelMagDipoleSpontaneousDecayRates[eigenSys_List, numE_Integer,
    OptionsPattern[]] := Module[
3884    {levMDlineStrength, eigenEnergies, energyDiffs,
3885    levelJs, spontaneousRatesInHartree, spontaneousRatesInSI,
```

```
    degenDivisor, units, nRef, nRefs, wavelengthsInNM},
    (
      nRef              = OptionValue["RefractiveIndex"];
      units             = OptionValue["Units"];
      levMDlineStrength =
    LowerTriangularize@LevelMagDipoleLineStrength[eigenSys,numE,"Units
    "->"Hartree"];
      levMDlineStrength = SparseArray[levMDlineStrength];
      eigenEnergies     = First /@ eigenSys;
      energyDiffs       = Outer[Subtract, eigenEnergies,
    eigenEnergies];
      energyDiffs       = kayserToHartree * energyDiffs;
      energyDiffs       = SparseArray[LowerTriangularize[energyDiffs
    ]];
      levelJs           = #[[2]]& /@ eigenSys;
      spontaneousRatesInHartree = 4/3 αFine^5 * energyDiffs^3 *
    levMDlineStrength;
      degenDivisor              = #1 / (2*levelJs[[#2[[1]]]] + 1)&;
      spontaneousRatesInHartree = MapIndexed[degenDivisor,
    spontaneousRatesInHartree, {2}];
      Which[nRef===1,
        True,
        NumberQ[nRef],
          (
            spontaneousRatesInHartree = nRef^3 *
    spontaneousRatesInHartree;
          ),
        True,
          (
            wavelengthsInNM    = Abs[kayserToHartree / energyDiffs] *
     10^7;
            nRefs              = Map[nRef, wavelengthsInNM];
            spontaneousRatesInHartree = nRefs^3 *
    spontaneousRatesInHartree;
          )
      ];
      If[units == "SI",
        (
          spontaneousRatesInSI = 1/hartreeTime *
    spontaneousRatesInHartree;
          Return[SparseArray@spontaneousRatesInSI];
        ),
        Return[SparseArray@spontaneousRatesInHartree];
      ];
    )
  ];

  (* ############# Optical Transitions for Levels ############## *)
  (* ########################################################### *)

  (* ########################################################### *)
  (* ################### Eigensystem analysis ################## *)

  PrettySaundersSL::usage = "PrettySaundersSL[SL] produces a human-
    redeable symbol for the spectroscopic term SL. SL can be either a
    string (in RS notation for the term) or a list of two numbers {S,
    L}. The option \"Representation\" can be used to specify whether
    the output is given as a symbol or as a ket. The default is \"Ket\
    ".";
  Options[PrettySaundersSL] = {"Representation" -> "Ket"};
  PrettySaundersSL[SL_, OptionsPattern[]] := (
    If[StringQ[SL],
    (
      {S,L} = FindSL[SL];
      L     = StringTake[SL,{2,-1}];
    ),
      {S,L}=SL
    ];
    pretty = RowBox[{
        AdjustmentBox[Style[2*S+1,Smaller], BoxBaselineShift->-1,
    BoxMargins->0],
        AdjustmentBox[PrintL[L]]
      }
    ];
    pretty = DisplayForm[pretty];
    pretty = Which[
```

```
      OptionValue["Representation"]=="Ket",
        Ket[pretty],
      OptionValue["Representation"]=="Symbol",
        pretty
    ];
    Return[pretty];
  );

  PrettySaundersSLJmJ::usage = "PrettySaundersSLJmJ[{SL, J, mJ}]
    produces a human-redeable symbol for the given basis vector {SL, J
    , mJ}.";
  Options[PrettySaundersSLJmJ] = {"Representation" -> "Ket"};
  PrettySaundersSLJmJ[{SL_, J_, mJ_}, OptionsPattern[]] := (If[
    StringQ[SL],
    ({S, L} = FindSL[SL];
      L = StringTake[SL, {2, -1}];
      ),
    {S, L} = SL];
    pretty = RowBox[{AdjustmentBox[Style[2*S + 1, Smaller],
        BoxBaselineShift -> -1, BoxMargins -> 0],
        AdjustmentBox[PrintL[L], BoxMargins -> -0.2],
        AdjustmentBox[
        Style[Row[{InputForm[J], ",", mJ}], Small],
        BoxBaselineShift -> 1,
        BoxMargins -> {{0.7, 0}, {0.4, 0.4}}]}];
    pretty = DisplayForm[pretty];
    If[OptionValue["Representation"] == "Ket",
      pretty = Ket[pretty]
    ];
    Return[pretty];
  );

  PrettySaundersSLJ::usage = "PrettySaundersSLJ[{SL, J}] produces a
    human-redeable symbol for the given basis vector {SL, J}. SL can
    be either a list of two numbers representing S and L or a string
    representing the spin multiplicity and the total orbital angular
    momentum J in spectroscopic notation. The option \"Representation\
    " can be used to specify whether the output is given as a symbol
    or as a ket. The default is \"Ket\".";
  Options[PrettySaundersSLJ] = {"Representation"->"Ket"};
  PrettySaundersSLJ[{SL_,J_},OptionsPattern[]] := (
    If[StringQ[SL],
    (
      {S,L}=FindSL[SL];
      L=StringTake[SL,{2,-1}];
    ),
      {S,L}=SL
    ];
    pretty = RowBox[{
        AdjustmentBox[Style[2*S+1,Smaller],BoxBaselineShift->-1,
    BoxMargins->0],
        AdjustmentBox[PrintL[L],BoxMargins->-0.2],
        AdjustmentBox[Style[InputForm[J],Small,FontTracking->"Narrow"
    ],BoxBaselineShift->1,BoxMargins->{{0.7,0},{0.4,0.4}}]
      }
    ];
    pretty = DisplayForm[pretty];
    pretty = Which[
      OptionValue["Representation"]=="Ket",
        Ket[pretty],
      OptionValue["Representation"]=="Symbol",
        pretty
    ];
    Return[pretty];
  );

  BasisVecInRusselSaunders::usage = "BasisVecInRusselSaunders[
    basisVec] takes a basis vector in the format {LSstring, Jval,
    mJval} and returns a human-readable symbol for the corresponding
    Russel-Saunders term.";
  BasisVecInRusselSaunders[basisVec_] := (
    {LSstring, Jval, mJval} = basisVec;
    Ket[PrettySaundersSLJmJ[basisVec]]
  );

  LSJMJTemplate =
```

```
    StringTemplate[
    "\!\(\*TemplateBox[{\nRowBox[{\"‘LS‘\", \",\", \nRowBox[{\"J\", \
\"=\", \"‘J‘\"}], \",\", \nRowBox[{\"mJ\", \"=\", \"‘mJ‘\"}]}]},\n\
\"Ket\"]\)"];

BasisVecInLSJMJ::usage = "BasisVecInLSJMJ[basisVec] takes a basis
  vector in the format {{{LSstring, Jval}, mJval}, nucSpin} and
  returns a human-readable symbol for the corresponding LSJMJ term
  in the form |LS, J=..., mJ=...>.";
BasisVecInLSJMJ[basisVec_] := (
  {LSstring, Jval, mJval} = basisVec;
  LSJMJTemplate[<|
    "LS" -> LSstring,
    "J" -> ToString[Jval, InputForm],
    "mJ" -> ToString[mJval, InputForm]|>]
);

ParseStates::usage = "ParseStates[eigenSys, basis] takes a list of
  eigenstates in terms of their coefficients in the given basis and
  returns a list of the same states in terms of their energy, LSJMJ
  symbol, J, mJ, S, L, LSJ symbol, and LS symbol. eigenSys is a list
   of lists with two elements, in each list the first element is the
   energy and the second one the corresponding eigenvector. The LS
  symbol returned corresponds to the term with the largest
  coefficient in the given basis.";
ParseStates[states_, basis_, OptionsPattern[]] := Module[
  {parsedStates},
  (
    parsedStates = Table[(
      {energy, eigenVec}      = state;
      maxTermIndex            = Ordering[Abs[eigenVec]][[-1]];
      {LSstring, Jval, mJval} = basis[[maxTermIndex]];
      LSJsymbol               = Subscript[LSstring, {Jval, mJval}];
      LSJMJsymbol             = LSstring <> ToString[Jval,
  InputForm];
      {S, L}                  = FindSL[LSstring];
      {energy, LSstring, Jval, mJval, S, L, LSJsymbol, LSJMJsymbol}
    ),
    {state, states}
    ];
    Return[parsedStates];
  )
];

ParseStatesByNumBasisVecs::usage = "ParseStatesByNumBasisVecs[
  eigenSys, basis, numBasisVecs, roundTo] takes a list of
  eigenstates (given in eigenSys) in terms of their coefficients in
  the given basis and returns a list of the same states in terms of
  their energy and the coefficients at most numBasisVecs basis
  vectors. By default roundTo is 0.01 and this is the value used to
  round the amplitude coefficients. eigenSys is a list of lists with
   two elements, in each list the first element is the energy and
  the second one the corresponding eigenvector.
The option \"Coefficients\" can be used to specify whether the
  coefficients are given as \"Amplitudes\" or \"Probabilities\". The
   default is \"Amplitudes\".
";
Options[ParseStatesByNumBasisVecs] = {
  "Coefficients" -> "Amplitudes",
  "Representation" -> "Ket",
  "ReturnAs" -> "Dot"
  };
ParseStatesByNumBasisVecs[eigensys_List, basis_List,
  numBasisVecs_Integer, roundTo_Real : 0.01, OptionsPattern[]] :=
  Module[
  {parsedStates, energy, eigenVec,
  probs, amplitudes, ordering,
  returnAs,
  chosenIndices, majorComponents,
  majorAmplitudes, majorRep},
  (
    returnAs     = OptionValue["ReturnAs"];
    parsedStates = Table[(
      {energy, eigenVec} = state;
      energy             = Chop[energy];
      probs              = Round[Abs[eigenVec^2], roundTo];
```

```
4062        amplitudes          = Round[eigenVec, roundTo];
4063        ordering            = Ordering[probs];
4064        chosenIndices       = ordering[[-numBasisVecs ;;]];
4065        majorComponents     = basis[[chosenIndices]];
4066        majorThings = If[OptionValue["Coefficients"] == "
    Probabilities",
4067          (
4068            probs[[chosenIndices]]
4069          ),
4070          (
4071            amplitudes[[chosenIndices]]
4072          )
4073        ];
4074        majorComponents     = PrettySaundersSLJmJ[#, "Representation"
    -> OptionValue["Representation"]] & /@ majorComponents;
4075        nonZ                = (# != 0.) & /@ majorThings;
4076        majorThings         = Pick[majorThings, nonZ];
4077        majorComponents     = Pick[majorComponents, nonZ];
4078        If[OptionValue["Coefficients"] == "Probabilities",
4079          (
4080            majorThings = majorThings * 100*"%"
4081          )
4082        ];
4083        majorRep  = Which[
4084                    returnAs == "Dot",
4085                      majorThings . majorComponents,
4086                    returnAs == "List",
4087                      Transpose[{Reverse@majorThings,
    Reverse@majorComponents}]
4088                    ];
4089        {energy, majorRep}
4090        ),
4091        {state, eigensys}];
4092      Return[parsedStates]
4093    )
4094  ];
4095
4096  FindThresholdPosition::usage = "FindThresholdPosition[list,
     threshold] returns the position of the first element in list that
     is greater than or equal to threshold. If no such element exists,
     it returns the length of list. The elements of the given list must
      be in ascending order.";
4097  FindThresholdPosition[list_, threshold_] := Module[
4098    {position},
4099    (
4100    position = Position[list, _?(# >= threshold &), 1, 1];
4101    thrPos = If[Length[position] > 0,
4102      position[[1, 1]],
4103      Length[list]];
4104    If[thrPos == 0,
4105      Return[1],
4106      Return[thrPos]]
4107    )
4108  ];
4109
4110  ParseStateByProbabilitySum[{energy_, eigenVec_}, probSum_, roundTo_
     :0.01, maxParts_:20] := Compile[
4111    {{energy, _Real, 0}, {eigenVec, _Complex, 1},
4112     {probSum, _Real, 0},{roundTo, _Real, 0},
4113     {maxParts, _Integer, 0}},
4114      Module[
4115        {numStates, state, amplitudes, probs, ordering,
4116        orderedProbs, truncationIndex, accProb, thresholdIndex,
    chosenIndices, majorComponents,
4117        majorAmplitudes, absMajorAmplitudes, notnullAmplitudes,
    majorRep},
4118        (
4119          numStates    = Length[eigenVec];
4120          (*Round them up*)
4121          amplitudes          = Round[eigenVec, roundTo];
4122          probs               = Round[Abs[eigenVec^2], roundTo];
4123          ordering            = Reverse[Ordering[probs]];
4124          (*Order the probabilities from high to low*)
4125          orderedProbs        = probs[[ordering]];
4126          (*To speed up Accumulate, assume that only as much as
    maxParts will be needed*)
```

```
4127            truncationIndex    = Min[maxParts, Length[orderedProbs]];
4128            orderedProbs       = orderedProbs[[;;truncationIndex]];
4129            (*Accumulate the probabilities*)
4130            accProb            = Accumulate[orderedProbs];
4131            (*Find the index of the first element in accProb that is
      greater than probSum*)
4132            thresholdIndex     = Min[Length[accProb],
      FindThresholdPosition[accProb, probSum]];
4133            (*Grab all the indicees up till that one*)
4134            chosenIndices      = ordering[[;; thresholdIndex]];
4135            (*Select the corresponding elements from the basis*)
4136            majorComponents    = basis[[chosenIndices]];
4137            (*Select the corresponding amplitudes*)
4138            majorAmplitudes    = amplitudes[[chosenIndices]];
4139            (*Take their absolute value*)
4140            absMajorAmplitudes = Abs[majorAmplitudes];
4141            (*Make sure that there are no effectively zero
      contributions*)
4142            notnullAmplitudes  = Flatten[Position[absMajorAmplitudes,
      x_ /; x != 0]];
4143            (* majorComponents    = PrettySaundersSLJmJ
      [{#[[1]],#[[2]],#[[3]]}] & /@ majorComponents; *)
4144            majorComponents    = PrettySaundersSLJmJ /@ majorComponents
      ;
4145            majorAmplitudes    = majorAmplitudes[[notnullAmplitudes]];
4146            (*Make them into Kets*)
4147            majorComponents    = Ket /@ majorComponents[[
      notnullAmplitudes]];
4148            (*Multiply and add to build the final Ket*)
4149            majorRep           = majorAmplitudes . majorComponents;
4150            Return[{energy, majorRep}];
4151          )
4152        ],
4153      CompilationTarget -> "C",
4154      RuntimeAttributes -> {Listable},
4155      Parallelization -> True,
4156      RuntimeOptions -> "Speed"
4157    ];
4158
4159    ParseStatesByProbabilitySum::usage = "ParseStatesByProbabilitySum[
        eigensys, basis, probSum] takes a list of eigenstates in terms of
        their coefficients in the given basis and returns a list of the
        same states in terms of their energy and the coefficients of the
        basis vectors that sum to at least probSum.";
4160    ParseStatesByProbabilitySum[eigensys_, basis_, probSum_, roundTo_ :
       0.01, maxParts_: 20] := Module[
4161      {parsedByProb, numStates, state, energy,
4162      eigenVec, amplitudes, probs, ordering,
4163      orderedProbs, truncationIndex, accProb,
4164      thresholdIndex, chosenIndices, majorComponents,
4165      majorAmplitudes, absMajorAmplitudes, notnullAmplitudes, majorRep
        },
4166      (
4167        numStates    = Length[eigensys];
4168        parsedByProb = Table[(
4169          state              = eigensys[[idx]];
4170          {energy, eigenVec} = state;
4171          (*Round them up*)
4172          amplitudes         = Round[eigenVec, roundTo];
4173          probs              = Round[Abs[eigenVec^2], roundTo];
4174          ordering           = Reverse[Ordering[probs]];
4175          (*Order the probabilities from high to low*)
4176          orderedProbs       = probs[[ordering]];
4177          (*To speed up Accumulate, assume that only as much as
      maxParts will be needed*)
4178          truncationIndex    = Min[maxParts, Length[orderedProbs]];
4179          orderedProbs       = orderedProbs[[;;truncationIndex]];
4180          (*Accumulate the probabilities*)
4181          accProb            = Accumulate[orderedProbs];
4182          (*Find the index of the first element in accProb that is
      greater than probSum*)
4183          thresholdIndex     = Min[Length[accProb],
      FindThresholdPosition[accProb, probSum]];
4184          (*Grab all the indicees up till that one*)
4185          chosenIndices      = ordering[[;; thresholdIndex]];
4186          (*Select the corresponding elements from the basis*)
```

```
4187          majorComponents    = basis[[chosenIndices]];
4188          (*Select the corresponding amplitudes*)
4189          majorAmplitudes    = amplitudes[[chosenIndices]];
4190          (*Take their absolute value*)
4191          absMajorAmplitudes = Abs[majorAmplitudes];
4192          (*Make sure that there are no effectively zero contributions
        *)
4193          notnullAmplitudes  = Flatten[Position[absMajorAmplitudes, x_
        /; x != 0]];
4194          (* majorComponents    = PrettySaundersSLJmJ
        [{#[[1]],#[[2]],#[[3]]}] & /@ majorComponents; *)
4195          majorComponents    = PrettySaundersSLJmJ /@ majorComponents;
4196          majorAmplitudes    = majorAmplitudes[[notnullAmplitudes]];
4197          majorComponents    = majorComponents[[notnullAmplitudes]];
4198          (*Multiply and add to build the final Ket*)
4199          majorRep           = majorAmplitudes . majorComponents;
4200          {energy, majorRep}
4201          ), {idx, numStates}];
4202        Return[parsedByProb];
4203      )
4204    ];
4205
4206    (* ################## Eigensystem analysis ################### *)
4207    (* ############################################################ *)
4208
4209    (* ############################################################ *)
4210    (* ########################### Misc ########################### *)
4211
4212    SymbToNum::usage = "SymbToNum[expr, numAssociation] takes an
        expression expr and returns what results after making the
        replacements defined in the given replacementAssociation. If
        replacementAssociation doesn't define values for expected keys,
        they are taken to be zero.";
4213    SymbToNum[expr_, replacementAssociation_] := (
4214      includedKeys = Keys[replacementAssociation];
4215      (*If a key is not defined, make its value zero.*)
4216      fullAssociation = Table[(
4217        If[MemberQ[includedKeys, key],
4218          ToExpression[key]->replacementAssociation[key],
4219          ToExpression[key]->0
4220        ]
4221      ),
4222      {key, paramSymbols}];
4223      Return[expr/.fullAssociation];
4224    );
4225
4226    SimpleConjugate::usage = "SimpleConjugate[expr] takes an expression
         and applies a simplified version of the conjugate in that all it
        does is that it replaces the imaginary unit I with -I. It assumes
        that every other symbol is real so that it remains the same under
        complex conjugation. Among other expressions it is valid for any
        rational or polynomial expression with complex coefficients and
        real variables.";
4227    SimpleConjugate[expr_] := expr /. Complex[a_, b_] :> a - I b;
4228
4229    ExportMZip::usage = "ExportMZip[\"dest.[zip,m]\"] saves a
        compressed version of expr to the given destination.";
4230    ExportMZip[filename_, expr_] := Module[
4231      {baseName, exportName, mImportName, zipImportName},
4232      (
4233        baseName    = FileBaseName[filename];
4234        exportName  = StringReplace[filename,".m"->".zip"];
4235        mImportName = StringReplace[exportName,".zip"->".m"];
4236        If[FileExistsQ[mImportName],
4237        (
4238          PrintTemporary[mImportName<>" exists already, deleting"];
4239          DeleteFile[mImportName];
4240          Pause[2];
4241        )
4242        ];
4243        Export[exportName, (baseName<>".m") -> expr];
4244      )
4245    ];
4246
4247    ImportMZip::usage = "ImportMZip[filename] imports a .m file inside
        a .zip file with corresponding filename. If the Option \"Leave
```

```
    Uncompressed\" is set to True (the default) then this function
    also leaves an umcompressed version of the object in the same
    folder of filename";
Options[ImportMZip]={"Leave Uncompressed" -> True};
ImportMZip[filename_String, OptionsPattern[]] := Module[
  {baseName, importKey, zipImportName, mImportName, imported},
  (
    baseName      = FileBaseName[filename];
    (*Function allows for the filename to be .m or .zip*)
    importKey     = baseName <> ".m";
    zipImportName = StringReplace[filename, ".m"->".zip"];
    mImportName   = StringReplace[zipImportName, ".zip"->".m"];
    mxImportName  = StringReplace[zipImportName, ".zip"->".mx"];
    Which[
      FileExistsQ[mxImportName],
    (
      PrintTemporary[".mx version exists already, importing that
  instead ..."];
      Return[Import[mxImportName]];
    ),
      FileExistsQ[mImportName],
    (
      PrintTemporary[".m version exists already, importing that
  instead ..."];
      Return[Import[mImportName]];
    )
    ];
    imported = Import[zipImportName, importKey];
    If[OptionValue["Leave Uncompressed"],
      (
        Export[mImportName, imported];
        Export[mxImportName, imported];
      )
    ];
    Return[imported];
  )
];

ReplaceInSparseArray::usage = "ReplaceInSparseArray[sparseArray,
  rules] takes a sparse array that may contain symbolic quantities
  and returns a sparse array in which the given rules have been used
   on every element.";
ReplaceInSparseArray[sparseA_SparseArray, rules_] := (
  SparseArray[Automatic,
    sparseA["Dimensions"],
    sparseA["Background"] /. rules,
    {
      1,
      {sparseA["RowPointers"], sparseA["ColumnIndices"]},
      sparseA["NonzeroValues"] /. rules
    }
    ]
);

MapToSparseArray::usage = "MapToSparseArray[sparseArray, function]
  takes a sparse array and returns a sparse array after the function
   has been applied to it.";
MapToSparseArray[sparseA_SparseArray, func_] := Module[
  {nonZ, backg, mapped},
  (
    nonZ   = func /@ sparseA["NonzeroValues"];
    backg  = func[sparseA["Background"]];
    mapped = SparseArray[Automatic,
      sparseA["Dimensions"],
      backg,
      {
        1,
        {sparseA["RowPointers"], sparseA["ColumnIndices"]},
        nonZ
      }
    ];
    Return[mapped];
  )
];

ParseTeXLikeSymbol::usage = "ParseTeXLikeSymbol[string] parses a
```

```
  string for a symbol given in LaTeX notation and returns a
  corresponding mathematica symbol. The string may have expressions
  for several symbols, they need to be separated by single spaces.
  In addition the _ and ^ symbols used in LaTeX notation need to
  have arguments that are enclosed in parenthesis, for example \"x_2
  \" is invalid, instead \"x_{2}\" should have been given.";
Options[ParseTeXLikeSymbol] = {"Form" -> "List"};
ParseTeXLikeSymbol[bigString_, OptionsPattern[]] := Module[
  {form, mainSymbol, symbols},
  (
    form = OptionValue["Form"];
    (* parse greek *)
    symbols = Table[(
        str = StringReplace[string, {"\\alpha" -> "α",
          "\\beta" -> "β",
          "\\gamma" -> "γ",
          "\\psi" -> "\[Psi]"}];
        symbol = Which[
          StringContainsQ[str, "_"] && Not[StringContainsQ[str, "^"
]],
          (
            (*yes sub no sup*)
            mainSymbol = StringSplit[str, "_"][[1]];
            mainSymbol = ToExpression[mainSymbol];

            subPart =
              StringCases[str,
                RegularExpression@"\\{(.*?)\\}" -> "$1"][[1]];
            Subscript[mainSymbol, subPart]
          ),
          Not[StringContainsQ[str, "_"]] && StringContainsQ[str, "^
"],
          (
            (*no sub yes sup*)
            mainSymbol = StringSplit[str, "^"][[1]];
            mainSymbol = ToExpression[mainSymbol];

            supPart =
              StringCases[str,
                RegularExpression@"\\{(.*?)\\}" -> "$1"][[1]];
            Superscript[mainSymbol, supPart]
          ),
          StringContainsQ[str, "_"] && StringContainsQ[str, "^"],
          (
            (*yes sub yes sup*)
            mainSymbol = StringSplit[str, "_"][[1]];
            mainSymbol = ToExpression[mainSymbol];
            {subPart, supPart} =
              StringCases[str, RegularExpression@"\\{(.*?)\\}" -> "
$1"];
            Subsuperscript[mainSymbol, subPart, supPart]
          ),
          True,
          (
            (*no sup or sub*)
            str
          )
          ];
        symbol
        ),
      {string, StringSplit[bigString, " "]}
    ];
    Which[
      form == "Row",
      Return[Row[symbols]],
      form == "List",
      Return[symbols]
    ]
  )
];

FromArrayToTable::usage = "FromArrayToTable[array, labels, energies
  ] takes a square array of values and returns a table with the
  labels of the rows and columns, the energies of the initial and
  final levels, the level energies, the vacuum wavelength of the
  transition, and the value of the array. The array must be square
```

```
    and the labels and energies must be compatible with the order
    implied by the array. The array must be a square array of values.
    The function returs a list of lists with the following elements:
4377    - Initial level index
4378    - Final level index
4379    - Initial level label
4380    - Final level label
4381    - Initial level energy
4382    - Final level energy
4383    - Vacuum wavelength
4384    - Value of the array element.
4385  Elements in which the array is zero are not included in the return
    of this function.";
4386  FromArrayToTable[array_,labels_,energies_] := Module[
4387    {tableFun, atl},
4388    (
4389      tableFun = {
4390        #2[[1]],
4391        #2[[2]],
4392        labels[[#2[[1]]]],
4393        labels[[#2[[2]]]],
4394        energies[[#2[[1]]]],
4395        energies[[#2[[2]]]],
4396        If[#2[[1]]==#2[[2]],"--",10^7/(energies[[#2[[1]]]]-energies
    [[#2[[2]]]])],
4397        #1
4398      }&;
4399      atl = Select[Flatten[MapIndexed[tableFun,array
    ,{2}],1],#[[-1]]=!=0.&];
4400      atl = Append[#,1/#[[-1]]]&/@atl;
4401      Return[atl]
4402    )
4403  ]
4404  (* ########################## Misc ########################## *)
4405  (* ########################################################## *)
4406
4407  (* ########################################################## *)
4408  (* ################## Some Plotting Routines ################## *)
4409
4410  EnergyLevelDiagram::usage = "EnergyLevelDiagram[states] takes
    states and produces a visualization of its energy spectrum.
4411  The resultant visualization can be navigated by clicking and
    dragging to zoom in on a region, or by clicking and dragging
    horizontally while pressing Ctrl. Double-click to reset the view."
    ;
4412  Options[EnergyLevelDiagram] = {
4413    "Title"->"",
4414    "ImageSize"->1000,
4415    "AspectRatio" -> 1/8,
4416    "Background"->"Automatic",
4417    "Epilog"->{},
4418    "Explorer"->True
4419    };
4420  EnergyLevelDiagram[states_, OptionsPattern[]] := Module[
4421    {energies, epi, explora},
4422    (
4423      energies = First/@states;
4424      epi = OptionValue["Epilog"];
4425      explora = If[OptionValue["Explorer"],
4426        ExploreGraphics,
4427        Identity
4428      ];
4429      explora@ListPlot[Tooltip[{{#, 0}, {#, 1}}, {Quantity
    [#/8065.54429, "eV"], Quantity[#, 1/"Centimeters"]}] &/@ energies,
4430        Joined       -> True,
4431        PlotStyle    -> Black,
4432        AspectRatio  -> OptionValue["AspectRatio"],
4433        ImageSize    -> OptionValue["ImageSize"],
4434        Frame        -> True,
4435        PlotRange    -> {All, {0, 1}},
4436        FrameTicks   -> {{None, None}, {Automatic, Automatic}},
4437        FrameStyle   -> Directive[15, Dashed, Thin],
4438        PlotLabel    -> Style[OptionValue["Title"], 15, Bold],
4439        Background   -> OptionValue["Background"],
4440        FrameLabel   -> {"\!\(\*FractionBox[\(E\), SuperscriptBox[\(
    cm\), \(-1\)]]\)"},
```

```
        Epilog       -> epi]
    )
];

ExploreGraphics::usage = "Pass a Graphics object to explore it.
  Zoom by clicking and dragging a rectangle. Pan by clicking and
  dragging while pressing Ctrl. Click twice to reset view.
Based on ZeitPolizei @ https://mathematica.stackexchange.com/
  questions/7142/how-to-manipulate-2d-plots.
The option \"OptAxesRedraw\" can be used to specify whether the
  axes should be redrawn. The default is False.";
Options[ExploreGraphics] = {OptAxesRedraw -> False};
ExploreGraphics[graph_Graphics, opts : OptionsPattern[]] := With[
  {
    gr  = First[graph],
    opt = DeleteCases[Options[graph],
          PlotRange -> PlotRange | AspectRatio | AxesOrigin -> _],
    plr = PlotRange /. AbsoluteOptions[graph, PlotRange],
    ar  = AspectRatio /. AbsoluteOptions[graph, AspectRatio],
    ao  = AbsoluteOptions[AxesOrigin],
    rectangle = {Dashing[Small],
      Line[{#1,
            {First[#2], Last[#1]},
            #2,
            {First[#1], Last[#2]},
            #1}]} &,
    optAxesRedraw = OptionValue[OptAxesRedraw]
  },
  DynamicModule[
      {dragging=False, first, second, rx1, rx2, ry1, ry2,
      range = plr},
      {{rx1, rx2}, {ry1, ry2}} = plr;
    Panel@
    EventHandler[
      Dynamic@Graphics[
        If[dragging, {gr, rectangle[first, second]}, gr],
        PlotRange -> Dynamic@range,
        AspectRatio -> ar,
        AxesOrigin -> If[optAxesRedraw,
          Dynamic@Mean[range\[Transpose]], ao],
        Sequence @@ opt],
      {{"MouseDown", 1} :> (
        first = MousePosition["Graphics"]
        ),
      {"MouseDragged", 1} :> (
        dragging = True;
        second = MousePosition["Graphics"]
        ),
      "MouseClicked" :> (
        If[CurrentValue@"MouseClickCount"==2,
          range = plr];
        ),
      {"MouseUp", 1} :> If[dragging,
        dragging = False;

        range = {{rx1, rx2}, {ry1, ry2}} =
          Transpose@{first, second};
        range[[2]] = {0, 1}],
      {"MouseDown", 2} :> (
        first = {sx1, sy1} = MousePosition["Graphics"]
        ),
      {"MouseDragged", 2} :> (
        second = {sx2, sy2} = MousePosition["Graphics"];
        rx1 = rx1 - (sx2 - sx1);
        rx2 = rx2 - (sx2 - sx1);
        ry1 = ry1 - (sy2 - sy1);
        ry2 = ry2 - (sy2 - sy1);
        range = {{rx1, rx2}, {ry1, ry2}};
        range[[2]] = {0, 1};
        )}]]];

LabeledGrid::usage = "LabeledGrid[data, rowHeaders, columnHeaders]
  provides a grid of given data interpreted as a matrix of values
  whose rows are labeled by rowHeaders and whose columns are labeled
   by columnHeaders. When hovering with the mouse over the grid
  elements, the row and column labels are displayed with the given
```

```
  separator between them.";
Options[LabeledGrid]={
    ItemSize->Automatic,
    Alignment->Center,
    Frame->All,
    "Separator"->",",
    "Pivot"->""
};
LabeledGrid[data_,rowHeaders_,columnHeaders_,OptionsPattern[]] :=
  Module[
   {gridList=data, rowHeads=rowHeaders, colHeads=columnHeaders},
   (
     separator=OptionValue["Separator"];
     pivot=OptionValue["Pivot"];
     gridList=Table[
             Tooltip[
               data[[rowIdx,colIdx]],
               DisplayForm[
                 RowBox[{rowHeads[[rowIdx]],
                         separator,
                         colHeads[[colIdx]]}
                       ]
                       ]
                     ],
         {rowIdx,Dimensions[data][[1]]},
         {colIdx,Dimensions[data][[2]]}];
     gridList=Transpose[Prepend[gridList,colHeads]];
     rowHeads=Prepend[rowHeads,pivot];
     gridList=Prepend[gridList,rowHeads]//Transpose;
     Grid[gridList,
         Frame->OptionValue[Frame],
         Alignment->OptionValue[Alignment],
         Frame->OptionValue[Frame],
         ItemSize->OptionValue[ItemSize]
         ]
   )
];

HamiltonianForm::usage = "HamiltonianForm[hamMatrix, basisLabels]
  takes the matrix representation of a hamiltonian together with a
  set of symbols representing the ordered basis in which the
  operator is represented. With this it creates a displayed form
  that has adequately labeled row and columns together with
  informative values when hovering over the matrix elements using
  the mouse cursor.";
Options[HamiltonianForm]={"Separator"->","Pivot"->""};
HamiltonianForm[hamMatrix_, basisLabels_List, OptionsPattern[]] :=
  (
     braLabels=DisplayForm[RowBox[{"\[LeftAngleBracket]",#,"\[
  RightBracketingBar]"}]]& /@ basisLabels;
     ketLabels=DisplayForm[RowBox[{"\[LeftBracketingBar]",#,"\[
  RightAngleBracket]"}]]& /@ basisLabels;
     LabeledGrid[hamMatrix,braLabels,ketLabels,"Separator"->
  OptionValue["Separator"],"Pivot"->OptionValue["Pivot"]]
     )

HamiltonianMatrixPlot::usage = "HamiltonianMatrixPlot[hamMatrix,
  basisLabels] creates a matrix plot of the given hamiltonian matrix
   with the given basis labels. The matrix elements can be hovered
  over to display the corresponding row and column labels together
  with the value of the matrix element. The option \"Overlay Values\
  " can be used to specify whether the matrix elements should be
  displayed on top of the matrix plot.";
Options[HamiltonianMatrixPlot] = Join[Options[MatrixPlot], {"Hover"
   -> True, "Overlay Values" -> True}];
HamiltonianMatrixPlot[hamMatrix_, basisLabels_, opts :
  OptionsPattern[]] := (
   braLabels = DisplayForm[RowBox[{"\[LeftAngleBracket]", #, "\[
  RightBracketingBar]"}]] & /@ basisLabels;
   ketLabels = DisplayForm[Rotate[RowBox[{"\[LeftBracketingBar]", #,
    "\[RightAngleBracket]"}],\[Pi]/2]] & /@ basisLabels;
   ketLabelsUpright = DisplayForm[RowBox[{"\[LeftBracketingBar]", #,
    "\[RightAngleBracket]"}]] & /@ basisLabels;
   numRows = Length[hamMatrix];
   numCols = Length[hamMatrix[[1]]];
   epiThings = Which[
```

```
      And[OptionValue["Hover"], Not[OptionValue["Overlay Values"]]],
      Flatten[
        Table[
          Tooltip[
            {
              Transparent,
              Rectangle[
              {j - 1, numRows - i},
              {j - 1, numRows - i} + {1, 1}
              ]
            },
          Row[{braLabels[[i]],ketLabelsUpright[[j]],"=",hamMatrix[[i, j]]}]
          ],
        {i, 1, numRows},
        {j, 1, numCols}
        ]
      ],
      And[OptionValue["Hover"], OptionValue["Overlay Values"]],
      Flatten[
        Table[
          Tooltip[
            {
              Transparent,
              Rectangle[
              {j - 1, numRows - i},
              {j - 1, numRows - i} + {1, 1}
              ]
            },
          DisplayForm[RowBox[{"\[LeftAngleBracket]", basisLabels[[i]], "\[LeftBracketingBar]", basisLabels[[j]], "\[RightAngleBracket]"}]]
          ],
        {i, numRows},
        {j, numCols}
        ]
      ],
      True,
      {}
      ];
    textOverlay = If[OptionValue["Overlay Values"],
      (
        Flatten[
        Table[
          Text[hamMatrix[[i, j]],
            {j - 1/2, numRows - i + 1/2}
          ],
        {i, 1, numRows},
        {j, 1, numCols}
        ]
        ]
      ),
      {}
      ];
    epiThings = Join[epiThings, textOverlay];
    MatrixPlot[hamMatrix,
      FrameTicks -> {
        {Transpose[{Range[Length[braLabels]], braLabels}], None},
        {None, Transpose[{Range[Length[ketLabels]], ketLabels}]}
        },
      Evaluate[FilterRules[{opts}, Options[MatrixPlot]]],
      Epilog -> epiThings
    ]
  );

  (* ################## Some Plotting Routines ################## *)
  (* ############################################################ *)

  (* ############################################################ *)
  (* ###################### Load Functions ###################### *)

  LoadAll::usage = "LoadAll[] executes most Load* functions.";
  LoadAll[] := (
    LoadTermLabels[];
    LoadCFP[];
    LoadUk[];
```

```
4635    LoadV1k[];
4636    LoadT22[];
4637    LoadSOOandECSOLS[];
4638
4639    LoadElectrostatic[];
4640    LoadSpinOrbit[];
4641    LoadSOOandECSO[];
4642    LoadSpinSpin[];
4643    LoadThreeBody[];
4644    LoadChenDeltas[];
4645    LoadCarnall[];
4646  );
4647
4648  fnTermLabels::usage = "This list contains the labels of f^n
        configurations. Each element of the list has four elements {LS,
        seniority, W, U}. At first sight this seems to only include the
        labels for the f^6 and f^7 configuration, however, all is included
         in these two.";
4649
4650  LoadTermLabels::usage = "LoadTermLabels[] loads into the session
        the labels for the terms in the f^n configurations.";
4651  LoadTermLabels[] := (
4652    If[ValueQ[fnTermLabels], Return[]];
4653    PrintTemporary["Loading data for state labels in the f^n
        configurations..."];
4654    fnTermsFname = FileNameJoin[{moduleDir, "data", "fnTerms.m"}];
4655
4656    If[!FileExistsQ[fnTermsFname],
4657      (PrintTemporary[">> fnTerms.m not found, generating ..."];
4658        fnTermLabels = ParseTermLabels["Export"->True];
4659      ),
4660      fnTermLabels = Import[fnTermsFname];
4661    ];
4662  );
4663
4664  Carnall::usage = "Association of data from Carnall et al (1989)
        with the following keys: {data, annotations, paramSymbols,
        elementNames, rawData, rawAnnotations, annnotatedData, appendix:Pr
        :Association, appendix:Pr:Calculated, appendix:Pr:RawTable,
        appendix:Headings}";
4665
4666  LoadCarnall::usage = "LoadCarnall[] loads data for trivalent
        lanthanides in LaF3 using the data from Bill Carnall's 1989 paper.
        ";
4667  LoadCarnall[] := (
4668    If[ValueQ[Carnall], Return[]];
4669    carnallFname = FileNameJoin[{moduleDir, "data", "Carnall.m"}];
4670    If[!FileExistsQ[carnallFname],
4671      (PrintTemporary[">> Carnall.m not found, generating ..."];
4672        Carnall = ParseCarnall[];
4673      ),
4674      Carnall = Import[carnallFname];
4675    ];
4676  );
4677
4678  LoadChenDeltas::usage = "LoadChenDeltas[] loads the differences
        noted by Chen.";
4679  LoadChenDeltas[] := (
4680    If[ValueQ[chenDeltas], Return[]];
4681    PrintTemporary["Loading the association of discrepancies found by
         Chen ..."];
4682    chenDeltasFname = FileNameJoin[{moduleDir, "data", "chenDeltas.m"
       }];
4683    If[!FileExistsQ[chenDeltasFname],
4684      (PrintTemporary[">> chenDeltas.m not found, generating ..."];
4685        chenDeltas = ParseChenDeltas[];
4686      ),
4687      chenDeltas = Import[chenDeltasFname];
4688    ];
4689  );
4690
4691  ParseChenDeltas::usage = "ParseChenDeltas[] parses the data found
        in ./data/the-chen-deltas-A.csv and ./data/the-chen-deltas-B.csv.
        If the option \"Export\" is set to True (True is the default),
        then the parsed data is saved to ./data/chenDeltas.m";
4692  Options[ParseChenDeltas] = {"Export" -> True};
```

```
ParseChenDeltas[OptionsPattern[]] := (
  chenDeltasRaw = Import[FileNameJoin[{moduleDir, "data", "the-chen-deltas-A.csv"}]];
  chenDeltasRaw = chenDeltasRaw[[2 ;;]];
  chenDeltas = <||>;
  chenDeltasA = <||>;
  Off[Power::infy];
  Do[
    ({right, wrong} = {chenDeltasRaw[[row]][[4 ;;]],
      chenDeltasRaw[[row + 1]][[4 ;;]]};
    key = chenDeltasRaw[[row]][[1 ;; 3]];
    repRule = (#[[1]] -> #[[2]]*#[[1]]) & /@
      Transpose[{{M0, M2, M4, P2, P4, P6}, right/wrong}];
    chenDeltasA[key] = <|"right" -> right, "wrong" -> wrong,
      "repRule" -> repRule|>;
    chenDeltasA[{key[[1]], key[[3]], key[[2]]}] = <|"right" -> right,
      "wrong" -> wrong, "repRule" -> repRule|>;
    ),
    {row, 1, Length[chenDeltasRaw], 2}];
  chenDeltas["A"] = chenDeltasA;

  chenDeltasRawB = Import[FileNameJoin[{moduleDir, "data", "the-chen-deltas-B.csv"}], "Text"];
  chenDeltasB = StringSplit[chenDeltasRawB, "\n"];
  chenDeltasB = StringSplit[#, ","] & /@ chenDeltasB;
  chenDeltasB = {ToExpression[StringTake[#[[1]], {2}]], #[[2]], #[[3]]} & /@ chenDeltasB;
  chenDeltas["B"] = chenDeltasB;
  On[Power::infy];
  If[OptionValue["Export"],
    (chenDeltasFname = FileNameJoin[{moduleDir, "data", "chenDeltas.m"}];
    Export[chenDeltasFname, chenDeltas];
    )
    ];
  Return[chenDeltas];
);

ParseCarnall::usage = "ParseCarnall[] parses the data found in ./data/Carnall.xls. If the option \"Export\" is set to True (True is the default), then the parsed data is saved to ./data/Carnall. This data is from the tables and appendices of Carnall et al (1989).";
Options[ParseCarnall] = {"Export" -> True};
ParseCarnall[OptionsPattern[]] := (
  ions          = {"Ce","Pr","Nd","Pm","Sm","Eu","Gd","Tb","Dy","Ho","Er","Tm","Yb"};
  templates     = StringTemplate/@StringSplit["appendix:`ion`:Association appendix:`ion`:Calculated appendix:`ion`:RawTable appendix:`ion`:Headings"," "];

  (* How many unique eigenvalues, after removing Kramer's degeneracy *)
  fullSizes     = AssociationThread[ions, {7, 91, 182, 1001, 1001, 3003, 1716, 3003, 1001, 1001, 182, 91, 7}];
  carnall       = Import[FileNameJoin[{moduleDir,"data","Carnall.xls"}]][[2]];
  carnallErr    = Import[FileNameJoin[{moduleDir,"data","Carnall.xls"}]][[3]];

  elementNames = carnall[[1]][[2;;]];
  carnall       = carnall[[2;;]];
  carnallErr    = carnallErr[[2;;]];
  carnall       = Transpose[carnall];
  carnallErr    = Transpose[carnallErr];
  paramNames    = ToExpression/@carnall[[1]][[1;;]];
  carnall       = carnall[[2;;]];
  carnallErr    = carnallErr[[2;;]];
  carnallData   = Table[(
                   data          = carnall[[i]];
                   data          = (#[[1]]->#[[2]])&/@Select[Transpose[{paramNames,data}],#[[2]]!=""&];
                   elementNames[[i]]->data
                   ),
                   {i,1,13}
```

```
                    ];
    carnallData  = Association[carnallData];
    carnallNotes = Table[(
                    data        = carnallErr[[i]];
                    elementName = elementNames[[i]];
                    dataFun     = (
                        #[[1]] -> If[#[[2]]=="[]",
                        "Not allowed to vary in fitting.",
                        If[#[[2]]=="[R]",
                            "Ratio constrained by: " <> <|"Eu"->"F4/F2=0.713; F6/F2=0.512",
                                "Gd"->"F4/F2=0.710]",
                                "Tb"->"F4/F2=0.707"|>[elementName],
                            If[#[[2]]=="i",
                                "Interpolated",
                                #[[2]]
                            ]
                        ]
                        ]) &;
                    data = dataFun /@ Select[Transpose[{paramNames,data}],#[[2]]!=""&];
                    elementName->data
                      ),
                {i,1,13}
                ];
    carnallNotes  = Association[carnallNotes];

    annotatedData = Table[
                    If[NumberQ[#[[1]]],Tooltip[#[[1]],#[[2]]],""] & /@ Transpose[{paramNames/.carnallData[element],
                      paramNames/.carnallNotes[element]
                        }],
                    {element,elementNames}
                    ];
    annotatedData = Transpose[annotatedData];

    Carnall = <|"data"      -> carnallData,
        "annotations"       -> carnallNotes,
        "paramSymbols"      -> paramNames,
        "elementNames"      -> elementNames,
        "rawData"           -> carnall,
        "rawAnnotations"    -> carnallErr,
        "includedTableIons" -> ions,
        "annnotatedData"    -> annotatedData
    |>;

    Do[(
        carnallData   = Import[FileNameJoin[{moduleDir,"data","Carnall.xls"}]][[sheetIdx]];
        headers       = carnallData[[1]];
        calcIndex     = Position[headers,"Calc (1/cm)"][[1,1]];
        headers       = headers[[2;;]];
        carnallLabels = carnallData[[1]];
        carnallData   = carnallData[[2;;]];
        carnallTerms  = DeleteDuplicates[First/@carnallData];
        parsedData    = Table[(
                            rows = Select[carnallData,#[[1]]==term&];
                            rows = #[[2;;]]&/@rows;
                            rows = Transpose[rows];
                            rows = Transpose[{headers,rows}];
                            rows = Association[(#[[1]]->#[[2]])&/@rows];
                            term->rows
                            ),
                      {term,carnallTerms}
                      ];
        carnallAssoc        = Association[parsedData];
        carnallCalcEnergies = #[[calcIndex]]&/@carnallData;
        carnallCalcEnergies = If[NumberQ[#],#,Missing[]]&/@carnallCalcEnergies;
        ion                 = ions[[sheetIdx-3]];
        carnallCalcEnergies = PadRight[carnallCalcEnergies, fullSizes[ion], Missing[]];
        keys                = #[<|"ion"->ion|>]&/@templates;
        Carnall[keys[[1]]]  = carnallAssoc;
        Carnall[keys[[2]]]  = carnallCalcEnergies;
```

```
4821          Carnall[keys[[3]]]  = carnallData;
4822          Carnall[keys[[4]]]  = headers;
4823          ),
4824      {sheetIdx,4,16}
4825      ];
4826
4827      goodions = Select[ions,#!="Pm"&];
4828      expData  = Select[Transpose[Carnall["appendix:"<>#<>":RawTable"
         ]][[1+Position[Carnall["appendix:"<>#<>":Headings"],"Exp (1/cm)"
         ][[1,1]]]],NumberQ]&/@goodions;
4829      Carnall["All Experimental Data"]=AssociationThread[goodions,
         expData];
4830      If[OptionValue["Export"],
4831        (
4832          carnallFname = FileNameJoin[{moduleDir, "data", "Carnall.m"
         }];
4833          Print["Exporting to "<>carnallFname];
4834          Export[carnallFname, Carnall];
4835        )
4836        ];
4837      Return[Carnall];
4838    );
4839
4840    CFP::usage = "CFP[{n, NKSL}] provides a list whose first element
       echoes NKSL and whose other elements are lists with two elements
       the first one being the symbol of a parent term and the second
       being the corresponding coefficient of fractional parentage. n
       must satisfy 1 <= n <= 7.
4841  These are according to the tables from Nielson & Koster.";
4842
4843  CFPAssoc::usage = " CFPAssoc is an association where keys are of
       lists of the form {num_electrons, daugherTerm, parentTerm} and
       values are the corresponding coefficients of fractional parentage.
        The terms given in string-spectroscopic notation. If a certain
       daughter term does not have a parent term, the value is 0. Loaded
       using LoadCFP[].
4844  These are according to the tables from Nielson & Koster.";
4845
4846  LoadCFP::usage = "LoadCFP[] loads CFP, CFPAssoc, and CFPTable into
       the session.";
4847  LoadCFP[] := (
4848    If[And[ValueQ[CFP], ValueQ[CFPTable], ValueQ[CFPAssoc]],Return
       []];
4849
4850    PrintTemporary["Loading CFPtable ..."];
4851    CFPTablefname = FileNameJoin[{moduleDir, "data", "CFPTable.m"}];
4852    If[!FileExistsQ[CFPTablefname],
4853      (PrintTemporary[">> CFPTable.m not found, generating ..."];
4854        CFPTable = GenerateCFPTable["Export"->True];
4855      ),
4856      CFPTable = Import[CFPTablefname];
4857    ];
4858
4859    PrintTemporary["Loading CFPs.m ..."];
4860    CFPfname = FileNameJoin[{moduleDir, "data", "CFPs.m"}];
4861    If[!FileExistsQ[CFPfname],
4862      (PrintTemporary[">> CFPs.m not found, generating ..."];
4863        CFP = GenerateCFP["Export"->True];
4864      ),
4865      CFP = Import[CFPfname];
4866    ];
4867
4868    PrintTemporary["Loading CFPAssoc.m ..."];
4869    CFPAfname = FileNameJoin[{moduleDir, "data", "CFPAssoc.m"}];
4870    If[!FileExistsQ[CFPAfname],
4871      (PrintTemporary[">> CFPAssoc.m not found, generating ..."];
4872        CFPAssoc = GenerateCFPAssoc["Export"->True];
4873      ),
4874      CFPAssoc = Import[CFPAfname];
4875    ];
4876  );
4877
4878  ReducedUkTable::usage = "ReducedUkTable[{n, l = 3, SL, SpLp, k}]
       provides reduced matrix elements of the unit spherical tensor
       operator Uk. See TASS section 11-9 \"Unit Tensor Operators\".
       Loaded using LoadUk[].";
```

```
4879
4880  LoadUk::usage = "LoadUk[] loads into session the reduced matrix
        elements for unit tensor operators.";
4881  LoadUk[] := (
4882    If[ValueQ[ReducedUkTable], Return[]];
4883    PrintTemporary["Loading the association of reduced matrix
      elements for unit tensor operators ..."];
4884    ReducedUkTableFname = FileNameJoin[{moduleDir, "data", "
      ReducedUkTable.m"}];
4885    If[!FileExistsQ[ReducedUkTableFname],
4886      (PrintTemporary[">> ReducedUkTable.m not found, generating ..."
      ];
4887        ReducedUkTable = GenerateReducedUkTable[7];
4888      ),
4889      ReducedUkTable = Import[ReducedUkTableFname];
4890    ];
4891  );
4892
4893  ElectrostaticTable::usage = "ElectrostaticTable[{n, SL, SpLp}]
        provides the calculated result of Electrostatic[{n, SL, SpLp}].
        Load using LoadElectrostatic[].";
4894
4895  LoadElectrostatic::usage = "LoadElectrostatic[] loads the reduced
        matrix elements for the electrostatic interaction.";
4896  LoadElectrostatic[] := (
4897    If[ValueQ[ElectrostaticTable], Return[]];
4898    PrintTemporary["Loading the association of matrix elements for
      the electrostatic interaction ..."];
4899    ElectrostaticTablefname = FileNameJoin[{moduleDir, "data", "
      ElectrostaticTable.m"}];
4900    If[!FileExistsQ[ElectrostaticTablefname],
4901      (PrintTemporary[">> ElectrostaticTable.m not found, generating
      ..."];
4902        ElectrostaticTable = GenerateElectrostaticTable[7];
4903      ),
4904      ElectrostaticTable = Import[ElectrostaticTablefname];
4905    ];
4906  );
4907
4908  LoadV1k::usage = "LoadV1k[] loads into session the matrix elements
        of V1k.";
4909  LoadV1k[] := (
4910    If[ValueQ[ReducedV1kTable], Return[]];
4911    PrintTemporary["Loading the association of matrix elements for
      V1k ..."];
4912    ReducedV1kTableFname = FileNameJoin[{moduleDir, "data", "
      ReducedV1kTable.m"}];
4913    If[!FileExistsQ[ReducedV1kTableFname],
4914      (PrintTemporary[">> ReducedV1kTable.m not found, generating ...
      "];
4915        ReducedV1kTable = GenerateReducedV1kTable[7];
4916      ),
4917      ReducedV1kTable = Import[ReducedV1kTableFname];
4918    ]
4919  );
4920
4921  LoadSpinOrbit::usage = "LoadSpinOrbit[] loads into session the
        matrix elements of the spin-orbit interaction.";
4922  LoadSpinOrbit[] := (
4923    If[ValueQ[SpinOrbitTable], Return[]];
4924    PrintTemporary["Loading the association of matrix elements for
      spin-orbit ..."];
4925    SpinOrbitTableFname = FileNameJoin[{moduleDir, "data", "
      SpinOrbitTable.m"}];
4926    If[!FileExistsQ[SpinOrbitTableFname],
4927      (
4928        PrintTemporary[">> SpinOrbitTable.m not found, generating ...
      "];
4929        SpinOrbitTable = GenerateSpinOrbitTable[7, "Export" -> True];
4930      ),
4931      SpinOrbitTable = Import[SpinOrbitTableFname];
4932    ]
4933  );
4934
4935  LoadSOOandECSOLS::usage = "LoadSOOandECSOLS[] loads into session
        the LS reduced matrix elements of the SOO-ECSO interaction.";
```

```
LoadSOOandECSOLS[] := (
  If[ValueQ[SOOandECSOLSTable], Return[]];
  PrintTemporary["Loading the association of LS reduced matrix elements for SOO-ECSO ..."];
  SOOandECSOLSTableFname = FileNameJoin[{moduleDir, "data", "ReducedSOOandECSOLSTable.m"}];
  If[!FileExistsQ[SOOandECSOLSTableFname],
    (PrintTemporary[">> ReducedSOOandECSOLSTable.m not found, generating ..."];
     SOOandECSOLSTable = GenerateSOOandECSOLSTable[7];
    ),
    SOOandECSOLSTable = Import[SOOandECSOLSTableFname];
  ];
);

LoadSOOandECSO::usage = "LoadSOOandECSO[] loads into session the LSJ reduced matrix elements of spin-other-orbit and electrostatically-correlated-spin-orbit.";
LoadSOOandECSO[] := (
  If[ValueQ[SOOandECSOTableFname], Return[]];
  PrintTemporary["Loading the association of matrix elements for spin-other-orbit and electrostatically-correlated-spin-orbit ..."];
  SOOandECSOTableFname = FileNameJoin[{moduleDir, "data", "SOOandECSOTable.m"}];
  If[!FileExistsQ[SOOandECSOTableFname],
    (PrintTemporary[">> SOOandECSOTable.m not found, generating ..."];
     SOOandECSOTable = GenerateSOOandECSOTable[7, "Export"->True];
    ),
    SOOandECSOTable = Import[SOOandECSOTableFname];
  ];
);

LoadT22::usage = "LoadT22[] loads into session the matrix elements of T22.";
LoadT22[] := (
  If[ValueQ[T22Table], Return[]];
  PrintTemporary["Loading the association of reduced T22 matrix elements ..."];
  T22TableFname = FileNameJoin[{moduleDir, "data", "ReducedT22Table.m"}];
  If[!FileExistsQ[T22TableFname],
    (PrintTemporary[">> ReducedT22Table.m not found, generating ..."];
     T22Table = GenerateT22Table[7];
    ),
    T22Table = Import[T22TableFname];
  ];
);

LoadSpinSpin::usage = "LoadSpinSpin[] loads into session the matrix elements of spin-spin.";
LoadSpinSpin[] := (
  If[ValueQ[SpinSpinTable], Return[]];
  PrintTemporary["Loading the association of matrix elements for spin-spin ..."];
  SpinSpinTableFname = FileNameJoin[{moduleDir, "data", "SpinSpinTable.m"}];
  If[!FileExistsQ[SpinSpinTableFname],
    (PrintTemporary[">> SpinSpinTable.m not found, generating ..."];
     SpinSpinTable = GenerateSpinSpinTable[7, "Export" -> True];
    ),
    SpinSpinTable = Import[SpinSpinTableFname];
  ];
);

LoadThreeBody::usage = "LoadThreeBody[] loads into session the matrix elements of three-body configuration-interaction effects.";
LoadThreeBody[] := (
  If[ValueQ[ThreeBodyTable], Return[]];
  PrintTemporary["Loading the association of matrix elements for three-body configuration-interaction effects ..."];
  ThreeBodyFname   = FileNameJoin[{moduleDir, "data", "ThreeBodyTable.m"}];
```

```
    ThreeBodiesFname = FileNameJoin[{moduleDir, "data", "ThreeBodyTables.m"}];
    If[!FileExistsQ[ThreeBodyFname],
      (PrintTemporary[">> ThreeBodyTable.m not found, generating ..."];
        {ThreeBodyTable, ThreeBodyTables} = GenerateThreeBodyTables[14, "Export" -> True];
      ),
      ThreeBodyTable  = Import[ThreeBodyFname];
      ThreeBodyTables = Import[ThreeBodiesFname];
    ];
  );

  (* ##################### Load Functions ###################### *)
  (* ########################################################### *)

End[];

LoadTermLabels[];
LoadCFP[];

EndPackage[];
```

17.2 fittings.m

This file has code useful for fitting the Hamiltonian.

```
(* ---------------------------------------------------------------------+

|~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~|

|~~~+----------------------------------------------------------------+~~~|

|~~~|                      _____ __   __   _                          |~~~|
|~~~|                     / __(_) /_/ /_(_)___   ____ ______          |~~~|
|~~~|                    / /_/ / __/ __/ / __ \/ __ `/ ___/           |~~~|
|~~~|                   / __/ / /_/ /_/ / / / / /_/ (__  )            |~~~|
|~~~|                  /_/ /_/\__/\__/_/_/ /_/\__, /____/             |~~~|
|~~~|                                        /____/                   |~~~|
|~~~|                                                                 |~~~|
|~~~+----------------------------------------------------------------+~~~|

|~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~|

|~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~|

|~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~|

|~~~~+--------------------------------------------------------------+~~~~|

|~~~~|                                                              |~~~~|
|~~~~|                                                              |~~~~|
|~~~~|  This script puts together some code useful for fitting the  |~~~~|
|~~~~|                  model Hamiltonian to data.                  |~~~~|
|~~~~|                                                              |~~~~|
|~~~~|                                                              |~~~~|
|~~~~+--------------------------------------------------------------+~~~~|

|~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~|

|~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~|
```

```
+--------------------------------------------------------------------
    *)

Get["qlanth.m"]
Get["qonstants.m"];
Get["misc.m"];
LoadCarnall[];
LoadFreeIon[];

Jiggle::usage = "Jiggle[num, wiggleRoom] takes a number and
    randomizes it a little by adding or subtracting a random fraction
    of itself. The fraction is controlled by wiggleRoom.";
Jiggle[num_, wiggleRoom_ : 0.1] := RandomReal[{1 - wiggleRoom, 1 +
    wiggleRoom}] * num;

AddToList::usage = "AddToList[list, element, maxSize, addOnlyNew]
    prepends the element to list and returns the list. If maxSize is
    reached, the last element is dropped. If addOnlyNew is True (the
    default), the element is only added if it is different from the
    last element.";
AddToList[list_, element_, maxSize_, addOnlyNew_ : True] := Module[{
    tempList = If[
      addOnlyNew,
      If[
       Length[list] == 0,
       {element},
       If[
        element != list[[-1]],
        Append[list, element],
        list
        ]
      ],
      Append[list, element]
      ]},
   If[Length[tempList] > maxSize,
    Drop[tempList, Length[tempList] - maxSize],
    tempList]
   ];

ProgressNotebook::usage="ProgressNotebook[] creates a progress
    notebook for the solver. This notebook includes a plot of the RMS
    history and the current parameter values. The notebook is returned
    . The RMS history and the parameter values are updated by setting
    the variables rmsHistory and paramSols. The variables
    stringPartialVars and paramSols are used to display the parameter
    values in the notebook. The notebook is created with the title \"
    Solver Progress\". The notebook is created with the option
    WindowSelected->True. The notebook is created with the option
    TextAlignment->Center. The notebook is created with the option
    WindowTitle->\"Solver Progress\".";
Options[ProgressNotebook] = {"Basic" -> True};
ProgressNotebook[OptionsPattern[]] := (
   nb = Which[
   OptionValue["Basic"],
   CreateDocument[(
      {
       Dynamic[
        TextCell[
         If[
          Length[paramSols] > 0,
          TableForm[
            Prepend[
              Transpose[{stringPartialVars,
              paramSols[[-1]]}],
              {"RMS",rmsHistory[[-1]]}]
              ],
           ""
          ],
         "Output"
         ],
        TrackedSymbols :> {paramSols, stringPartialVars}
        ]
       }
      ),
     WindowSize -> {600, 1000},
     WindowSelected -> True,
```

```
      TextAlignment -> Center,
      WindowTitle -> "Solver Progress"
      ],
    True,
    CreateDocument[(
       {
         "",
         Dynamic[Framed[progressMessage]],
         Dynamic[
         GraphicsColumn[
          {ListPlot[rmsHistory,
            PlotMarkers -> "OpenMarkers",
            Frame -> True,
            FrameLabel -> {"Iteration", "RMS"},
            ImageSize -> 800,
            AspectRatio -> 1/3,
            FrameStyle -> Directive[Thick, 15],
            PlotLabel -> If[Length[rmsHistory] != 0, rmsHistory[[-1]],
     ""]
           ],
          ListPlot[(#/#[[1]]) & /@ Transpose[paramSols],
           Joined -> True,
           PlotRange -> {All, {-5, 5}},
           Frame -> True,
           ImageSize -> 800,
           AspectRatio -> 1,
           FrameStyle -> Directive[Thick, 15],
           FrameLabel -> {"Iteration", "Params"}
           ]
          }
         ],
         TrackedSymbols :> {rmsHistory, paramSols}],
        Dynamic[
         TextCell[
          If[
           Length[paramSols] > 0,
           TableForm[Transpose[{stringPartialVars, paramSols[[-1]]}]],
           ""
          ],
         "Output"
         ],
         TrackedSymbols :> {paramSols, stringPartialVars}
        ]
       }
      ),
      WindowSize -> {600, 1000},
      WindowSelected -> True,
      TextAlignment -> Center,
      WindowTitle -> "Solver Progress"
      ]
    ];
    Return[nb];
    );

energyCostFunTemplate::usage="energyCostFunTemplate is template used
    to define the cost function for the energy matching. The template
    is used to define a function TheRightEnergyPath that takes a list
    of variables and returns the RMS of the energy differences between
     the computed and the experimental energies. The template requires
     the values to the following keys to be provided: `vars` and `
    varPatterns`";
energyCostFunTemplate = StringTemplate["
TheRightEnergyPath[`varPatterns`]:= (
  {eigenEnergies, eigenVecs} = Eigensystem[compHam[`vars`]];
  ordering      = Ordering[eigenEnergies];
  eigenEnergies = eigenEnergies - Min[eigenEnergies];
  states        = Transpose[{eigenEnergies, eigenVecs}];
  states        = states[[ordering]];
  coarseStates  = ParseStates[states, basis];
  coarseStates  = {#[[1]],#[[-1]]}& /@ coarseStates;
  (* The eigenvectors need to be simplified in order to compare
    labels to labels *)
  missingLevels = Length[coarseStates]-Length[expData];
  (* The energies are in the first element of the tuples. *)
  energyDiffFun = (Abs[#1[[1]]-#2[[1]]])&;
  (* match disregarding labels *)
```

```
  energyFlow    = FlowMatching[coarseStates,
                  expData,
                  \"notMatched\" -> missingLevels,
                  \"CostFun\"    -> energyDiffFun
                  ];
  energyPairs   = {#[[1]][[1]], #[[2]][[1]]} & /@ energyFlow[[1]];
  energyRms     = Sqrt[Total[(Abs[#[[2]]-#[[1]]])^2 & /@ energyPairs]
    / Length[energyPairs]];
  Return[energyRms];
)"];

AppendToLog[message_, file_String] := Module[
  {timestamp = DateString["ISODateTime"], msgString},
  (
    msgString = ToString[message, InputForm]; (* Convert any
    expression to a string *)
    OpenAppend[file];
    WriteString[file, timestamp, " - ", msgString, "\n"];
    Close[file];
  )
  ];

energyAndLabelCostFunTemplate::usage="energyAndLabelCostFunTemplate
    is a template used to define the cost function that includes both
    the differences between energies and the differences between
    labels. The template is used to define a function
    TheRightSignedPath that takes a list of variables and returns the
    RMS of the energy differences between the computed and the
    experimental energies together with a term that depends on the
    differences between the labels. The template requires the values
    to the following keys to be provided: `vars` and `varPatterns`";
energyAndLabelCostFunTemplate = StringTemplate["
TheRightSignedPath[`varPatterns`] := Module[
  {energyRms, eigenEnergies, eigenVecs, ordering, states,
    coarseStates, missingLevels, energyDiffFun, energyFlow,
    energyPairs, energyAndLabelFun, energyAndLabelFlow, totalAvgCost},
  (
    {eigenEnergies, eigenVecs} = Eigensystem[compHam[`vars`]];
    ordering      = Ordering[eigenEnergies];
    eigenEnergies = eigenEnergies - Min[eigenEnergies];
    states        = Transpose[{eigenEnergies, eigenVecs}];
    states        = states[[ordering]];
    coarseStates  = ParseStates[states, basis];

    (* The eigenvectors need to be simplified in order to compare
    labels to labels *)
    coarseStates  = {#[[1]],#[[-1]]}& /@ coarseStates;
    missingLevels = Length[coarseStates]-Length[expData];

    (* The energies are in the first element of the tuples. *)
    energyDiffFun = ( Abs[#1[[1]]-#2[[1]]] ) &;

    (* matching disregarding labels to get overall scale for scaling
    differences in labels *)
    energyFlow    = FlowMatching[coarseStates,
                    expData,
                    \"notMatched\" -> missingLevels,
                    \"CostFun\"    -> energyDiffFun
                    ];
    energyPairs   = {#[[1]][[1]], #[[2]][[1]]}&/@energyFlow[[1]];
    energyRms     = Sqrt[Total[(Abs[#[[2]]-#[[1]]])^2 & /@
    energyPairs]/Length[energyPairs]];

    (* matching using both labels and energies  *)
    energyAndLabelFun  = With[{del=energyRms},
                (Abs[#1[[1]]-#2[[1]]] +
                If[#1[[2]]==#2[[2]],
                  0.,
                  del])&];

    (* energyAndLabelFun  = With[{del=energyRms},
                (Abs[#1[[1]]-#2[[1]]] +
                del*EditDistance[#1[[2]],#2[[2]]])&]; *)
    energyAndLabelFun  = ( Abs[#1[[1]] - #2[[1]]] + EditDistance
    [#1[[2]],#2[[2]]] )&;
    energyAndLabelFlow = FlowMatching[coarseStates,
```

```
                        expData,
                        \"notMatched\" -> missingLevels,
                        \"CostFun\"    -> energyAndLabelFun
                        ];
    totalAvgCost       = Total[energyAndLabelFun@@# & /@
    energyAndLabelFlow[[1]]]/Length[energyAndLabelFlow[[1]]];
    Return[totalAvgCost];
  )
]"];

truncatedEnergyCostTemplate = StringTemplate["
TheTruncatedAndSignedPath[`varsWithNumericQ`] :=
(
  (* Calculate the truncated Hamiltonian *)
  numericalFreeIonHam = compileIntermediateTruncatedHam[`
    varsMixedWithFixedVals`];

  (* Diagonalize it *)
  {truncatedEigenvalues, truncatedEigenVectors} = Eigensystem[
    numericalFreeIonHam];

  (* Using the truncated eigenvectors push them up to the full state
    space *)
  pulledTruncatedEigenVectors = truncatedEigenVectors.Transpose[
    truncatedIntermediateBasis];
  states = Transpose[{truncatedEigenvalues,
    pulledTruncatedEigenVectors}];
  states = SortBy[states, First];
  states = ShiftedLevels[states];

  (* Coarsen the resulting eigenstates *)
  coarseStates = ParseStates[states, basis];

  (* Grab the parts that are needed for fitting *)
  coarseStates = {#[[1]], #[[-1]]} & /@ coarseStates;

  (* This cost function takes into account both labels and energies a
     random factor is added for the sake of stability of the solver*)
  energyAndLabelFun = (
        (
          Abs[#1[[1]] - #2[[1]]] +
          EditDistance[#1[[2]], #2[[2]]]
        ) *
        (1 + RandomReal[{-10^-6, 10^-6}])) &;

  (* This one only takes into account the energies *)
  energyFun = (Abs[#1[[1]] - #2[[1]]]*(1 + RandomReal[{0, 10^-6}]) &)
    ;

  (* Choose which cost function to use *)
  costFun = energyAndLabelFun;

  (* Not all states are to be matched to the experimental data *)
  missingLevels = Length[coarseStates] - Length[expData];

  (* If there are more experimental data than calculated ones, don't
    leave any state unmatched to those*)
  missingLevels = If[missingLevels < 0, 0, missingLevels];

  (* Apply the Hungarian algorithm to match the two sets of data *)
  energyAndLabelFlow = FlowMatching[coarseStates,
    expData,
    \"notMatched\" -> missingLevels,
    \"CostFun\" -> costFun];
  totalCosts   = (costFun @@ #)& /@ energyAndLabelFlow[[1]];
  totalAvgCost = Total[totalCosts] / Length[energyAndLabelFlow[[1]]];
  Return[totalAvgCost]
)"
];

Constrainer::usage = "Constrainer[problemVars, ln] returns a list of
    constraints for the variables in problemVars for trivalent
    lanthanide ion ln. problemVars are standard model symbols (F2, F4,
     ...). The ranges returned are based in the fitted parameters for
    LaF3 as found in Carnall et al. They could probably be more fine
    grained, but these ranges are seen to describe all the ions in
```

```
    that case.";
Constrainer[problemVars_, ln_] := (
  slater = Which[
    MemberQ[{"Ce", "Yb"}, ln],
    {},
    True,
    {#, (20000. < # < 120000.)} & /@ {F2, F4, F6}
    ];
  alpha = Which[
    MemberQ[{"Ce", "Yb"}, ln],
    {},
    True,
    {{α, 14. < α < 22.}}
    ];
  zeta = {{ζ, 500. < ζ < 3200.}};
  beta = Which[
    MemberQ[{"Ce", "Yb"}, ln],
    {},
    True,
    {{β, -1000. < β < -400.}}
    ];
  gamma = Which[
    MemberQ[{"Ce", "Yb"}, ln],
    {},
    True,
    {{γ, 1000. < γ < 2000.}}
    ];
  tees = Which[
    ln == "Tm",
    {100. < T2 < 500.},
    MemberQ[{"Ce", "Pr", "Yb"}, ln],
    {},
    True,
    {#, -500. < # < 500.} & /@ {T2, T3, T4, T6, T7, T8}];
  marvins = Which[
    MemberQ[{"Ce", "Yb"}, ln],
    {},
    True,
    {{M0, 1.0 < M0 < 5.0}}
    ];
  peas = Which[
    MemberQ[{"Ce", "Yb"}, ln],
    {},
    True,
    {{P2, -200. < P2 < 1200.}}
    ];
  crystalRanges = {#, (-2000. < # < 2000.)} & /@ (Intersection[
      cfSymbols, problemVars]);
  allCons =
   Join[slater, zeta, alpha, beta, gamma, tees, marvins, peas,
    crystalRanges];
  allCons = Select[allCons, MemberQ[problemVars, #[[1]]] &];
  Return[Flatten[Rest /@ allCons]]
  )

Options[LogSol] = {"PrintFun" -> PrintTemporary};
LogSol::usage = "LogSol[expr, solHistory, prefix] saves the given
    expression to a file. The file is named with the given prefix and
    a created UUID. The file is saved in the \"log\" directory under
    the current directory. The file is saved in the format of a .m
    file. The function returns the name of the file.";
LogSol[theSolution_, prefix_, OptionsPattern[]] := (
  PrintFun = OptionValue["PrintFun"];
  fname = prefix <> "-sols-" <> CreateUUID[] <> ".m";
  fname = FileNameJoin[{".", "log", fname}];
  PrintFun["Saving solution to: ", fname];
  Export[fname, theSolution];
  Return[fname];
  );


FitToHam::usage = "FitToHam[numE, expData, fitToSymbols, simplifier,
    OptionsPattern[]] fits the model Hamiltonian to the experimental
    data for the trivalent lanthanide ion with number numE. The
    experimental data is given in the form of a list of tuples. The
    first element of the tuple is the energy and the second element is
```

```
     the label. The function saves the results to a file, with the
    string filePrefix prepended to it, by default this is an empty
    string, in which case the filePrefix is modified to be the name of
     the lanthanide.
340 The fitToSymbols is a list of the symbols to be fit. The simplifier
    is a list of rules that simplify the Hamiltonian.
341 The options and their defaults are:
342 \"PrintFun\"->PrintTemporary,
343 \"FilePrefix\"->\"\",
344 \"SlackChannel\"->None,
345 \"MaxHistory\"->100,
346 \"MaxIters\"->100,
347 \"NumCycles\"->10,
348 \"ProgressWindow\"->True
349 The PrintFun option is the function used to print progress messages.
350 The FilePrefix option is the prefix to use for the file name, by
    default this is the symbol for the lanthanide.
351 The SlackChannel option is the channel to post progress messages to.
352 The MaxHistory option is the maximum number of iterations to keep in
    the history.
353 The MaxIters option is the maximum number of iterations for the
    solver.
354 The NumCycles option is the number of cycles to run the solver for.
355 The function returns a list of solutions. The solutions are the
    results of the NMinimize function. The solutions are a list of
    tuples. The first element of the tuple is the RMS error and the
    second element is the parameter values
356 The function also saves the solutions to a file. The file is named
    with a prefix and a UUID. The file is saved in the current
    directory. The file is saved in the format of a .m file.";
357 Options[FitToHam] = {
358       "PrintFun"-> PrintTemporary,
359       "FilePrefix" -> "",
360       "SlackChannel" -> None,
361       "MaxHistory" -> 100,
362       "ProgressWindow"-> True,
363       "MaxIters" -> 100,
364       "NumCycles" -> 10};
365 FitToHam[numE_Integer, expData_List, fitToSymbols_List,
    simplifier_List, OptionsPattern[]] :=
366   (
367     PrintFun         = OptionValue["PrintFun"];
368     fitToVars        = ToExpression[ToString[#] <> "v"] & /@
    fitToSymbols;
369     stringfitToVars  = ToString /@ fitToVars;
370     slackChan        = OptionValue["SlackChannel"];
371     maxHistory       = OptionValue["MaxHistory"];
372     maxIters         = OptionValue["MaxIters"];
373     numCycles        = OptionValue["NumCycles"];
374     ln               = theLanthanides[[numE]];
375     logFilePrefix    = If[OptionValue["FilePrefix"] == "",
376                           ToString[theLanthanides[[numE]]],
377                           OptionValue["FilePrefix"]];
378     PrintFun["Assembling the Hamiltonian for f^", numE, " ..."];
379     ham = HamMatrixAssembly[numE];
380     PrintFun["Simplifying the symbolic expression for the Hamiltonian
     in terms of the given simplifier..."];
381     ham = ReplaceInSparseArray[ham, simplifier];
382     PrintFun["Determining the variables to be fit for ..."];
383     (* as they remain after simplifying *)
384     fitVars = Variables[Normal[ham]];
385     (* append v to symbols *)
386     varVars = ToExpression[ToString[#] <> "v"] & /@ fitVars;
387
388     PrintFun[
389     "Compiling a function for efficient evaluation of the Hamiltonian
     matrix ..."];
390     compHam = Compile[Evaluate[fitVars], Evaluate[N[Normal[ham]]]];
391
392     PrintFun[
393     "Defining the cost function according to given energies and state
     labels ..."];
394
395     varPatterns = StringJoin[{ToString[#], "_?NumericQ"}] & /@
    fitVars;
396     varPatterns = Riffle[varPatterns, ", "];
```

```
397     varPatterns = StringJoin[varPatterns];
398     vars = ToString[#] & /@ fitVars;
399     vars = Riffle[vars, ", "];
400     vars = StringJoin[vars];
401
402     basis = BasisLSJMJ[numE];
403
404     (* define the cost functions given the problem variables *)
405     energyCostFunString =
406     energyCostFunTemplate[<|
407       "varPatterns" -> varPatterns,
408       "vars" -> vars|>];
409     ToExpression[energyCostFunString];
410     energyAndLabelCostFunString = energyAndLabelCostFunTemplate[<|"
      varPatterns" -> varPatterns, "vars" -> vars|>];
411     ToExpression[energyAndLabelCostFunString];
412
413     PrintFun["getting starting values from LaF3..."];
414     lnParams = LoadLaF3Parameters[ln];
415     bills = Table[lnParams[ToExpression[StringTake[ToString[varvar],
      {1, -2}]]], {varvar, varVars}];
416
417     (* define the function arguments with the frozen args in place *)
418     activeArgs = Table[
419       If[MemberQ[fitToVars, varvar],
420       varvar,
421       lnParams[ToExpression[StringTake[ToString[varvar], {1, -2}]]]],
422     {varvar, varVars}
423     ];
424     activeArgs = StringJoin[Riffle[ToString /@ activeArgs, ", "]];
425     (* the constraints, very important *)
426     constraints = N[Constrainer[fitToVars, ln]];
427     complementaryArgs = Table[
428       If[MemberQ[fitToVars, varvar],
429       varvar,
430       lnParams[ToExpression[StringTake[ToString[varvar], {1, -2}]]]],
431     {varvar, varVars}
432     ];
433
434     fromBill = {B02v -> B02, B04v -> B04, B06v -> B06, B22v -> B22,
435     B24v -> B24, B26v -> B26, B44v -> B44, B46v -> B46, B66v -> B66,
436     M0v -> M0, P2v -> P2} /. lnParams;
437
438     If[Not[ValueQ[noteboo]] && OptionValue["ProgressWindow"],
439     noteboo = ProgressNotebook["Basic" -> False];
440     ];
441
442     threadHeaderTemplate = StringTemplate[
443     "(`idx`/`reps`) Fitting data for `ln` using `freeVars`."
444     ];
445     solutions = {};
446     Do[
447     (
448       (* Remove the downvalues of the cost function *)
449       (* DownValues[TheRightSignedPath] = {DownValues[
      TheRightSignedPath][[-1]]}; *)
450       (* start history anew *)
451       rmsHistory = {};
452       paramSols  = {};
453       startTime  = Now;
454       threadMessage = threadHeaderTemplate[
455           <|"reps" -> numCycles,
456           "idx" -> rep,
457           "ln" -> ln,
458           "freeVars" -> ToString[fitToVars]|>];
459       If[slackChan =!= None,
460         threadTS = PostMessageToSlack[threadMessage, slackChan]["ts"]
461       ];
462       solverTemplateNMini = StringTemplate["
463         numIter = 0;
464         sol = NMinimize[
465           Evaluate[
466             Join[{TheRightSignedPath[`activeArgs`]},
467               constraints
468             ]
469           ],
```

```
        fitToVars,
        MaxIterations->`maxIterations`,
        Method->`Method`,
        `Monitor`:>(
          currentErr = TheRightSignedPath[`activeArgs`];
          numIter   += 1;
          rmsHistory = AddToList[rmsHistory, currentErr, maxHistory, False];
          paramSols  = AddToList[paramSols, fitToVars, maxHistory, False];
        )
      ]
    "];
    solverCode = solverTemplateNMini[<|
      "maxIterations" -> maxIters,
      "Method" -> "{\"DifferentialEvolution\",
          \"PostProcess\"   -> False,
          \"ScalingFactor\" -> 0.9,
          \"RandomSeed\"    -> RandomInteger[{0,1000000}],
          \"SearchPoints\"  -> 10}",
      "Monitor" -> "StepMonitor",
      "activeArgs" -> activeArgs|>];
    ToExpression[solverCode];
    timeTaken = QuantityMagnitude[Now - startTime, "Seconds"];
    Print["Took " <> ToString[timeTaken] <> "s"];
    Print[sol];
    {bestError, bestParams} = sol;
    resultMessage = "sigma=" <> ToString[Round[bestError, 0.1]];
    logFname = LogSol[sol, logFilePrefix];
    If[slackChan =!= None,
    (
      PostMessageToSlack[resultMessage,   slackChan, "threadTS" -> threadTS];
      PostFileToSlack[logFname, logFname, slackChan, "threadTS" -> threadTS];
    )
    ];

    vsBill = TableForm[
    Transpose[{
      First /@ fromBill,
      Last /@ fromBill,
      Round[Last /@ bestParams, 1.]}],
    TableHeadings -> {None, {"Param", "Bill Bkq", "ql Bkq"}}
    ];
    If[slackChan =!= None,
      PostPdfToSlack[logFname, vsBill, slackChan, "threadTS" -> threadTS]
    ];

    (* analysis code *)

    finalHam = compHam @@ (complementaryArgs /. bestParams);
    {eigenEnergies, eigenVecs} = Eigensystem[finalHam];
    ordering = Ordering[eigenEnergies];
    eigenEnergies = eigenEnergies - Min[eigenEnergies];
    states = Transpose[{eigenEnergies, eigenVecs}];
    states = states[[ordering]];
    coarseStates = ParseStates[states, basis];

    (* The eigenvectors need to be simplified in order to compare labels to labels *)
    coarseStates = {#[[1]], #[[-1]]} & /@ coarseStates;
    missingLevels = Length[coarseStates] - Length[expData];
    (* The energies are in the first element of the tuples. *)
    energyDiffFun = (Abs[#1[[1]] - #2[[1]]]) &;
    (* matching disregarding labels to get overall scale for scaling differences in labels *)
    energyFlow = FlowMatching[coarseStates,
            expData,
            "notMatched" -> missingLevels,
            "CostFun" -> energyDiffFun];
    energyPairs = {#[[1]][[1]], #[[2]][[1]]} & /@ energyFlow[[1]];
    energyRms = Sqrt[Total[(Abs[#[[2]] - #[[1]]])^2 & /@ energyPairs] / Length[energyPairs]];
    (* matching using both labels and energies *)
```

```
538       energyAndLabelFun = (Abs[#1[[1]] - #2[[1]]] + EditDistance
      [#1[[2]],#2[[2]]]) &;
539       energyAndLabelFlow = FlowMatching[coarseStates,
540             expData,
541             "notMatched" -> (Length[coarseStates] - Length[expData]),
542             "CostFun" -> energyAndLabelFun];
543       totalAvgCost = Total[energyAndLabelFun @@ # & /@
      energyAndLabelFlow[[1]]] / Length[energyAndLabelFlow[[1]]];
544
545       compa = (Flatten /@ energyAndLabelFlow[[1]]);
546       compa = Join[
547           #,
548           {
549             #[[2]] == #[[4]],
550             If[NumberQ[#[[1]]],
551               Round[#[[1]] - #[[3]],1],
552               ""
553             ],
554           #[[5]] - #[[3]],
555           Which[
556             Round[Abs[#[[1]] - #[[3]]]] < Round[Abs[#[[5]] -
      #[[3]]]],
557               "Better",
558             Round[Abs[#[[1]] - #[[3]]]] == Round[Abs[#[[5]] -
      #[[3]]]],
559               "Equal",
560             True,
561               "Worse"
562           ]
563           }
564       ] & /@ compa;
565       atable = TableForm[compa,
566         TableHeadings -> {None,
567           {"ql", "ql", "Bill (exp)", "Bill (exp)",
568           "Bill (calc)", "labels=", "ql - exp", "bill - exp"}}
569       ];
570       atable = Framed[atable, FrameMargins -> 20];
571       upsAndDowns = {
572         {"Better", Length[Select[compa, #[[-1]] == "Better" &]]},
573         {"Equal",  Length[Select[compa, #[[-1]] == "Equal" &]]},
574         {"Worse",  Length[Select[compa, #[[-1]] == "Worse" &]]}
575       };
576       upsAndDowns = TableForm[upsAndDowns];
577       If[slackChan =!= None,
578         PostPdfToSlack["table", atable, slackChan, "threadTS" ->
      threadTS];
579       ];
580       solutions = Append[solutions, sol];
581     ),
582     {rep, 1, numCycles}
583     ];
584   )
585
586 TruncationFit::usage="TruncationFit[numE, expData, numReps,
      activeVars, startingValues, Options] fits the given expData in an
      f^numE configuration, generating numReps different solutions, and
      varying the symbols in activeVars. The list startingValues is a
      list with all of the parameters needed to define the Hamiltonian (
      including values for activeVars, which will be disregarded but are
       required as position placeholders). The function returns a list
      of solutions. The solutions are the results of the NMinimize
      function using the Differential Evolution method. The solutions
      are a list of tuples. The first element of the tuple is the RMS
      error and the second element is a list of replacement rules for
      the fitted parameters. Once each NMinimize is done, the function
      saves the solutions to a file. The file is named with a prefix and
       a UUID. The file is saved in the log sub-directory as a .m file.
      The solver is always constrained by the relevant subsets of
      constraints for the parameters as provided by the Constrainer
      function. By default the Differential Evolution method starts with
       a generation of points within the given constraints, however it
      is also possible here to have a different region from which the
      initial points are chosen with the option \"StartingForVars\".
587
588 The following options can be used:
589   \"SignatureCheck\" : if True then then the function ends
```

```
    prematurely, printing a list with the symbols that would have
    defined the Hamiltonian after all simplifications have been
    applied. Useful to check the entire parameter set that the
    Hamiltonian has, which has to match one-to-one what is provided by
     startingValues.
  \"FilePrefix\" : the prefix to use for the file name, by default
    this is the symbol for the lanthanide.
  \"AccuracyGoal\": sets the accuracy goal for NMinimize, the default
     is 3.
  \"MaxHistory\" : determines how long the logs for the solver can be
    .
  \"MaxIterations\": determines the maximum number of iterations used
     by NMinimize.

  \"AccuracyGoal\": the accuracy goal used by NMinimize, default of
    3.
  \"TrucationEnergy\": if Automatic then the maximum energy in
    expData is taken, else it takes the value set by this option. In
    all cases the energies in expData are truncated to this value.
  \"PrintFun\": the function used to print progress messages, the
    default is PrintTemporary.
  \"SlackChannel\": name of the Slack channel to which to dump
    progress messaages, the default is None which disables this option
     entirely.
  \"ProgressView\": whether or not a progress window will be opened
    to show the progress of the solver, the default is True.

  \"ReturnHashFileNameAndExit\": if True then the function returns
    the name of the file with the solutions and exits, the default is
    False.
  \"StartingForVars\": if different from {} then it has to be a list
    with two elements. The first element being a number that
    determines the fraction half-width of the interval used for
    choosing the initial generation of points. The second element
    being a list with as many elements as activeVars corresponding to
    the midpoints from which the intial generation points are chosen.
    The default is {}.
  \"DE:CrossProbability\": the cross probability used by the
    Differential Evolution method, the default is 0.5.
  \"DE:ScalingFactor\": the scaling factor used by the Differential
    Evolution method, the default is 0.6.
  \"DE:SearchPoints\": the number of search points used by the
    Differential Evolution method, the default is Automatic.

  \"MagneticSimplifier\": a list of replacement rules to simplify the
     Marvin and pesudo-magnetic paramters.
  \"MagFieldSimplifier\": a list of replacement rules to specify a
    magnetic field (in T), if set to {}, then {Bx, By, Bz} can also
    then be used as variables to be fitted for.
  \"SymmetrySimplifier\": a list of replacements rules to simplify
    the crystal field.
  \"OtherSimplifier\": an additiona list of replacement rules that
    are applied to the Hamiltonian before computing with it.
  \"ThreeBodySimplifier\": the default is an Association that simply
    states which three body parameters Tk are zero in different
    configurations, if a list of replacement rules is used then that
    is used instead for the given problem.

  \"FreeIonSymbols\": a list with the symbols to be included in the
    intermediate coupling basis.
  \"AppendToLogFile\": an association appended to the log file under
    the key \"Appendix\".
  ";
Options[TruncationFit]={
  "MaxHistory"       -> 200,
  "MaxIterations"    -> 100,
  "FilePrefix"       -> "",
  "AccuracyGoal"     -> 3,
  "TruncationEnergy" -> Automatic,
  "PrintFun"         -> PrintTemporary,
  "SlackChannel"     -> None,
  "ProgressView"     -> True,
  "SignatureCheck"   -> False,
  "AppendToLogFile"  -> <||>,
  "StartingForVars"  -> {},
  "ReturnHashFileNameAndExit" -> False,
```

```
  "DE:CrossProbability" -> 0.5,
  "DE:ScalingFactor"    -> 0.6,
  "DE:SearchPoints"     -> Automatic,
  "MagneticSimplifier"  -> {
    M2 -> 56/100 M0,
    M4 -> 31/100 M0,
    P4 -> 1/2 P2,
    P6 -> 1/10 P2},
  "MagFieldSimplifier" -> {
    Bx->0,By->0,Bz->0
    },
  "SymmetrySimplifier" -> {
    B12->0,B14->0,B16->0,B34->0,B36->0,B56->0,
    S12->0,S14->0,S16->0,S22->0,S24->0,S26->0,S34->0,S36->0,
    S44->0,S46->0,S56->0,S66->0
    },
"OtherSimplifier" -> {
    F0->0,
    P0->0,
    \[Sigma]SS->0,
    T11p->0,T12->0,T14->0,T15->0,
    T16->0,T18->0,T17->0,T19->0,T2p->0
    },
"ThreeBodySimplifier" -> <|
    1  -> {
      T2->0,T3->0,T4->0,T6->0,T7->0,T8->0,T11p->0,T12->0,T14->0,T15
    ->0,T16->0,T18->0,T17->0,T19->0,T2p->0},2->{T2->0,T3->0,T4->0,T6
    ->0,T7->0,T8->0,T11p->0,T12->0,T14->0,T15->0,T16->0,T18->0,T17->0,
    T19->0,T2p->0
      },
    3  -> {},
    4  -> {},
    5  -> {},
    6  -> {},
    7  -> {},
    8  -> {},
    9  -> {},
    10 -> {},
    11 -> {},
    12 -> {
      T3->0,T4->0,T6->0,T7->0,T8->0,T11p->0,T12->0,T14->0,T15->0,T16
    ->0,T18->0,T17->0,T19->0,T2p->0
      },
    13->{
      T2->0,T3->0,T4->0,T6->0,T7->0,T8->0,T11p->0,T12->0,T14->0,T15
    ->0,T16->0,T18->0,T17->0,T19->0,T2p->0
      }
    |>,
"FreeIonSymbols" -> {F0, F2, F4, F6, M0, P2, α, β, γ, ζ, T2, T3, T4,
    T6, T7, T8}
};
TruncationFit[numE_Integer, expData0_List, numReps_Integer,
    activeVars_List, startingValues_List, OptionsPattern[]]:=(
  ln               = theLanthanides[[numE]];
  expData          = expData0;
  PrintFun         = OptionValue["PrintFun"];
  truncationEnergy = If[OptionValue["TruncationEnergy"]===Automatic,
    Max[First/@expData],
    OptionValue["TruncationEnergy"]
  ];
  oddsAndEnds    = <||>;
  expData        = Select[expData, #[[1]] <= truncationEnergy &];
  maxIterations  = OptionValue["MaxIterations"];
  maxHistory     = OptionValue["MaxHistory"];
  slackChan      = OptionValue["SlackChannel"];
  accuracyGoal   = OptionValue["AccuracyGoal"];
  logFilePrefix  = If[OptionValue["FilePrefix"] == "",
                      ToString[theLanthanides[[numE]]],
                      OptionValue["FilePrefix"]];

  usingInitialRange  = Not[OptionValue["StartingForVars"] === {}];
  If[usingInitialRange,
    (
      PrintFun["Using the solver for initial values in range ..."];
      {fractionalWidth, startVarValues} = OptionValue["
    StartingForVars"];
```

```
    )
  ];

  magneticSimplifier  = OptionValue["MagneticSimplifier"];
  magFieldSimplifier  = OptionValue["MagFieldSimplifier"];
  symmetrySimplifier  = OptionValue["SymmetrySimplifier"];
  otherSimplifier     = OptionValue["OtherSimplifier"];
  threeBodySimplifier = If[Head[OptionValue["ThreeBodySimplifier"]]
    == Association,
    OptionValue["ThreeBodySimplifier"][numE],
    OptionValue["ThreeBodySimplifier"]
  ];
  simplifier          = Join[magneticSimplifier,
                        magFieldSimplifier,
                        symmetrySimplifier,
                        threeBodySimplifier,
                        otherSimplifier];
  freeIonSymbols = OptionValue["FreeIonSymbols"];
  runningInteractive = (Head[$ParentLink] === LinkObject);

  oddsAndEnds["simplifier"] = simplifier;
  oddsAndEnds["freeIonSymbols"] = freeIonSymbols;
  oddsAndEnds["truncationEnergy"] = truncationEnergy;
  oddsAndEnds["numE"] = numE;
  oddsAndEnds["expData"] = expData;
  oddsAndEnds["numReps"] = numReps;
  oddsAndEnds["activeVars"] = activeVars;
  oddsAndEnds["startingValues"] = startingValues;
  oddsAndEnds["maxIterations"] = maxIterations;
  oddsAndEnds["PrintFun"] = PrintFun;
  oddsAndEnds["ln"] = ln;
  oddsAndEnds["numE"] = numE;
  oddsAndEnds["accuracyGoal"] = accuracyGoal;
  oddsAndEnds["Appendix"] = OptionValue["AppendToLogFile"];

  hamDim         = Binomial[14, numE];
  modelSymbols   = Sort[Select[paramSymbols, Not[MemberQ[Join[
    racahSymbols, chenSymbols,{t2Switch, \[Epsilon],gs}],#]]&]];
  (* Remove the symbols that will be removed by the simplifier, no
    symbol should remain here that is not in the symbolic hamiltonian
    *)
  reducedModelSymbols = Select[modelSymbols, Not[MemberQ[Keys[
    simplifier],#]]&];
  If[OptionValue["SignatureCheck"],
    (
    Print["Given the model parameters and the simplifying assumptions
    , the resultant model parameters are:"];
    Print[{reducedModelSymbols}];
    Print["The ordering in these needs to be respected in the
    startValues parameter ..."];
    Print["Exiting ..."];
    Return[""];
    )
  ];

  (*calculate the basis*)
  basis          = BasisLSJMJ[numE];
  (* grab the Hamiltonian preserving its block structure *)
  PrintFun["Assembling the Hamiltonian for f^",numE," keeping the
    block structure ..."];
  ham            = HamMatrixAssembly[numE, "ReturnInBlocks"->True];
  (* apply the simplifier *)
  PrintFun["Simplifying using the given aggregate set of
    simplification rules ..."];
  ham            = Map[ReplaceInSparseArray[#, simplifier]&, ham, {2}];

  (* Get the reference parameters from LaF3 *)
  PrintFun["Getting reference parameters for ",ln," using LaF3 ..."];
  lnParams = LoadLaF3Parameters[ln];
  freeBies = Prepend[Values[(#->(#/.lnParams))&/@freeIonSymbols],numE
    ];
  (* a more explicit alias *)
  allVars            = reducedModelSymbols;

  oddsAndEnds["allVars"]  = allVars;
  oddsAndEnds["freeBies"] = freeBies;
```

```
763
764   (* reload compiled version if found *)
765   varHash                   = Hash[{numE, allVars, freeBies,
        truncationEnergy}];
766   compileIntermediateFname = "compileIntermediateTruncatedHam-"<>
        ToString[varHash]<>".mx";
767   truncadedFname            = "TheTruncatedAndSignedPath-"<>ToString[
        varHash]<>".mx";
768   If[OptionValue["ReturnHashFileNameAndExit"],
769     (
770       Print[varHash];
771       Return[truncadedFname];
772     )
773   ];
774   If[FileExistsQ[compileIntermediateFname],
775     PrintFun["This ion and free-ion params have been compiled before
        (as determined by {numE, allVars, freeBies, truncationEnergy}).
        Loading the previously saved function and intermediate coupling
        basis ..."];
776     {compileIntermediateTruncatedHam, truncatedIntermediateBasis} =
        Import[compileIntermediateFname];,
777   (
778     PrintFun["Zeroing out every symbol in the Hamiltonian that is not
         a free-ion parameter ..."];
779     (* Get the free ion symbols *)
780     freeIonSimplifier = (#->0) & /@ Complement[reducedModelSymbols,
        freeIonSymbols];
781     (* Take the diagonal blocks for the intermediate analysis *)
782     PrintFun["Grabbing the diagonal blocks of the Hamiltonian ..."];
783     diagonalBlocks       = Diagonal[ham];
784     (* simplify them to only keep the free ion symbols *)
785     PrintFun["Simplifying the diagonal blocks to only keep the free
        ion symbols ..."];
786     diagonalScalarBlocks = ReplaceInSparseArray[#,freeIonSimplifier
        ]&/@diagonalBlocks;
787     (* these include the MJ quantum numbers, remove that *)
788     PrintFun["Contracting the basis vectors by removing the MJ
        quantum numbers from the diagonal blocks ..."];
789     diagonalScalarBlocks = FreeHam[diagonalScalarBlocks, numE];
790
791     argsOfTheIntermediateEigensystems         = StringJoin[Riffle[
        Prepend[(ToString[#]<>"v_") & /@ freeIonSymbols,"numE_"],", "]];
792     argsForEvalInsideOfTheIntermediateSystems = StringJoin[Riffle[(
        ToString[#]<>"v") & /@ freeIonSymbols,", "]];
793     PrintFun["argsOfTheIntermediateEigensystems = ",
        argsOfTheIntermediateEigensystems];
794     PrintFun["argsForEvalInsideOfTheIntermediateSystems = ",
        argsForEvalInsideOfTheIntermediateSystems];
795     PrintFun["If the following fails, make sure to modify the
        arguments of TheIntermediateEigensystems to match the ones above
        ..."];
796
797     (* Compile a function that will effectively calculate the
        spectrum of all of the scalar blocks given the parameters of the
        free-ion part of the Hamiltonian *)
798     (* Compile one function for each of the blocks *)
799     PrintFun["Compiling functions for the diagonal blocks of the
        Hamiltonian ..."];
800     compiledDiagonal = Compile[Evaluate[freeIonSymbols], Evaluate[N[
        Normal[#]]]]&/@diagonalScalarBlocks;
801     (* Use that to create a function that will calculate the free-ion
         eigensystem *)
802     TheIntermediateEigensystems[numEv_, F0v_, F2v_, F4v_, F6v_, M0v_,
         P2v_, αv_, βv_, γv_, ζv_, T2v_, T3v_, T4v_, T6v_, T7v_, T8v_] :=
        (
803       theNumericBlocks = (#[F0v, F2v, F4v, F6v, M0v, P2v, αv, βv, γv,
         ζv, T2v, T3v, T4v, T6v, T7v, T8v]&)/@compiledDiagonal;
804       theIntermediateEigensystems = Eigensystem/@theNumericBlocks;
805       Js      = AllowedJ[numEv];
806       basisJ = BasisLSJMJ[numEv,"AsAssociation"->True];
807       (* Having calculated the eigensystems with the removed
        degeneracies, put the degeneracies back in explicitly *)
808       elevatedIntermediateEigensystems = MapIndexed[EigenLever[#1,2Js
        [[#2[[1]]]]+1]&, theIntermediateEigensystems];
809       pivot = If[EvenQ[numEv],0,-1/2];
810       LSJmultiplets = (#[[1]]<>ToString[InputForm[#[[2]]]])&/@Select[
```

```
    BasisLSJMJ[numEv],#[[-1]]== pivot &];
811    (* Calculate the multiplet assignments that the intermediate
    basis eigenvectors have *)
812    multipletAssignments = Table[
813      (
814        J          = Js[[idx]];
815        eigenVecs = theIntermediateEigensystems[[idx]][[2]];
816        majorComponentIndices        = Ordering[Abs[#]][[-1]]&/
    @eigenVecs;
817        majorComponentAssignments    = LSJmultiplets[[#]]&/
    @majorComponentIndices;
818        (* All of the degenerate eigenvectors belong to the same
    multiplet*)
819        elevatedMultipletAssignments = ListRepeater[
    majorComponentAssignments,2J+1];
820        elevatedMultipletAssignments
821      ),
822    {idx, 1, Length[Js]}
823    ];
824    (* Put together the multiplet assignments and the energies *)
825    freeIenergiesAndMultiplets = Transpose/@Transpose[{First/
    @elevatedIntermediateEigensystems, multipletAssignments}];
826    freeIenergiesAndMultiplets = Flatten[freeIenergiesAndMultiplets
    , 1];
827    (* Calculate the change of basis matrix using the intermediate
    coupling eigenvectors *)
828    basisChanger = BlockDiagonalMatrix[Transpose/@Last/
    @elevatedIntermediateEigensystems];
829    basisChanger = SparseArray[basisChanger];
830    Return[{theIntermediateEigensystems, multipletAssignments,
    elevatedIntermediateEigensystems, freeIenergiesAndMultiplets,
    basisChanger}]
831  );
832
833  PrintFun["Calculating the intermediate eigensystems for ",ln,"
    using free-ion params from LaF3 ..."];
834  (* Calculate intermediate coupling basis using the free-ion
    params for LaF3 *)
835  {theIntermediateEigensystems, multipletAssignments,
    elevatedIntermediateEigensystems, freeIenergiesAndMultiplets,
    basisChanger} = TheIntermediateEigensystems@@freeBies;
836
837  (* Use that intermediate coupling basis to compile a function for
     the full Hamiltonian *)
838  allFreeEnergies = Flatten[First/@elevatedIntermediateEigensystems
    ];
839  (* Important that the intermediate coupling basis have attached
    energies, which make possible the truncation *)
840  ordering = Ordering[allFreeEnergies];
841  (* Sort the free ion energies and determine which indices should
    be included in the truncation *)
842  allFreeEnergiesSorted          = Sort[allFreeEnergies];
843  {minFreeEnergy, maxFreeEnergy} = MinMax[allFreeEnergies];
844  (* Determine the index at which the energy is equal or larger
    than the truncation energy *)
845  sortedTruncationIndex = Which[
846    truncationEnergy > (maxFreeEnergy-minFreeEnergy),
847    hamDim,
848    True,
849    FirstPosition[allFreeEnergiesSorted-Min[allFreeEnergiesSorted],
    x_/;x>truncationEnergy,{0},1][[1]]
850  ];
851  (* The actual energy at which the truncation is made *)
852  roundedTruncationEnergy = allFreeEnergiesSorted[[
    sortedTruncationIndex]];
853
854  (* The indices that enact the truncation *)
855  truncationIndices = ordering[[;;sortedTruncationIndex]];
856
857  (* Using the ham (with all the symbols) change the basis to the
    computed one *)
858  PrintFun["Changing the basis of the Hamiltonian to the
    intermediate coupling basis ..."];
859  intermediateHam            = Transpose[basisChanger].ArrayFlatten
    [ham].basisChanger;
860  (* Using the truncation indices truncate that one *)
```

```
861     PrintFun["Truncating the Hamiltonian ..."];
862     truncatedIntermediateHam    = intermediateHam[[truncationIndices,
        truncationIndices]];
863     (* These are the basis vectors for the truncated hamiltonian *)
864     PrintFun["Saving the truncated intermediate basis ..."];
865     truncatedIntermediateBasis = basisChanger[[All,truncationIndices
        ]];
866
867     PrintFun["Compiling a function for the truncated Hamiltonian ..."
        ];
868     (* Compile a function that will calculate the truncated
        Hamiltonian given the parameters in allVars, this is the function
        to be use in fitting *)
869     compileIntermediateTruncatedHam = Compile[Evaluate[allVars],
870                                       Evaluate[N[Normal[
        truncatedIntermediateHam]]]];
871     (* Save the compiled function *)
872     PrintFun["Saving the compiled function for the truncated
        Hamiltonian and the truncatedIntermediateBasis..."];
873     Export[compileIntermediateFname, {compileIntermediateTruncatedHam
        , truncatedIntermediateBasis}];
874   )
875   ];
876
877   TheTruncatedAndSignedPathGenerator::usage = "This function puts
        together the necessary expression for defining a function which
        has as arguments all the symbolic values in varsMixedWithVals and
        which feeds to compileIntermediateTruncatedHam the arguments as
        given in varsMixedWithVals. varsMixedWithVals needs to respect the
         order of aruments expected by compileIntermediateTruncatedHam.
        Once the necessary template has been used this function then
        results in the definition of the function
        TheTruncatedAndSignedPath.";
878   TheTruncatedAndSignedPathGenerator[varsMixedWithVals_List]:=(
879     variableVars   = Select[varsMixedWithVals,Not[NumericQ[#]]&];
880     numQSignature = StringJoin[Riffle[(ToString[#]<>"_?NumericQ")&/
        @variableVars,", "]];
881     varWithValsSignature = StringJoin[Riffle[(ToString[#]<>"")&/
        @varsMixedWithVals,", "]];
882     funcString     = truncatedEnergyCostTemplate[<|"varsWithNumericQ"
        ->numQSignature,"varsMixedWithFixedVals" -> varWithValsSignature
        |>];
883     ClearAll[TheTruncatedAndSignedPath];
884     ToExpression[funcString]
885   );
886
887   (* We need to create a function call that has all the frozen
        parameters in place and all the active symbols unevaluated *)
888   (* find the indices of the activeVars to create the function
        signature *)
889   activeVarIndices = Flatten[Position[allVars,#]&/@activeVars];
890   (* we start from the numerical values in the current best*)
891   jobVars          = startingValues;
892   (* we then put back the symbols that should be unevaluated *)
893   jobVars[[activeVarIndices]] = activeVars;
894
895   oddsAndEnds["jobVars"] = jobVars;
896   (* calculate the constraints *)
897   constraints                = N[Constrainer[activeVars,ln]];
898   oddsAndEnds["constraints"] = constraints;
899   (* This is useful for the progress window *)
900   activeVarsString  = StringJoin[Riffle[ToString/@activeVars,", "]];
901   TheTruncatedAndSignedPathGenerator[jobVars];
902   stringPartialVars = ToString/@activeVars;
903
904   activeVarsWithRange = If[usingInitialRange,
905     MapIndexed[Flatten[{#1,
906         (1-Sign[startVarValues[[#2]]]*fractionalWidth) *
        startVarValues[[#2]],
907         (1+Sign[startVarValues[[#2]]]*fractionalWidth) *
        startVarValues[[#2]]
908         }]&, activeVars],
909     activeVars
910   ];
911
912   (* this is the template for the minimizer *)
```

```
913  solverTemplateNMini = StringTemplate["
914  numIter = 0;
915  sol = NMinimize[
916    Evaluate[
917      Join[{TheTruncatedAndSignedPath[`activeVarsString`]},
918        constraints
919      ]
920    ],
921    activeVarsWithRange,
922    AccuracyGoal   -> `accuracyGoal`,
923    MaxIterations  -> `maxIterations`,
924    Method->`Method`,
925    `Monitor`:>(
926      currentErr = TheTruncatedAndSignedPath[`activeVarsString`];
927      currentParams = activeVars;
928      numIter   += 1;
929      rmsHistory = AddToList[rmsHistory, currentErr, maxHistory,
     False];
930      paramSols  = AddToList[paramSols, activeVars, maxHistory, False
     ];
931      If[Not[runningInteractive],(
932        Print[numIter,\"/\",`maxIterations`];
933        Print[\"err    = \", ToString[NumberForm[Round[currentErr
     ,0.001],{Infinity,3}]]];
934        Print[\"params = \", ToString[NumberForm[Round[#,0.0001],{
     Infinity,4}]] &/@ currentParams];
935        )
936      ];
937    )
938  ]
939  "];
940  methodStringTemplate = StringTemplate["
941      {\"DifferentialEvolution\",
942        \"PostProcess\"   -> False,
943        \"ScalingFactor\" -> `DE:ScalingFactor`,
944        \"CrossProbability\" -> `DE:CrossProbability`,
945        \"RandomSeed\"    -> RandomInteger[{0,1000000}],
946        \"SearchPoints\"  -> `DE:SearchPoints`}"];
947  methodString = methodStringTemplate[<|
948    "DE:ScalingFactor" -> OptionValue["DE:ScalingFactor"],
949    "DE:CrossProbability" -> OptionValue["DE:CrossProbability"],
950    "DE:SearchPoints" -> OptionValue["DE:SearchPoints"]|>];
951  (* Evaluate the template *)
952  solverCode = solverTemplateNMini[<|
953    "accuracyGoal"  -> accuracyGoal,
954    "maxIterations" -> maxIterations,
955    "Method"->"{\"DifferentialEvolution\",
956                \"PostProcess\"   -> False,
957                \"ScalingFactor\" -> 0.6,
958                \"CrossProbability\" -> 0.25,
959                \"RandomSeed\"    -> RandomInteger[{0,1000000}],
960                \"SearchPoints\"  -> Automatic}",
961    "Monitor"->"StepMonitor",
962    "activeVarsString"->activeVarsString|>
963  ];
964  threadHeaderTemplate = StringTemplate[ "(`idx`/`reps`) Fitting data
       for `ln` using `freeVars`."];
965  (* Find as many solutions as numReps *)
966  sols = Table[(
967    rmsHistory        = {};
968    paramSols         = {};
969    openNotebooks     = If[runningInteractive,
970              ("WindowTitle"/.NotebookInformation[#]) & /@ Notebooks
     [],
971              {}];
972    If[Not[MemberQ[openNotebooks,"Solver Progress"]] && OptionValue["
     ProgressView"],
973      ProgressNotebook["Basic"->False]
974    ];
975    If[Not[slackChan === None],
976    (
977      threadMessage = threadHeaderTemplate[<|"reps" -> numReps, "idx"
      -> rep, "ln" -> ln,
978        "freeVars" -> ToString[activeVars]|>];
979      threadTS = PostMessageToSlack[threadMessage, slackChan]["ts"];
980    )
```

```
    ];
    startTime = Now;
    ToExpression[solverCode];

    timeTaken = QuantityMagnitude[Now - startTime, "Seconds"];
    Print["Took " <> ToString[timeTaken] <> "s"];
    Print[sol];
    bestError     = sol[[1]];
    bestParams    = sol[[2]];
    resultMessage = "sigma=" <> ToString[Round[bestError, 0.1]];
    solAssoc = <|
      "bestRMS"      -> bestError,
      "solHistory"   -> rmsHistory,
      "bestParams"   -> bestParams,
      "paramHistory" -> paramSols,
      "timeTaken/s"    -> timeTaken
      |>;
    solAssoc = Join[solAssoc,   oddsAndEnds];
    logFname = LogSol[solAssoc, logFilePrefix];

    If[Not[slackChan===None],(
      PostMessageToSlack[resultMessage,   slackChan, "threadTS" ->
    threadTS];
      PostFileToSlack[StringSplit[logFname,"/"][[-1]], logFname,
    slackChan, "threadTS" -> threadTS]
    )
    ];
    solAssoc
    ),
    {rep,1,numReps}
  ];
  Return[sols];
);

ClassicalFit::usage="ClassicalFit[numE, expData, excludeDataIndices,
    problemVars, startValues, \[Sigma]exp, constraints_List, Options]
    fits the given expData in an f^numE configuration, by using the
    symbols in problemVars. The symbols given in problemVars may be
    constrained or held constant, this being controlled by constraints
     list which is a list of replacement rules expressing desired
    constraints. The constraints list additional constraints imposed
    upon the model parameters that remain once other simplifications
    have been \"baked\" into the compiled Hamiltonians that are used
    to increase the speed of the calculation.

Important, note that in the case of odd number of electrons the given
     data must explicitly include the Kramers degeneracy;
    excludeDataIndices must be compatible with this.

The list expData needs to be a list of lists with the only
    restriction that the first element of them corresponds to energies
     of levels. In this list, an empty value can be used to indicate
    known gaps in the data. Even if the energy value for a level is
    known (and given in expData) certain values can be omitted from
    the fitting procedure through the list excludeDataIndices, which
    correspond to indices in expData that should be skipped over.

The Hamiltonian used for fitting is version that has been truncated
    either by using the maximum energy given in expData or by manually
     setting a truncation energy using the option \"TruncationEnergy\"
    .

The argument \[Sigma]exp is the estimated uncertainty in the
    differences between the calculated and the experimental energy
    levels. This is used to estimate the uncertainty in the fitted
    parameters. Admittedly this will be a rough estimate (at least on
    the contribution of the calculated uncertainty), but it is better
    than nothing and may at least provide a lower bound to the
    uncertainty in the fitted parameters. It is assumed that the
    uncertainty in the differences between the calculated and the
    experimental energy levels is the same for all of them.

The list startValues is a list with all of the parameters needed to
    define the Hamiltonian (including the initial values for
    problemVars).

```

```
1025 The function saves the solution to a file. The file is named with a
         prefix (controlled by the option \"FilePrefix\") and a UUID. The
         file is saved in the log sub-directory as a .m file.
1026
1027 Here's a description of the different parts of this function: first
         the Hamiltonian is assembled and simplified using the given
         simplifications. Then the intermediate coupling basis is
         calculated using the free-ion parameters for the given lanthanide.
          The Hamiltonian is then changed to the intermediate coupling
         basis and truncated. The truncated Hamiltonian is then compiled
         into a function that can be used to calculate the energy levels of
          the truncated Hamiltonian. The function that calculates the
         energy levels is then used to fit the experimental data. The
         fitting is done using FindMinimum with the Levenberg-Marquardt
         method.
1028
1029 The function returns an association with the following keys:
1030
1031 - \"bestRMS\" which is the best \[Sigma] value found.
1032 - \"bestParams\" which is the best set of parameters found for the
         variables that were not constrained.
1033 - \"bestParamsWithConstraints\" which has the best set of parameters
         (from - \"bestParams\") together with the used constraints. These
         include all the parameters in the model, even those that were not
         fitted for.
1034 - \"paramSols\" which is a list of the parameters trajectories during
          the stepping of the fitting algorithm.
1035 - \"timeTaken/s\" which is the time taken to find the best fit.
1036 - \"simplifier\" which is the simplifier used to simplify the
         Hamiltonian.
1037 - \"excludeDataIndices\" as given in the input.
1038 - \"startValues\" as given in the input.
1039
1040 - \"freeIonSymbols\" which are the symbols used in the intermediate
         coupling basis.
1041 - \"truncationEnergy\" which is the energy used to truncate the
         Hamiltonian, if it was set to Automatic, the value here is the
         actual energy used.
1042 - \"numE\" which is the number of electrons in the f^numE
         configuration.
1043 - \"expData\" which is the experimental data used for fitting.
1044 - \"problemVars\" which are the symbols considered for fitting
1045
1046 - \"maxIterations\" which is the maximum number of iterations used by
          NMinimize.
1047 - \"hamDim\" which is the dimension of the full Hamiltonian.
1048 - \"allVars\" which are all the symbols defining the Hamiltonian
         under the aggregate simplifications.
1049 - \"freeBies\" which are the free-ion parameters used to define the
         intermediate coupling basis.
1050 - \"truncatedDim\" which is the dimension of the truncated
         Hamiltonian.
1051 - \"compiledIntermediateFname\" the file name of the compiled
         function used for the truncated Hamiltonian.
1052
1053 - \"fittedLevels\" which is the number of levels fitted for.
1054 - \"actualSteps\" the number of steps that FindMiniminum actually
         took.
1055 - \"solWithUncertainty\" which is a list of replacement rules of the
         form (paramSymbol -> {bestEstimate, uncertainty}).
1056 - \"rmsHistory\" which is a list of the \[Sigma] values found during
         the fitting.
1057 - \"Appendix\" which is an association appended to the log file under
          the key \"Appendix\".
1058 - \"presentDataIndices\" which is the list of indices in expData that
          were used for fitting, this takes into account both the empty
         indices in expData and also the indices in excludeDataIndices.
1059
1060 - \"states\" which contains a list of eigenvalues and eigenvectors
         for the fitted model, this is only available if the option \"
         SaveEigenvectors\" is set to True; if a general shift of energy
         was allowed for in the fitting, then the energies are shifted
         accordingly.
1061 - \"energies\" which is a list of the energies of the fitted levels,
         this is only available if the option \"SaveEigenvectors\" is set
         to False. If a general shift of energy was allowed for in the
```

```
    fitting, then the energies are shifted accordingly.
- \"degreesOfFreedom\" which is equal to the nunber of fitted state
    energies minus the number of parameters used in fitting.

The function admits the following options with corresponding default
    values:
- \"MaxHistory\" : determines how long the logs for the solver can be
    .
- \"MaxIterations\": determines the maximum number of iterations used
     by NMinimize.
- \"FilePrefix\" : the prefix to use for the subfolder in the log
    filder, in which the solution files are saved, by default this is
    \"calcs\" so that the calculation files are saved under the
    directory \"log/calcs\".
- \"AddConstantShift\" : if True then a constant shift is allowed in
    the fitting, default is False. If this is the case the variable \"
    \[Epsilon]\" is added to the list of variables to be fitted for,
    it must not be included in problemVars.

- \"AccuracyGoal\": the accuracy goal used by NMinimize, default of
    5.
- \"TrucationEnergy\": if Automatic then the maximum energy in
    expData is taken, else it takes the value set by this option. In
    all cases the energies in expData are only considered up to this
    value.
- \"PrintFun\": the function used to print progress messages, the
    default is PrintTemporary.
- \"RefParamsVintage\": the vintage of the reference parameters to
    use. The reference parameters are both used to determine the
    truncated Hamiltonian, and also as starting values for the solver.
     It may be \"LaF3\", in which case reference parameters from
    Carnall are used. It may also be \"LiYF4\", in which case the
    reference parameters from the LiYF4 paper are used. It may also be
     Automatic, in which case the given experimental data is used to
    determine starting values for F^k and ζ. It may also be a list or
    association that provides values for the Slater integrals and spin
    -orbit coupling, the remaining necessary parameters complemented
    by using \"LaF3\".

- \"SlackChannel\": name of the Slack channel to which to dump
    progress messaages, the default is None which disables this option
    .
- \"ProgressView\": whether or not a progress window will be opened
    to show the progress of the solver, the default is True.
- \"SignatureCheck\": if True then then the function returns
    prematurely, returning a list with the symbols that would have
    defined the Hamiltonian after all simplifications have been
    applied. Useful to check the entire parameter set that the
    Hamiltonian has, which has to match one-to-one what is provided by
     startingValues.
- \"SaveEigenvectors\": if True then the both the eigenvectors and
    eigenvalues are saved under the \"states\" key of the returned
    association. If False then only the energies are saved, the
    default is False.

- \"AppendToLogFile\": an association appended to the log file under
    the key \"Appendix\".
- \"MagneticSimplifier\": a list of replacement rules to simplify the
     Marvin and pesudo-magnetic paramters. Here the ratios of the
    Marvin parameters and the pseudo-magnetic parameters are defined
    to simplify the magnetic part of the Hamiltonian.
- \"MagFieldSimplifier\": a list of replacement rules to specify a
    magnetic field (in T), if set to {}, then {Bx, By, Bz} can also be
     used as variables to be fitted for.

- \"SymmetrySimplifier\": a list of replacements rules to simplify
    the crystal field.
- \"OtherSimplifier\": an additional list of replacement rules that
    are applied to the Hamiltonian before computing with it. Here the
    spin-spin contribution can be turned off by setting \[Sigma]SS->0,
     which is the default.
";
Options[ClassicalFit] = {
  "MaxHistory"       -> 200,
  "MaxIterations"    -> 100,
  "FilePrefix"       -> "calcs",
```

```
  "ProgressView"     -> True,
  "TruncationEnergy" -> Automatic,
  "AccuracyGoal"     -> 5,
  "PrintFun"         -> PrintTemporary,
  "SlackChannel"     -> None,
  "RefParamsVintage" -> "LaF3",
  "ProgressView"     -> True,
  "SignatureCheck"   -> False,
  "AddConstantShift" -> False,
  "SaveEigenvectors" -> False,
  "AppendToLogFile"  -> <||>,
  "SaveToLog"        -> False,
  "Energy Uncertainty in K" -> Automatic,
  "MagneticSimplifier" -> {
    M2 -> 56/100 M0,
    M4 -> 31/100 M0,
    P4 -> 1/2 P2,
    P6 -> 1/10 P2
    },
  "MagFieldSimplifier" -> {
    Bx -> 0,
    By -> 0,
    Bz -> 0
    },
  "SymmetrySimplifier" -> {
    B12->0, B14->0, B16->0, B34->0, B36->0, B56->0,
    S12->0 ,S14->0, S16->0, S22->0, S24->0, S26->0,
    S34->0 ,S36->0, S44->0, S46->0, S56->0, S66->0
    },
  "OtherSimplifier" -> {
    F0->0,
    P0->0,
    \[Sigma]SS->0,
    T11p->0, T12->0, T14->0, T15->0,
    T16->0, T18->0, T17->0, T19->0, T2p->0,
    wChErrA ->0, wChErrB->0
    },
  "ThreeBodySimplifier" -> <|
    1  -> {
      T2->0, T3->0, T4->0, T6->0, T7->0, T8->0,
      T11p->0, T12->0, T14->0, T15->0, T16->0, T18->0, T17->0, T19
    ->0,
      T2p->0},
    2 -> {
      T2->0, T3->0, T4->0, T6->0, T7->0, T8->0,
      T11p->0, T12->0, T14->0, T15->0, T16->0, T18->0, T17->0, T19
    ->0,
      T2p->0
      },
    3  -> {},
    4  -> {},
    5  -> {},
    6  -> {},
    7  -> {},
    8  -> {},
    9  -> {},
    10 -> {},
    11 -> {},
    12 -> {
      T3->0, T4->0, T6->0, T7->0, T8->0,
      T11p->0, T12->0, T14->0, T15->0, T16->0, T18->0, T17->0, T19
    ->0,
      T2p->0
      },
    13->{
      T2->0, T3->0, T4->0, T6->0, T7->0, T8->0,
      T11p->0, T12->0, T14->0, T15->0, T16->0, T18->0, T17->0, T19
    ->0,
      T2p->0
      }
    |>,
    "FreeIonSymbols" -> {F0, F2, F4, F6, ζ}
};
ClassicalFit[numE_Integer, expData_List, excludeDataIndices_List,
    problemVars_List, startValues_Association, constraints_List,
    OptionsPattern[]]:=Module[
```

```
1161  {accuracyGoal, activeVarIndices, activeVars, activeVarsString,
      activeVarsWithRange, allFreeEnergies, allFreeEnergiesSorted,
      allVars, allVarsVec, argsForEvalInsideOfTheIntermediateSystems,
      argsOfTheIntermediateEigensystems, aVar, aVarPosition, basis,
      basisChanger, basisChangerBlocks, bestError, bestParams, bestRMS,
      blockShifts, blockSizes, colIdx, compiledDiagonal,
      compiledIntermediateFname, constrainedProblemVars,
      constrainedProblemVarsList, covMat, currentRMS, degressOfFreedom,
      dependentVars, diagonalBlocks, diagonalScalarBlocks, diff,
      eigenEnergies, eigenvalueDispenserTemplate, eigenVectors,
      elevatedIntermediateEigensystems, endTime, fmSol, fmSolAssoc,
      fractionalWidth, freeBies, freeIenergiesAndMultiplets,
      freeionSymbols, fullHam, fullSolVec, funcString, ham, hamDim,
      hamEigenvaluesTemplate, hamString, hess, indepSolVecVec, indepVars
      , intermediateHam, isolationValues, jobVars, lin, linMat, ln,
      lnParams, logFilePrefix, logFname, magneticSimplifier,
      maxFreeEnergy, maxHistory, maxIterations, methodString,
      methodStringTemplate, minFreeEnergy, minpoly, modelSymbols,
      multipletAssignments, needlePosition, numBlocks, numQSignature,
      numReps, solCompendium, openNotebooks, ordering, othersFixed,
      otherSimplifier, p0, paramBest, paramSigma, perHam, polySols,
      presentDataIndices, PrintFun, problemVarsPositions, problemVarsQ,
      problemVarsQString, problemVarsVec, problemVarsWithStartValues,
      reducedModelSymbols, resultMessage, roundedTruncationEnergy,
      rowIdx, runningInteractive, shiftToggle, simplifier, slackChan,
      sol, solAssoc, sols, solWithUncertainty, sortedTruncationIndex,
      sqdiff, standardValues, starTime, startingValues, startTime,
      startVarValues, states, steps, symmetrySimplifier,
      theIntermediateEigensystems, TheIntermediateEigensystems,
      TheTruncatedAndSignedPathGenerator, thisPoly, threadHeaderTemplate
      , threadMessage, threadTS, timeTaken, totalVariance,
      truncadedFname, truncatedIntermediateBasis,
      truncatedIntermediateHam, truncationEnergy, truncationIndices,
      RefParams, truncationUmbral, usingInitialRange, varHash, varIdx,
      varsWithConstants, varWithValsSignature, \[Lambda]0Vec, \[Lambda]
      exp},
1162  (
1163    \[Sigma]exp   = OptionValue["Energy Uncertainty in K"];
1164    solCompendium = <||>;
1165    refParamsVintage = OptionValue["RefParamsVintage"];
1166    RefParams = Which[
1167      refParamsVintage === "LaF3",
1168      LoadLaF3Parameters,
1169      refParamsVintage === "LiYF4",
1170      LoadLiYF4Parameters,
1171      True,
1172      refParamsVintage
1173    ];
1174    hamDim        = Binomial[14, numE];
1175    addShift      = OptionValue["AddConstantShift"];
1176    ln            = theLanthanides[[numE]];
1177    maxHistory    = OptionValue["MaxHistory"];
1178    maxIterations = OptionValue["MaxIterations"];
1179    logFilePrefix = If[OptionValue["FilePrefix"] == "",
1180                       ToString[theLanthanides[[numE]]],
1181                       OptionValue["FilePrefix"]
1182                     ];
1183    accuracyGoal = OptionValue["AccuracyGoal"];
1184    slackChan    = OptionValue["SlackChannel"];
1185    PrintFun     = OptionValue["PrintFun"];
1186    freeIonSymbols      = OptionValue["FreeIonSymbols"];
1187    runningInteractive  = (Head[$ParentLink] === LinkObject);
1188    magneticSimplifier  = OptionValue["MagneticSimplifier"];
1189    magFieldSimplifier  = OptionValue["MagFieldSimplifier"];
1190    symmetrySimplifier  = OptionValue["SymmetrySimplifier"];
1191    otherSimplifier     = OptionValue["OtherSimplifier"];
1192    threeBodySimplifier = If[Head[OptionValue["ThreeBodySimplifier"]]
      == Association,
1193                             OptionValue["ThreeBodySimplifier"][numE],
1194                             OptionValue["ThreeBodySimplifier"]
1195                           ];
1196
1197    truncationEnergy = If[OptionValue["TruncationEnergy"] ===
      Automatic,
1198      (
1199        PrintFun["Truncation energy set to Automatic, using the
```

```
    maximum energy (+20%) in the data ..."];
1200        Round[1.2 * Max[Select[First /@ expData, NumericQ[#] &]]]
1201      ),
1202      OptionValue["TruncationEnergy"]
1203      ];
1204    truncationEnergy = Max[50000, truncationEnergy];
1205    PrintFun["Using a truncation energy of ", truncationEnergy, " K"
    ];
1206
1207    simplifier = Join[magneticSimplifier,
1208                      magFieldSimplifier,
1209                      symmetrySimplifier,
1210                      threeBodySimplifier,
1211                      otherSimplifier];
1212
1213    PrintFun["Determining gaps in the data ..."];
1214    (* whatever is non-numeric is assumed as a known gap *)
1215    presentDataIndices = Flatten[Position[expData, {_?(NumericQ[#] &)
    , ___}]];
1216    (* some indices omitted here based on the excludeDataIndices
    argument *)
1217    presentDataIndices = Complement[presentDataIndices,
    excludeDataIndices];
1218
1219    solCompendium["simplifier"]          = simplifier;
1220    solCompendium["excludeDataIndices"] = excludeDataIndices;
1221    solCompendium["startValues"]         = startValues;
1222    solCompendium["freeIonSymbols"]      = freeIonSymbols;
1223    solCompendium["truncationEnergy"]    = truncationEnergy;
1224    solCompendium["numE"]                = numE;
1225    solCompendium["expData"]             = expData;
1226    solCompendium["problemVars"]         = problemVars;
1227    solCompendium["maxIterations"]       = maxIterations;
1228    solCompendium["hamDim"]              = hamDim;
1229    solCompendium["constraints"]         = constraints;
1230
1231    modelSymbols  = Sort[Select[paramSymbols, Not[MemberQ[Join[
    racahSymbols, juddOfeltIntensitySymbols, chenSymbols,{t2Switch, \[
    Epsilon], gs, nE}],#]]&]];
1232    (* remove the symbols that will be removed by the simplifier, no
    symbol should remain here that is not in the symbolic Hamiltonian
    *)
1233    reducedModelSymbols = Select[modelSymbols, Not[MemberQ[Keys[
    simplifier],#]]&];
1234
1235    (* this is useful to understand what are the arguments of the
    truncated compiled Hamiltonian *)
1236    If[OptionValue["SignatureCheck"],
1237      (
1238        Print["Given the model parameters and the simplifying
    assumptions, the resultant model parameters are:"];
1239        Print[{reducedModelSymbols}];
1240        Print["Exiting ..."];
1241        Return[""];
1242      )
1243    ];
1244
1245    (* calculate the basis *)
1246    PrintFun["Retrieving the LSJMJ basis for f^", numE, " ..."];
1247    basis    = BasisLSJMJ[numE];
1248
1249    Which[refParamsVintage === Automatic,
1250      (
1251        PrintFun["Using the automatic vintage with freshly fitted
    free-ion parameters and others as in LaF3 ..."];
1252        lnParams      = LoadLaF3Parameters[ln];
1253        freeIonSol    = FreeIonSolver[expData, numE];
1254        freeIonParams = freeIonSol["bestParams"];
1255        lnParams      = Join[lnParams, freeIonParams];
1256      ),
1257      MemberQ[{List, Association}, Head[RefParams]],
1258      (
1259        RefParams = Association[RefParams];
1260        PrintFun["Using the given parameters as a starting point ..."
    ];
1261        lnParams    = RefParams;
```

```
1262          extraParams = LoadLaF3Parameters[ln];
1263          lnParams    = Join[extraParams, lnParams];
1264        ),
1265        True,
1266        (
1267          (* get the reference parameters from the given vintage *)
1268          PrintFun["Getting reference free-ion parameters for ", ln, "
      using ", refParamsVintage, " ..."];
1269          lnParams = ParamPad[RefParams[ln], "PrintFun" -> PringFun];
1270        )
1271      ];
1272      freeBies = Prepend[Values[(#->(#/.lnParams)) &/@ freeIonSymbols],
        numE];
1273      (* a more explicit alias *)
1274      allVars            = reducedModelSymbols;
1275      numericConstraints = Association@Select[constraints, NumericQ
      [#[[2]]] &];
1276      standardValues     = allVars /. Join[lnParams, numericConstraints
      ];
1277      solCompendium["allVars"]  = allVars;
1278      solCompendium["freeBies"] = freeBies;
1279
1280      (* reload compiled version if found *)
1281      varHash                   = Hash[{numE, allVars, freeBies,
      truncationEnergy, simplifier}];
1282      compiledIntermediateFname = ln <> "-compiled-intermediate-
      truncated-ham-" <> ToString[varHash] <> ".mx";
1283      compiledIntermediateFname = FileNameJoin[{moduleDir, "compiled",
      compiledIntermediateFname}];
1284      solCompendium["compiledIntermediateFname"] =
      compiledIntermediateFname;
1285
1286      If[FileExistsQ[compiledIntermediateFname],
1287        PrintFun["This ion, free-ion params, and full set of variables
      have been used before (as determined by {numE, allVars, freeBies,
      truncationEnergy, simplifier}). Loading the previously saved
      compiled function and intermediate coupling basis ..."];
1288        PrintFun["Using : ", compiledIntermediateFname];
1289        {compileIntermediateTruncatedHam, truncatedIntermediateBasis} =
       Import[compiledIntermediateFname];,
1290      (
1291        If[truncationEnergy == Infinity,
1292        (
1293            ham = HamMatrixAssembly[numE, "ReturnInBlocks" -> False];
1294            theSimplifier = simplifier;
1295            ham = Normal@ReplaceInSparseArray[ham, simplifier];
1296            PrintFun["Compiling a function for the Hamiltonian with no
      truncation ..."];
1297            (* compile a function that will calculate the truncated
      Hamiltonian given the parameters in allVars, this is the function
      to be use in fitting *)
1298            compileIntermediateTruncatedHam = Compile[Evaluate[allVars
      ], Evaluate[ham]];
1299            truncatedIntermediateBasis = SparseArray@IdentityMatrix[
      Binomial[14, numE]];
1300            (* save the compiled function *)
1301            PrintFun["Saving the compiled function for the Hamiltonian
      with no truncation and a placeholder intermediate basis ..."];
1302            Export[compiledIntermediateFname, {
      compileIntermediateTruncatedHam, truncatedIntermediateBasis}];
1303        ),
1304        (
1305          (* grab the Hamiltonian preserving the block structure *)
1306          PrintFun["Assembling the Hamiltonian for f^",numE," keeping
      the block structure ..."];
1307          ham          = HamMatrixAssembly[numE, "ReturnInBlocks"->True
      ];
1308          (* apply the simplifier *)
1309          PrintFun["Simplifying using the aggregate set of
      simplification rules ..."];
1310          ham          = Map[ReplaceInSparseArray[#, simplifier]&, ham,
       {2}];
1311          PrintFun["Zeroing out every symbol in the Hamiltonian that is
       not a free-ion parameter ..."];
1312          (* Get the free ion symbols *)
1313          freeIonSimplifier = (#->0) & /@ Complement[
```

```
    reducedModelSymbols, freeIonSymbols];
1314        (* Take the diagonal blocks for the intermediate analysis *)
1315        PrintFun["Grabbing the diagonal blocks of the Hamiltonian ...
    "];
1316        diagonalBlocks       = Diagonal[ham];
1317        (* simplify them to only keep the free ion symbols *)
1318        PrintFun["Simplifying the diagonal blocks to only keep the
    free ion symbols ..."];
1319        diagonalScalarBlocks = ReplaceInSparseArray[#,
    freeIonSimplifier]&/@diagonalBlocks;
1320        (* these include the MJ quantum numbers, remove that *)
1321        PrintFun["Contracting the basis vectors by removing the MJ
    quantum numbers from the diagonal blocks ..."];
1322        diagonalScalarBlocks = FreeHam[diagonalScalarBlocks, numE];
1323
1324        argsOfTheIntermediateEigensystems         = StringJoin[Riffle
    [Prepend[(ToString[#]<>"v_") & /@ freeIonSymbols,"numE_"],", "]];
1325        argsForEvalInsideOfTheIntermediateSystems = StringJoin[Riffle
    [(ToString[#]<>"v") & /@ freeIonSymbols,", "]];
1326        PrintFun["argsOfTheIntermediateEigensystems = ",
    argsOfTheIntermediateEigensystems];
1327        PrintFun["argsForEvalInsideOfTheIntermediateSystems = ",
    argsForEvalInsideOfTheIntermediateSystems];
1328        PrintFun["(if the following fails, it might help to see if
    the arguments of TheIntermediateEigensystems match the ones shown
    above)"];
1329
1330        (* compile a function that will effectively calculate the
    spectrum of all of the scalar blocks given the parameters of the
    free-ion part of the Hamiltonian *)
1331        (* compile one function for each of the blocks *)
1332        PrintFun["Compiling functions for the diagonal blocks of the
    Hamiltonian ..."];
1333        compiledDiagonal = Compile[Evaluate[freeIonSymbols], Evaluate
    [N[Normal[#]]]]&/@diagonalScalarBlocks;
1334        (* use that to create a function that will calculate the free
    -ion eigensystem *)
1335        TheIntermediateEigensystems[numEv_, F0v_, F2v_, F4v_, F6v_, ζ
    v_] := (
1336          theNumericBlocks = (#[F0v, F2v, F4v, F6v, ζv]&) /@
    compiledDiagonal;
1337          theIntermediateEigensystems = Eigensystem /@
    theNumericBlocks;
1338          Js     = AllowedJ[numEv];
1339          basisJ = BasisLSJMJ[numEv,"AsAssociation"->True];
1340          (* having calculated the eigensystems with the removed
    degeneracies, put the degeneracies back in explicitly *)
1341          elevatedIntermediateEigensystems = MapIndexed[EigenLever
    [#1, 2Js[[#2[[1]]]]+1 ]&, theIntermediateEigensystems];
1342          (* Identify a single MJ to keep *)
1343          pivot          = If[EvenQ[numEv],0,-1/2];
1344          LSJmultiplets = (#[[1]]<>ToString[InputForm[#[[2]]]])&/
    @Select[BasisLSJMJ[numEv],#[[-1]]== pivot &];
1345          (* calculate the multiplet assignments that the
    intermediate basis eigenvectors have *)
1346          needlePosition = 0;
1347          multipletAssignments = Table[
1348            (
1349              J         = Js[[idx]];
1350              eigenVecs = theIntermediateEigensystems[[idx]][[2]];
1351              majorComponentIndices        = Ordering[Abs[#]][[-1]]&/
    @eigenVecs;
1352              majorComponentIndices       += needlePosition;
1353              needlePosition              += Length[
    majorComponentIndices];
1354              majorComponentAssignments    = LSJmultiplets[[#]]&/
    @majorComponentIndices;
1355              (* All of the degenerate eigenvectors belong to the
    same multiplet*)
1356              elevatedMultipletAssignments = ListRepeater[
    majorComponentAssignments, 2J+1];
1357              elevatedMultipletAssignments
1358            ),
1359          {idx, 1, Length[Js]}
1360          ];
1361          (* put together the multiplet assignments and the energies
```

```
    *)
1362        freeIenergiesAndMultiplets = Transpose/@Transpose[{First/
    @elevatedIntermediateEigensystems, multipletAssignments}];
1363        freeIenergiesAndMultiplets = Flatten[
    freeIenergiesAndMultiplets, 1];
1364        (* calculate the change of basis matrix using the
    intermediate coupling eigenvectors *)
1365        basisChanger = BlockDiagonalMatrix[Transpose/@Last/
    @elevatedIntermediateEigensystems];
1366        basisChanger = SparseArray[basisChanger];
1367        Return[{theIntermediateEigensystems, multipletAssignments,
    elevatedIntermediateEigensystems, freeIenergiesAndMultiplets,
    basisChanger}]
1368      );
1369
1370      PrintFun["Calculating the intermediate eigensystems for ",ln,
    " using free-ion params from LaF3 ..."];
1371      (* calculate intermediate coupling basis using the free-ion
    params for LaF3 *)
1372      {theIntermediateEigensystems, multipletAssignments,
    elevatedIntermediateEigensystems, freeIenergiesAndMultiplets,
    basisChanger} = TheIntermediateEigensystems@@freeBies;
1373
1374      (* use that intermediate coupling basis to compile a function
     for the full Hamiltonian *)
1375      allFreeEnergies = Flatten[First/
    @elevatedIntermediateEigensystems];
1376      (* important that the intermediate coupling basis have
    attached energies, which make possible the truncation *)
1377      ordering = Ordering[allFreeEnergies];
1378      (* sort the free ion energies and determine which indices
    should be included in the truncation *)
1379      allFreeEnergiesSorted           = Sort[allFreeEnergies];
1380      {minFreeEnergy, maxFreeEnergy} = MinMax[allFreeEnergies];
1381      (* determine the index at which the energy is equal or larger
     than the truncation energy *)
1382      sortedTruncationIndex = Which[
1383        truncationEnergy > (maxFreeEnergy-minFreeEnergy),
1384        hamDim,
1385        True,
1386        FirstPosition[allFreeEnergiesSorted - Min[
    allFreeEnergiesSorted],x_/;x>truncationEnergy,{0},1][[1]]
1387      ];
1388      (* the actual energy at which the truncation is made *)
1389      roundedTruncationEnergy = allFreeEnergiesSorted[[
    sortedTruncationIndex]];
1390
1391      (* the indices that participate in the truncation *)
1392      truncationIndices = ordering[[;;sortedTruncationIndex]];
1393      PrintFun["Computing the block structure of the change of
    basis array ..."];
1394      blockSizes         = BlockArrayDimensionsArray[ham];
1395      basisChangerBlocks = ArrayBlocker[basisChanger, blockSizes];
1396      blockShifts        = First /@ Diagonal[blockSizes];
1397      numBlocks          = Length[blockSizes];
1398      (* using the ham (with all the symbols) change the basis to
    the computed one *)
1399      PrintFun["Changing the basis of the Hamiltonian to the
    intermediate coupling basis ..."];
1400      intermediateHam = BlockMatrixMultiply[ham, basisChangerBlocks
    ];
1401      PrintFun["Distributing products inside of symbolic matrix
    elements to keep complexity in check ..."];
1402      Do[
1403        intermediateHam[[rowIdx, colIdx]] = MapToSparseArray[
    intermediateHam[[rowIdx, colIdx]], Distribute /@ # &];,
1404        {rowIdx, 1, numBlocks},
1405        {colIdx, 1, numBlocks}
1406      ];
1407      intermediateHam = BlockMatrixMultiply[BlockTranspose[
    basisChangerBlocks],intermediateHam];
1408      PrintFun["Distributing products inside of symbolic matrix
    elements to keep complexity in check ..."];
1409      Do[
1410        intermediateHam[[rowIdx, colIdx]] = MapToSparseArray[
    intermediateHam[[rowIdx, colIdx]], Distribute /@ # &];,
```

```
1411          {rowIdx, 1, numBlocks},
1412          {colIdx, 1, numBlocks}
1413        ];
1414        (* using the truncation indices truncate that one *)
1415        PrintFun["Truncating the Hamiltonian ..."];
1416        truncatedIntermediateHam = TruncateBlockArray[intermediateHam
    , truncationIndices, blockShifts];
1417        (* these are the basis vectors for the truncated hamiltonian
    *)
1418        PrintFun["Saving the truncated intermediate basis ..."];
1419        truncatedIntermediateBasis = basisChanger[[All,
    truncationIndices]];
1420
1421        PrintFun["Compiling a function for the truncated Hamiltonian
    ..."];
1422        (* compile a function that will calculate the truncated
    Hamiltonian given the parameters in allVars, this is the function
    to be use in fitting *)
1423        compileIntermediateTruncatedHam = Compile[Evaluate[allVars],
    Evaluate[truncatedIntermediateHam]];
1424        (* save the compiled function *)
1425        PrintFun["Saving the compiled function for the truncated
    Hamiltonian and the truncated intermediate basis ..."];
1426        Export[compiledIntermediateFname, {
    compileIntermediateTruncatedHam, truncatedIntermediateBasis}];
1427      )
1428    ];
1429    )
1430    ];
1431
1432    truncationUmbral = Dimensions[truncatedIntermediateBasis][[2]];
1433    PrintFun["The truncated Hamiltonian has a dimension of ",
    truncationUmbral, "x", truncationUmbral, " ..."];
1434    presentDataIndices = Select[presentDataIndices, # <=
    truncationUmbral &];
1435    solCompendium["presentDataIndices"] = presentDataIndices;
1436
1437    (* the problemVars are the symbols that will be fitted for *)
1438
1439    PrintFun["Starting up the fitting process using the Levenberg-
    Marquardt method ..."];
1440    (* using the problemVars I need to create the argument list
    including _?NumericQ *)
1441    problemVarsQ       = (ToString[#] <> "_?NumericQ") & /@
    problemVars;
1442    problemVarsQString = StringJoin[Riffle[problemVarsQ, ", "]];
1443    (* we also need to have the padded arguments with the variables
    in the right position and the fixed values in the remaining ones
    *)
1444    problemVarsPositions = Position[allVars, #][[1, 1]] & /@
    problemVars;
1445    problemVarsString    = StringJoin[Riffle[ToString /@ problemVars,
     ", "]];
1446    (* to feed parameters to the Hamiltonian, which includes all
    parameters, we need to form the set of arguments, with fixed
    values where needed, and the variables in the right position *)
1447    varsWithConstants                          = standardValues;
1448    varsWithConstants[[problemVarsPositions]] = problemVars;
1449    varsWithConstantsString                    = ToString[
    varsWithConstants];
1450
1451    (* this following function serves eigenvalues from the
    Hamiltonian, has memoization so it might grow to use a lot of RAM
    *)
1452    Clear[HamSortedEigenvalues];
1453    hamEigenvaluesTemplate = StringTemplate["
1454    HamSortedEigenvalues[`problemVarsQ`]:=(
1455      ham         = compileIntermediateTruncatedHam@@`
    varsWithConstants`;
1456      eigenValues = Chop[Sort@Eigenvalues@ham];
1457      eigenValues = eigenValues - Min[eigenValues];
1458      HamSortedEigenvalues[`problemVarsString`] = eigenValues;
1459      Return[eigenValues]
1460    )"];
1461    hamString = hamEigenvaluesTemplate[<|
1462        "problemVarsQ"      -> problemVarsQString,
```

```
        "varsWithConstants" -> varsWithConstantsString,
        "problemVarsString" -> problemVarsString
        |>];
    ToExpression[hamString];

    (* we also need a function that will pick the i-th eigenvalue,
    this seems unnecessary but it's needed to form the right
    functional form expected by the Levenberg-Marquardt method *)
    eigenvalueDispenserTemplate = StringTemplate["
    PartialHamEigenvalues[`problemVarsQ`][i_]:=(
      eigenVals = HamSortedEigenvalues[`problemVarsString`];
      eigenVals[[i]]
    )
    "];
    eigenValueDispenserString = eigenvalueDispenserTemplate[<|
        "problemVarsQ"      -> problemVarsQString,
        "problemVarsString" -> problemVarsString
        |>];
    ToExpression[eigenValueDispenserString];

    PrintFun["Determining the free variables after constraints ..."];
    constrainedProblemVars     = (problemVars /. constraints);
    constrainedProblemVarsList = Variables[constrainedProblemVars];
    If[addShift,
      PrintFun["Adding a constant shift to the fitting parameters ...
    "];
      constrainedProblemVarsList = Append[constrainedProblemVarsList,
     \[Epsilon]]
    ];

    indepVars = Complement[problemVars, #[[1]] & /@ constraints];
    stringPartialVars = ToString/@constrainedProblemVarsList;

    paramSols  = {};
    rmsHistory = {};
    steps      = 0;
    problemVarsWithStartValues = KeyValueMap[{#1,#2} &, startValues];
    If[addShift,
      problemVarsWithStartValues = Append[problemVarsWithStartValues,
     {\[Epsilon] ,0}];
    ];
    openNotebooks     = If[runningInteractive,
              ("WindowTitle"/.NotebookInformation[#]) & /@ Notebooks
    [],
              {}];
    If[Not[MemberQ[openNotebooks,"Solver Progress"]] && OptionValue["
    ProgressView"],
      ProgressNotebook["Basic"->False]
    ];
    degressOfFreedom = Length[presentDataIndices] - Length[
    problemVars] - 1;
    PrintFun["Fitting for ", Length[presentDataIndices], " data
    points with ", Length[problemVars], " free parameters.", " The
    effective degrees of freedom are ", degressOfFreedom, " ..."];

    PrintFun["Fitting model to data ..."];
    startTime   = Now;
    shiftToggle = If[addShift, 1, 0];
    sol = FindMinimum[
      Sum[(expData[[j]][[1]] - (PartialHamEigenvalues @@
    constrainedProblemVars)[j] - shiftToggle * \[Epsilon])^2,
      {j, presentDataIndices}],
      problemVarsWithStartValues,
      Method        -> "LevenbergMarquardt",
      MaxIterations -> OptionValue["MaxIterations"],
      AccuracyGoal  -> OptionValue["AccuracyGoal"],
      StepMonitor :> (
        steps      += 1;
        currentSqSum = Sum[(expData[[j]][[1]] - (
    PartialHamEigenvalues @@ constrainedProblemVars)[j] - shiftToggle
    * \[Epsilon])^2, {j, presentDataIndices}];
        currentRMS = Sqrt[currentSqSum / degressOfFreedom];
        paramSols  = AddToList[paramSols, constrainedProblemVarsList,
     maxHistory];
        rmsHistory = AddToList[rmsHistory, currentRMS, maxHistory];
        )
```

```
1525        ];
1526      endTime = Now;
1527      timeTaken = QuantityMagnitude[endTime - startTime, "Seconds"];
1528      PrintFun["Solution found in ", timeTaken, "s"];
1529
1530      solVec = constrainedProblemVars /. sol[[-1]];
1531      indepSolVec = indepVars /. sol[[-1]];
1532      If[addShift,
1533        \[Epsilon]Best = \[Epsilon]/. sol[[-1]],
1534        \[Epsilon]Best = 0
1535      ];
1536      fullSolVec = standardValues;
1537      fullSolVec[[problemVarsPositions]] = solVec;
1538      PrintFun["Calculating the truncated numerical Hamiltonian
        corresponding to the solution ..."];
1539      fullHam = compileIntermediateTruncatedHam @@ fullSolVec;
1540      PrintFun["Calculating energies and eigenvectors ..."];
1541      {eigenEnergies, eigenVectors} = Eigensystem[fullHam];
1542      states = Transpose[{eigenEnergies, eigenVectors}];
1543      states = SortBy[states, First];
1544      eigenEnergies = First /@ states;
1545      PrintFun["Shifting energies to make ground state zero of energy
        ..."];
1546      eigenEnergies = eigenEnergies - eigenEnergies[[1]];
1547      PrintFun["Calculating the linear approximant to each eigenvalue
        ..."];
1548      allVarsVec = Transpose[{allVars}];
1549      p0 = Transpose[{fullSolVec}];
1550      linMat = {};
1551      If[addShift,
1552        tail = -2,
1553        tail = -1];
1554      Do[
1555        (
1556          aVarPosition = Position[allVars, aVar][[1, 1]];
1557          isolationValues = ConstantArray[0, Length[allVars]];
1558          isolationValues[[aVarPosition]] = 1;
1559          dependentVars = KeyValueMap[{#1, D[#2, aVar]} &, Association[
        constraints]];
1560          Do[
1561            isolationValues[[Position[allVars, dVar[[1]]][[1, 1]]]] =
        dVar[[2]],
1562            {dVar, dependentVars}
1563          ];
1564          perHam  = compileIntermediateTruncatedHam @@ isolationValues;
1565          lin     = FirstOrderPerturbation[Last /@ states, perHam];
1566          linMat  = Append[linMat, lin];
1567        ),
1568        {aVar, constrainedProblemVarsList[[;;tail]]}
1569      ];
1570      PrintFun["Removing the gradient of the ground state ..."];
1571      linMat = (# - #[[1]] & /@ linMat);
1572      PrintFun["Transposing derivative matrices into columns ..."];
1573      linMat  = Transpose[linMat];
1574
1575      PrintFun["Calculating the eigenvalue vector at solution ..."];
1576      \[Lambda]0Vec = Transpose[{eigenEnergies[[presentDataIndices]]}];
1577      PrintFun["Putting together the experimental vector ..."];
1578      \[Lambda]exp = Transpose[{First /@ expData[[presentDataIndices
        ]]}];
1579      problemVarsVec = If[addShift,
1580        Transpose[{constrainedProblemVarsList[[;;-2]]}],
1581        Transpose[{constrainedProblemVarsList}]
1582      ];
1583      indepSolVecVec = Transpose[{indepSolVec}];
1584      PrintFun["Calculating the difference between eigenvalues at
        solution ..."];
1585      diff = If[linMat == {},
1586        (\[Lambda]0Vec - \[Lambda]exp)  + \[Epsilon]Best,
1587        (\[Lambda]0Vec - \[Lambda]exp)  + \[Epsilon]Best + linMat[[
        presentDataIndices]].(problemVarsVec - indepSolVecVec)
1588      ];
1589      PrintFun["Calculating the sum of squares of differences around
        solution ... "];
1590      sqdiff        = Expand[(Transpose[diff] . diff)[[1, 1]]];
1591      PrintFun["Calculating the minimum (which should coincide with sol
```

```
    ) ..."];
1592    minpoly       = sqdiff /. AssociationThread[problemVars -> solVec
    ];
1593    fmSolAssoc    = Association[sol[[2]]];
1594    If[\[Sigma]exp == Automatic,
1595      \[Sigma]exp = Sqrt[minpoly / degressOfFreedom];
1596    ];
1597    \[CapitalDelta]\[Chi]2 = Sqrt[degressOfFreedom];
1598    Amat = (1/\[Sigma]exp^2) * Transpose[linMat[[presentDataIndices
    ]]].linMat[[presentDataIndices]];
1599    paramIntervals = EllipsoidBoundingBox[Amat, \[CapitalDelta]\[Chi
    ]2];
1600    PrintFun["Calculating the uncertainty in the parameters ..."];
1601    solWithUncertainty = Table[
1602      (
1603        aVar        = constrainedProblemVarsList[[varIdx]];
1604        paramBest   = aVar /. fmSolAssoc;
1605        (aVar -> {paramBest, paramIntervals[[varIdx, 2]]})
1606      ),
1607    {varIdx, 1, Length[constrainedProblemVarsList]-shiftToggle}
1608    ];
1609    PrintFun["Calculating the covariance matrix ..."];
1610    hess = If[linmat=={},
1611      {{Infinity}},
1612      2 * Transpose[linMat[[presentDataIndices]]] . linMat[[
    presentDataIndices]]
1613    ];
1614    covMat  = If[linmat=={},
1615      {{0}},
1616      \[Sigma]exp^2 * Inverse[hess]
1617    ];
1618    bestRMS    = Sqrt[minpoly / degressOfFreedom];
1619    bestParams = sol[[2]];
1620    bestWithConstraints = Association@Join[constraints, bestParams];
1621    bestWithConstraints = bestWithConstraints /. bestWithConstraints;
1622    bestWithConstraints = (# + 0.) & /@ bestWithConstraints;
1623
1624    solCompendium["degreesOfFreedom"]    = degressOfFreedom;
1625    solCompendium["solWithUncertainty"]  = solWithUncertainty;
1626    solCompendium["truncatedDim"]        = truncationUmbral;
1627    solCompendium["fittedLevels"]        = Length[presentDataIndices
    ];
1628    solCompendium["actualSteps"]         = steps;
1629    solCompendium["bestRMS"]             = bestRMS;
1630    solCompendium["problemVars"]         = problemVars;
1631    solCompendium["paramSols"]           = paramSols;
1632    solCompendium["rmsHistory"]          = rmsHistory;
1633    solCompendium["Appendix"]            = OptionValue["
    AppendToLogFile"];
1634    solCompendium["timeTaken/s"]         = timeTaken;
1635    solCompendium["bestParams"]          = bestParams;
1636    solCompendium["bestParamsWithConstraints"] = bestWithConstraints;
1637
1638    If[OptionValue["SaveEigenvectors"],
1639        solCompendium["states"] = {#[[1]] + \[Epsilon]Best, #[[2]]}
    &/@ (Chop /@ ShiftedLevels[states]),
1640        (
1641          finalEnergies = Sort[First /@ states];
1642          finalEnergies = finalEnergies - finalEnergies[[1]];
1643          finalEnergies = finalEnergies + \[Epsilon]Best;
1644          finalEnergies  = Chop /@ finalEnergies;
1645          solCompendium["energies"] = finalEnergies;
1646      )
1647    ];
1648    If[OptionValue["SaveToLog"],
1649      PrintFun["Saving the solution to the log file ..."];
1650      LogSol[solCompendium, logFilePrefix];
1651    ];
1652    PrintFun["Finished ..."];
1653    Return[solCompendium];
1654  )
1655];
1656
1657
1658caseConstraints::usage="This Association contains the constraints
    that are not the same across all of the lanthanides. For instance,
```

```
    since the ratio between M2 and M0 is assumed the same for all the
    trivalent lanthanides, that one is not included here.
This association has keys equal to symbols of lanthanides and values
    equal to lists of rules that express either a parameter being held
    fixed or made proportional to another.
In Table I of Carnall 1989 these correspond to cases were values are
    given in square brackets.";
caseConstraints = <|
"Ce" -> {
    B02 -> -218.,
    B04 -> 738.,
    B06 -> 679.,
    B22 -> -50.,
    B24 -> 431.,
    B26 -> -921.,
    B44 -> 616.,
    B46 -> -348.,
    B66 -> -788.
    },
"Pr" -> {},
"Nd" -> {},
"Pm" -> {},
"Sm" -> {
    B22 -> -50.,
    T2 -> 300.,
    T3 -> 36.,
    T4 -> 56.,
    γ -> 1500.
    },
"Eu" -> {
    F4 -> 0.713 F2,
    F6 -> 0.512 F2,
    B22 -> -50.,
    B24 -> 597.,
    B26 -> -706.,
    B44 -> 408.,
    B46 -> -508.,
    B66 -> -692.,
    M0 -> 2.1,
    P2 -> 360.,
    T2 -> 300.,
    T3 -> 40.,
    T4 -> 60.,
    T6 -> -300.,
    T7 -> 370.,
    T8 -> 320.,
    α -> 20.16,
    β  -> -566.9,
    γ -> 1500.
    },
"Pm" -> {
    B02 -> -245.,
    B04 -> 470.,
    B06 -> 640.,
    B22 -> -50.,
    B24 -> 525.,
    B26 -> -750.,
    B44 -> 490.,
    B46 -> -450.,
    B66 -> -760.,
    F2 -> 76400.,
    F4 -> 54900.,
    F6 -> 37700.,
    M0 -> 2.4,
    P2 -> 275.,
    T2 -> 300.,
    T3 -> 35.,
    T4 -> 58.,
    T6 -> -310.,
    T7 -> 350.,
    T8 -> 320.,
    α -> 20.5,
    β -> -560.,
    γ -> 1475.,
    ζ -> 1025.},
"Gd" -> {
```

```
    F4 -> 0.710 F2,
    B02 -> -231.,
    B04 -> 604.,
    B06 -> 280.,
    B22 -> -99.,
    B24 -> 340.,
    B26 -> -721.,
    B44 -> 452.,
    B46 -> -204.,
    B66 -> -509.,
    T2 -> 300.,
    T3 -> 42.,
    T4 -> 62.,
    T6 -> -295.,
    T7 -> 350.,
    T8 -> 310.,
    β -> -600.,
    γ -> 1575.
    },
"Tb" -> {
    F4 -> 0.707 F2,
    T2 -> 320.,
    T3 -> 40.,
    T4 -> 50.,
    γ -> 1650.
    },
"Dy" -> {},
"Ho" -> {
    B02 -> -240.,
    T2 -> 400.,
    γ -> 1800.
    },
"Er" -> {
    T2 -> 400.,
    γ -> 1800.
    },
"Tm" -> {
    T2 -> 400.,
    γ -> 1820.
    },
"Yb" -> {
    B02 -> -249.,
    B04 -> 457.,
    B06 -> 282.,
    B22 -> -105.,
    B24 -> 320.,
    B26 -> -482.,
    B44 -> 428.,
    B46 -> -234.,
    B66 -> -492.
}
|>;

variedSymbols =<|
    "Ce" -> {ζ},
    "Pr" -> {B02, B04, B06, B22, B24, B26, B44, B46, B66,
             F2, F4, F6,
             M0, P2,
             α, β, γ,
             ζ},
    "Nd" -> {B02, B04, B06, B22, B24, B26, B44, B46, B66,
             F2, F4, F6,
             M0, P2,
             T2, T3, T4, T6, T7, T8,
             α, β, γ,
             ζ},
    "Pm" -> {},
    "Sm" -> {B02, B04, B06, B24, B26, B44, B46, B66,
             F2, F4, F6, M0, P2,
             T6, T7, T8,
             α, β, ζ},
    "Eu" -> {B02, B04, B06,
             F2, F4, F6, ζ},
    "Gd" -> {F2, F4, F6,
             M0, P2,
             α, ζ},
```

```
    "Tb" -> {B02, B04, B06, B22, B24, B26, B44, B46, B66,
             F2, F4, F6,
             M0, P2,
             T6, T7, T8,
             α, β, ζ},
    "Dy" -> {B02, B04, B06, B22, B24, B26, B44, B46, B66,
             F2, F4, F6,
             M0, P2,
             T2, T3, T4, T6, T7, T8,
             α, β, γ, ζ},
    "Ho" -> {B04, B06, B22, B24, B26, B44, B46, B66,
             F2, F4, F6,
             M0, P2,
             T3, T4, T6, T7, T8,
             α, β, ζ},
    "Er" -> {B02, B04, B06, B22, B24, B26, B44, B46, B66,
             F2, F4, F6,
             M0, P2,
             T3, T4, T6, T7, T8, α, β, ζ},
    "Tm" -> {B02, B04, B06, B22, B24, B26, B44, B46, B66,
             F2, F4, F6,
             M0, P2,
             α, β, ζ},
    "Yb" -> {ζ}
    |>;

caseConstraintsLiYF4 = <|
  "Ce" -> {
    B04 -> -1043.,
    B44 -> -1249.,
    B06 -> -65.,
    B46 -> -1069.
    },
  "Pr" -> {
    β -> -644.,
    γ -> 1413.,
    M0 -> 1.88,
    P2 -> 244.
    },
  "Nd" -> {
    M0 -> 1.85
    },
  "Sm" -> {
    α -> 20.5,
    β -> -616.,
    γ -> 1565.,
    T2 -> 282.,
    T3 -> 26.,
    T4 -> 71.,
    T6 -> -257.,
    T7 -> 314.,
    T8 -> 328.,
    M0 -> 2.38,
    P2 -> 336.
    },
  "Eu" -> {
    T2 -> 370.,
    T3 -> 40.,
    T4 -> 40.,
    T6 -> -300.,
    T7 -> 380.,
    T8 -> 370.
    },
  "Tb" -> {
    F4 -> 0.709 F2,
    F6 -> 0.503 F2,
    α -> 17.6,
    β -> -581.,
    γ -> 1792.,
    T2 -> 330.,
    T3 -> 40.,
    T4 -> 45.,
    T6 -> -365.,
    T7 -> 320.,
    T8 -> 349.,
    M0 -> 2.7,
```

```
    P2 -> 482.
    },
  "Dy" -> {
    (* F4 -> 0.707 F2,
    F6 -> 0.516 F2, *)
    F2 -> 90421,
    F4 -> 63928,
    F6 -> 46657,
    α -> 17.9,
    β -> -628.,
    γ -> 1790.,
    T2 -> 326.,
    T3 -> 23.,
    T4 -> 83.,
    T6 -> -294.,
    T7 -> 403.,
    T8 -> 340.,
    M0 -> 4.46,
    P2 -> 610.,
    B46 -> -700.
    },
  "Ho" -> {
    α -> 17.2,
    β -> -596.,
    γ -> 1839.,
    T2 -> 365.,
    T3 -> 37.,
    T4 -> 95.,
    T6 -> -274.,
    T7 -> 331.,
    T8 -> 343.,
    P2 -> 582.
    },
  "Er" -> {},
  "Tm" -> {
    α -> 17.3,
    β -> -665.,
    γ -> 1936.,
    M0 -> 4.93,
    P2 -> 730.,
    T2 -> 400.
    },
  "Yb" -> {
    B06 -> -23.,
    B46 -> -512.
    }
  |>;

variedSymbolsLiYF4 = <|
  "Ce" -> {
    B02, ζ
    },
  "Pr" -> {
    B02, B04, B06, B44, B46,
    F2, F4, F6,
    α, ζ
    },
  "Nd" -> {
    B02, B04, B06, B44, B46,
    F2, F4, F6,
    P2,
    T2, T3, T4, T6, T7, T8,
    α, β, γ, ζ
    },
  "Sm" -> {
    B02, B04, B06, B44, B46,
    F2, F4, F6,
    ζ
    },
  "Eu" -> {
    B02, B04, B06, B44, B46,
    F2, F4, F6,
    M0, P2,
    α, β, γ, ζ
    },
  "Tb" -> {
```

```
    B02, B04, B06, B44, B46,
    F2, F4, F6,
    ζ
    },
  "Dy" -> {
    B02, B04, B06, B44,
    F2, F4, F6,
    ζ
    },
  "Ho" -> {
    B02, B04, B06, B44, B46,
    F2, F4, F6,
    M0,
    ζ
    },
  "Er" -> {
    B02, B04, B06, B44, B46,
    F2, F4, F6,
    M0, P2,
    T2, T3, T4, T6, T7,  T8,
    α, β, γ,
    ζ
    },
  "Tm" -> {
    B02, B04, B06, B44, B46,
    F2, F4, F6,
    ζ
    },
  "Yb" -> {
    B02, B04, B44,
    ζ
    }
  |>

paramsChengLiYF4::usage="This association has the model parameters as
    fitted by Cheng et. al \"Crystal-field analyses for trivalent
    lanthanide ions in LiYF4\".";
paramsChengLiYF4 = <|
  "Ce" -> {
    ζ -> 630.,
    B02 -> 354., B04 -> -1043.,
    B44 -> -1249., B06 -> -65.,
    B46 -> -1069.
    },
  "Pr" -> {
    F2 -> 68955., F4 -> 50505., F6 -> 33098.,
    ζ -> 748.,
    α -> 23.3, β -> -644., γ -> 1413.,
    M0 -> 1.88, P2 -> 244.,
    B02 -> 512.,   B04 -> -1127.,
    B44 -> -1239., B06 -> -85.,
    B46 -> -1205.
    },
 "Nd" -> {
    F2 -> 72952., F4 -> 52681., F6 -> 35476.,
    ζ -> 877.,
    α -> 21., β -> -579., γ -> 1446.,
    T2 -> 210., T3 -> 41., T4 -> 74., T6 -> -293., T7 -> 321., T8 ->
    205.,
    M0 -> 1.85, P2 -> 304.,
    B02 -> 391.,   B04 -> -1031.,
    B44 -> -1271., B06 -> -28.,
    B46 -> -1046.
    },
 "Sm" -> {
    F2 -> 79515., F4 -> 56766., F6 -> 40078.,
    ζ -> 1168.,
    α -> 20.5, β -> -616., γ -> 1565.,
    T2 -> 282., T3 -> 26., T4 -> 71., T6 -> -257., T7 -> 314., T8 ->
    328.,
    M0 -> 2.38, P2 -> 336.,
    B02 -> 370.,  B04 -> -757.,
    B44 -> -941., B06 -> -67.,
    B46 -> -895.
    },
 "Eu" -> {
```

```
    F2 -> 82573., F4 -> 59646., F6 -> 43203.,
    ζ -> 1329.,
    α -> 21.6, β -> -482., γ -> 1140.,
    T2 -> 370., T3 -> 40., T4 -> 40., T6 -> -300., T7 -> 380., T8 ->
   370.,
    M0 -> 2.41, P2 -> 332.,
    B02 -> 339.,   B04 -> -733.,
    B44 -> -1067., B06 -> -36.,
    B46 -> -764.
    },
 "Tb" -> {
    F2 -> 90972., F4 -> 64499., F6 -> 45759.,
    ζ -> 1702.,
    α -> 17.6, β -> -581., γ -> 1792.,
    T2 -> 330., T3 -> 40., T4 -> 45., T6 -> -365., T7 -> 320., T8 ->
   349.,
    M0 -> 2.7, P2 -> 482.,
    B02 -> 413.,   B04 -> -867.,
    B44 -> -1114., B06 -> -41.,
    B46 -> -736.
    },
 "Dy" -> {
    F0 -> 0,
    F2 -> 90421., F4 -> 63928., F6 -> 46657.,
    ζ -> 1895.,
    α -> 17.9, β -> -628., γ -> 1790.,
    T2 -> 326., T3 -> 23., T4 -> 83., T6 -> -294., T7 -> 403., T8 ->
   340.,
    M0 -> 4.46, P2 -> 610.,
    B02 -> 360.,  B04 -> -737.,
    B44 -> -943., B06 -> -35.,
    B46 -> -700.
    },
 "Ho" -> {
    F2 -> 93512., F4 -> 66084., F6 -> 49765.,
    ζ -> 2126.,
    α -> 17.2, β -> -596., γ -> 1839.,
    T2 -> 365., T3 -> 37., T4 -> 95., T6 -> -274., T7 -> 331., T8 ->
   343.,
    M0 -> 3.92, P2 -> 582.,
    B02 -> 386.,  B04 -> -629.,
    B44 -> -841., B06 -> -33.,
    B46 -> -687.
    },
 "Er" -> {
    F2 -> 97326., F4 -> 67987., F6 -> 53651.,
    ζ -> 2377.,
    α -> 18.1, β -> -599., γ -> 1870.,
    T2 -> 380., T3 -> 41., T4 -> 69., T6 -> -356., T7 -> 239., T8 ->
   390.,
    M0 -> 4.41, P2 -> 795.,
    B02 -> 325.,   B04 -> -749.,
    B44 -> -1014., B06 -> -19.,
    B46 -> -635.
    },
 "Tm" -> {
    F0 -> 0.,
    T2 -> 0.,
    F2 -> 101938., F4 -> 71553., F6 -> 51359.,
    ζ -> 2632.,
    α -> 17.3, β -> -665., γ -> 1936.,
    M0 -> 4.93, P2 -> 730.,
    B02 -> 339.,  B04 -> -627.,
    B44 -> -913., B06 -> -39.,
    B46 -> -584.
    },
 "Yb" -> {
    ζ -> 2916.,
    B02 -> 446.,  B04 -> -560.,
    B44 -> -843., B06 -> -23.,
    B46 -> -512.
    }
  |>

StringToSLJ[string_] := Module[
  {stringed = string, LS, J, LSindex},
```

```
  (
  If[StringContainsQ[stringed, "+"],
   Return["mixed"]
   ];
  LS = StringTake[stringed, {1, 2}];
  If[StringContainsQ[stringed, "("],
   (
     LSindex =
     StringCases[stringed, RegularExpression["\\(([^)]*)\\)"] :> "$1"
   ];
    LS = LS <> LSindex;
    stringed = StringSplit[stringed, ")"][[-1]];
    J = ToExpression[stringed];
    ),
   (
    J = ToExpression@StringTake[stringed, {3, -1}];
    )
   ];
  {LS, J}
  )
];

FreeIonSolver::usage="This function takes a list of experimental data and the number of electrons in the lanthanide ion and returns the free-ion parameters that best fit the data. The options are:
  - F4F6_SlaterRatios: a list of two numbers that represent the ratio of F4 to F2 and F6 to F2, respectively.
  - PrintFun: a function that will be used to print the progress of the fitting process.
  - MaxIterations: the maximum number of iterations that the fitting process will run.
  - MaxMultiplets: the maximum number of multiplets that will be used in the fitting process.
  - MaxPercent: the maximum percentage of the data that can be off by the fitting.
  - SubSetBounds: a list of two numbers that represent the minimum and maximum number of multiplets that will be used in the fitting process.
The function returns an association with the following keys:
  - bestParams: the best parameters found in the fitting.
  - worstRelativeError: the worst relative error in the fitting.
  - SlaterRatios: the Slater ratios used in the fitting.
  - usedBaricenters: the baricenters used in the fitting.
If no acceptable solution is found, the function will return all solutions that are not worse than 10*MaxPercent. A solution is acceptable if the worst relative error is less than the MaxPercent option.
";
Options[FreeIonSolver] = {
  "F4F6_SlaterRatios" -> {0.707, 0.516},
  "PrintFun" -> PrintTemporary,
  "MaxIterations" -> 10000,
  "MaxMultiplets" -> 12,
  "MaxPercent" -> 3.,
  "SubSetBounds" -> {5, 12}
  };
FreeIonSolver[expData_, numE_, OptionsPattern[]] := Module[
  (* {maxMultiplets, maxPercent, F4overF2, F6overF2, PrintFun, minSubSetSize, maxSubSetSize, multipletEnergies, numMultiplets, allEqns, subsetSizes, ln, solutions, subsets, subset, eqns, m, b, meritFun, sol, goodThings, bestThings, bestOfAll, finalSol, usedMultiplets, usedBaricenters}, *)
  {},
  (
    maxMultiplets = OptionValue["MaxMultiplets"];
    maxIterations = OptionValue["MaxIterations"];
    maxPercent    = OptionValue["MaxPercent"];
    F4overF2      = OptionValue["F4F6_SlaterRatios"][[1]];
    F6overF2      = OptionValue["F4F6_SlaterRatios"][[2]];
    PrintFun      = OptionValue["PrintFun"];
    minSubSetSize = OptionValue["SubSetBounds"][[1]];
    maxSubSetSize = OptionValue["SubSetBounds"][[2]];
    freeIonParams = {F0, F2, F4, F6, ζ};
    ln            = theLanthanides[[numE]];

    PrintFun["Parsing the barycenters of the different multiplets ...
```

```
"];
multipletEnergies = Map[First, #] & /@ GroupBy[expData, #[[2]] &];
multipletEnergies = Mean[Select[#, NumberQ]] & /@ multipletEnergies;
multipletEnergies = Select[multipletEnergies, FreeQ[#, Mean] &];
multipletEnergies = KeySelect[KeyMap[StringToSLJ, multipletEnergies], # =!= "mixed" &];
multipletEnergies = KeyMap[Prepend[#, numE] &, multipletEnergies];
numMultiplets     = Length[multipletEnergies];

PrintFun["Composing the system of equations for the free-ion energies ..."];
allEqns     = KeyValueMap[FreeIonTable[#1] == #2 &, multipletEnergies];
allEqns     = Append[Coefficient[#[[1]], {F0, F2, F4, F6, ζ}], #[[2]]] & /@ allEqns;
allEqns     = allEqns[[;; Min[Length[allEqns], maxMultiplets]]];
subsetSizes = Range[1, numMultiplets];
numSubsets = {#, Binomial[numMultiplets, #]} & /@ subsetSizes;
numSubsets = Transpose@SortBy[numSubsets, Last];
accSizes = Accumulate[numSubsets[[2]]];
numSubsets = Transpose@Append[numSubsets, accSizes];
lastSub = SelectFirst[numSubsets, #[[3]] > 1000 &, Last[numSubsets]];
lastPosition = Position[numSubsets, lastSub][[1, 1]];
chosenSubsetSizes = #[[1]] & /@ numSubsets[[;; lastPosition]];
solutions   = <||>;

PrintFun["Selecting subsets of different lengths and fitting with ratio-constraints ..."];
Do[
  subsets = Subsets[Range[1, Length[allEqns]], {subsetSize}];
  PrintFun["Considering ", Length[subsets], " barycenter subsets of size ", subsetSize, " ..."];
  Do[
  (
    subset = subsets[[subsetIndex]];
    eqns   = allEqns[[subset]];
    m      = #[[;; 5]] & /@ eqns;
    b      = #[[6]] & /@ eqns;
    meritFun = Max[100 * Expand[Abs[(m . freeIonParams - b)]/b]];
    sol = NMinimize[{meritFun,
      F0 > 0,
      F2 > 0,
      F4 == F4overF2 * F2,
      F6 == F6overF2 * F2,
      ζ > 0},
      freeIonParams,
      MaxIterations -> maxIterations,
      Method -> "Convex"];
    solutions[{subsetSize, subset}] = sol;
    )
  , {subsetIndex, 1, Length[subsets]}
  ],
  {subsetSize, chosenSubsetSizes}
];

PrintFun["Collecting solutions of different subset size ..."];
goodThings = Table[Normal[Sort[KeySelect[#[[1]] & /@
        solutions, #[[1]] == subSize &]][[1]],
        {subSize, subsetSizes}];

PrintFun["Picking the solutions that are not worse than ", maxPercent, "% ..."];
bestThings = Select[goodThings, #[[2]] <= maxPercent &];
If[bestThings == {},
  Print["No acceptable solution found, consider increasing maxPercent or inspecting the given data ..."];
  Return[goodThings];
];

PrintFun["Keeping the solution with the largest number of used barycenters ..."];
bestOfAll = bestThings[[-1]];
```

```
    sol        = solutions[bestOfAll[[1]]];
    subset     = bestOfAll[[1, 2]];
    eqns       = allEqns[[subset]];
    m          = #[[;; 5]] & /@ eqns;
    b          = #[[6]] & /@ eqns;
    usedMultiplets  = Keys[multipletEnergies][[subset]];
    usedBaricenters = {#, multipletEnergies[#]} & /@ usedMultiplets;
    uniqeLS = DeleteDuplicates[#[[2]] &/@ Keys[multipletEnergies]];
    solAssoc = Association[sol[[2]]];
    usedLaF3 = False;
    If[Length[uniqeLS] == 1,
      (
        Print["There is too little data to find Slater parameters,
    using the ones for LaF3, and keeping the fitted spin-orbit zeta
    ..."];
        laf3params = LoadLaF3Parameters[ln];
        usedLaF3   = True;
        solAssoc[F0] = laf3params[F0];
        solAssoc[F2] = laf3params[F2];
        solAssoc[F4] = laf3params[F4];
        solAssoc[F6] = laf3params[F6];
      )
    ];
    finalSol = <|
      "bestParams" -> solAssoc,
      "usedLaF3" -> usedLaF3,
      "worstRelativeError" -> sol[[1]],
      "SlaterRatios" -> {F4overF2, F6overF2},
      "usedBaricenters" -> usedBaricenters|>;
    Return[finalSol];
)
];
```

17.3 qplotter.m

This module has a few useful plotting routines.

```

BeginPackage["qplotter`"];

GetColor;
IndexMappingPlot;
ListLabelPlot;
AutoGraphicsGrid;
SpectrumPlot;
WaveToRGB;

Begin["`Private`"];

  AutoGraphicsGrid::usage="AutoGraphicsGrid[graphsList] takes a list
    of graphics and creates a GraphicsGrid with them. The number of
    columns and rows is chosen automatically so that the grid has a
    squarish shape.";
  Options[AutoGraphicsGrid] = Options[GraphicsGrid];
  AutoGraphicsGrid[graphsList_, opts : OptionsPattern[]] :=
    (
      numGraphs = Length[graphsList];
      width = Floor[Sqrt[numGraphs]];
      height = Ceiling[numGraphs/width];
      groupedGraphs = Partition[graphsList, width, width, 1, Null];
      GraphicsGrid[groupedGraphs, opts]
    )

  Options[IndexMappingPlot] = Options[Graphics];
  IndexMappingPlot::usage =
    "IndexMappingPlot[pairs] take a list of pairs of integers and
    creates a visual representation of how they are paired. The first
    indices being depicted in the bottom and the second indices being
    depicted on top.";
  IndexMappingPlot[pairs_, opts : OptionsPattern[]] := Module[{width,
     height}, (
    width = Max[First /@ pairs];
    height = width/3;
    Return[
      Graphics[{{Tooltip[Point[{#[[1]], 0}],#[[1]]]}, Tooltip[Point
    [{#[[2]], height}],#[[2]]],
```

```
          Line[{{#[[1]], 0}, {#[[2]], height}}]} & /@ pairs, opts,
  ImageSize -> 800]]
  )
  ]

TickCompressor[fTicks_] :=
Module[{avgTicks, prevTickLabel, groupCounter, groupTally, idx,
  tickPosition, tickLabel, avgPosition, groupLabel}, (avgTicks =
  {};
  prevTickLabel = fTicks[[1, 2]];
  groupCounter = 0;
  groupTally = 0;
  idx = 1;
  Do[({tickPosition, tickLabel} = tick;
    If[
    tickLabel === prevTickLabel,
    (groupCounter += 1;
      groupTally += tickPosition;
      groupLabel = tickLabel;),
    (
      avgPosition = groupTally/groupCounter;
      avgTicks = Append[avgTicks, {avgPosition, groupLabel}];
      groupCounter = 1;
      groupTally = tickPosition;
      groupLabel = tickLabel;
      )
    ];
    If[idx != Length[fTicks],
    prevTickLabel = tickLabel;
    idx += 1;]
    ), {tick, fTicks}];
  If[Or[Not[prevTickLabel === tickLabel], groupCounter > 1],
  (
    avgPosition = groupTally/groupCounter;
    avgTicks = Append[avgTicks, {avgPosition, groupLabel}];
    )
  ];
  Return[avgTicks];)]

GetColor[s_Style] := s /. Style[_, c_] :> c
GetColor[_] := Black

ListLabelPlot::usage="ListLabelPlot[data, labels] takes a list of
  numbers with corresponding labels. The data is grouped according
  to the labels and a ListPlot is created with them so that each
  group has a different color and their corresponding label is shown
   in the horizontal axis.";
Options[ListLabelPlot] = Join[Options[ListPlot], {"TickCompression"
  ->True,
"LabelLevels"->1}];
ListLabelPlot[data_, labels_, opts : OptionsPattern[]] := Module[
  {uniqueLabels, pallete, groupedByTerm, groupedKeys, scatterGroups
  ,
  groupedColors, frameTicks, compTicks, bottomTicks, topTicks},
  (
  uniqueLabels  = DeleteDuplicates[labels];
  pallete = Table[ColorData["Rainbow", i], {i, 0, 1,
      1/(Length[uniqueLabels] - 1)}];
  uniqueLabels  = (#[[1]] -> #[[2]]) & /@ Transpose[{RandomSample[
  uniqueLabels], pallete}];
  uniqueLabels  = Association[uniqueLabels];
  groupedByTerm = GroupBy[Transpose[{labels, Range[Length[data]],
  data}], First];
  groupedKeys   = Keys[groupedByTerm];
  scatterGroups = Transpose[Transpose[#][[2 ;; 3]]] & /@ Values[
  groupedByTerm];
  groupedColors = uniqueLabels[#] & /@ groupedKeys;
  frameTicks    = {Transpose[{Range[Length[data]],
    Style[Rotate[#, 90 Degree], uniqueLabels[#]] & /@ labels}],
    Automatic};
    If[OptionValue["TickCompression"], (
        compTicks = TickCompressor[frameTicks[[1]]];
        bottomTicks =
            MapIndexed[
            If[EvenQ[First[#2]], {#1[[1]],
                Tooltip[Style["\[SmallCircle]", GetColor
```

```
    [#1[[2]]]],#1[[2]]]
97                  }, #1] &, compTicks];
98          topTicks =
99              MapIndexed[
100             If[OddQ[First[#2]], {#1[[1]],
101                 Tooltip[Style["\[SmallCircle]", GetColor
    [#1[[2]]]],#1[[2]]]
102                 }, #1] &, compTicks];
103         frameTicks = {{Automatic, Automatic}, {bottomTicks,
    topTicks}};)
104   ];
105   ListPlot[scatterGroups,
106     opts,
107     Frame       -> True,
108     AxesStyle   -> {Directive[Black, Dotted], Automatic},
109     PlotStyle   -> groupedColors,
110     FrameTicks -> frameTicks]
111   )
112   ]
113
114 WaveToRGB::usage="WaveToRGB[wave, gamma] takes a wavelength in nm
    and returns the corresponding RGB color. The gamma parameter is
    optional and defaults to 0.8. The wavelength wave is assumed to be
     in nm. If the wavelength is below 380 the color will be the same
    as for 380 nm. If the wavelength is above 750 the color will be
    the same as for 750 nm. The function returns an RGBColor object.
    REF: https://www.noah.org/wiki/wave_to_rgb_in_Python. ";
115 WaveToRGB[wave_, gamma_ : 0.8] := (
116   wavelength = (wave);
117   Which[
118     wavelength < 380,
119       wavelength = 380,
120     wavelength > 750,
121       wavelength = 750
122   ];
123   Which[380 <= wavelength <= 440,
124   (
125     attenuation = 0.3 + 0.7*(wavelength - 380)/(440 - 380);
126     R = ((-(wavelength - 440)/(440 - 380))*attenuation)^gamma;
127     G = 0.0;
128     B = (1.0*attenuation)^gamma;
129     ),
130   440 <= wavelength <= 490,
131   (
132     R = 0.0;
133     G = ((wavelength - 440)/(490 - 440))^gamma;
134     B = 1.0;
135     ),
136   490 <= wavelength <= 510,
137   (
138     R = 0.0;
139     G = 1.0;
140     B = (-(wavelength - 510)/(510 - 490))^gamma;
141     ),
142   510 <= wavelength <= 580,
143   (
144     R = ((wavelength - 510)/(580 - 510))^gamma;
145     G = 1.0;
146     B = 0.0;
147     ),
148   580 <= wavelength <= 645,
149   (
150     R = 1.0;
151     G = (-(wavelength - 645)/(645 - 580))^gamma;
152     B = 0.0;
153     ),
154   645 <= wavelength <= 750,
155   (
156     attenuation = 0.3 + 0.7*(750 - wavelength)/(750 - 645);
157     R = (1.0*attenuation)^gamma;
158     G = 0.0;
159     B = 0.0;
160     ),
161   True,
162   (
163     R = 0;
```

```
      G = 0;
      B = 0;
      )];
    Return[RGBColor[R, G, B]]
    )

FuzzyRectangle::usage = "FuzzyRectangle[xCenter, width, ymin,
  height, color] creates a polygon with a fuzzy edge. The polygon is
   centered at xCenter and has a full horizontal width of width. The
   bottom of the polygon is at ymin and the height is height. The
  color of the polygon is color. The left edge and the right edge of
   the resulting polygon will be transparent and the middle will be
  colored. The polygon is returned as a list of polygons.";
FuzzyRectangle[xCenter_, width_, ymin_, height_, color_, intensity_
  :1] := Module[
    {intenseColor, nocolor, ymax, polys},
(
    nocolor = Directive[Opacity[0], color];
    ymax = ymin + height;
    intenseColor = Directive[Opacity[intensity], color];
    polys = {
      Polygon[{
        {xCenter - width/2, ymin},
        {xCenter, ymin},
        {xCenter, ymax},
        {xCenter - width/2, ymax}},
        VertexColors -> {
          nocolor,
          intenseColor,
          intenseColor,
          nocolor,
          nocolor}],
      Polygon[{
        {xCenter, ymin},
        {xCenter + width/2, ymin},
        {xCenter + width/2, ymax},
        {xCenter, ymax}},
        VertexColors -> {
          intenseColor,
          nocolor,
          nocolor,
          intenseColor,
          intenseColor}]
      };
    Return[polys]
    );
]

Options[SpectrumPlot] = Options[Graphics];
Options[SpectrumPlot] = Join[Options[SpectrumPlot], {"Intensities"
  -> {},"Tooltips" -> True, "Comments" -> {}, "SpectrumFunction" ->
  WaveToRGB}];
SpectrumPlot::usage="SpectrumPlot[lines, widthToHeightAspect,
  lineWidth] takes a list of spectral lines and creates a visual
  representation of them. The lines are represented as fuzzy
  rectangles with a width of lineWidth and a height that is
  determined by the overall condition that the width to height ratio
   of the resulting graph is widthToHeightAspect. The color of the
  lines is determined by the wavelength of the line. The function
  assumes that the lines are given in nm.
If the lineWidth parameter is a single number, then every line
  shares that width. If the lineWidth parameter is a list of numbers
  , then each line has a different width. The function returns a
  Graphics object. The function also accepts any options that
  Graphics accepts. The background of the plot is black by default.
  The plot range is set to the minimum and maximum wavelength of the
   given lines.
Besides the options for Graphics the function also admits the
  option Intensities. This option is a list of numbers that
  determines the intensity of each line. If the Intensities option
  is not given, then the lines are drawn with full intensity. If the
   Intensities option is given, then the lines are drawn with the
  given intensity. The intensity is a number between 0 and 1.
The function also admits the option \"Tooltips\". If this option is
   set to True, then the lines will have a tooltip that shows the
  wavelength of the line. If this option is set to False, then the
```

```
    lines will not have a tooltip. The default value for this option
    is True.
  If \"Tooltips\" is set to True and the option \"Comments\" is a non
    -empty list, then the tooltip will append the wavelength and the
    values in the comments list for the tooltips.
  The function also admits the option \"SpectrumFunction\". This
    option is a function that takes a wavelength and returns a color.
    The default value for this option is WaveToRGB.
  ";
  SpectrumPlot[lines_, widthToHeightAspect_, lineWidth_, opts :
    OptionsPattern[]] := Module[
    {minWave, maxWave, height, fuzzyLines},
  (
    colorFun = OptionValue["SpectrumFunction"];
    {minWave, maxWave} = MinMax[lines];
    height     = (maxWave - minWave)/widthToHeightAspect;
    fuzzyLines = Which[
      NumberQ[lineWidth] && Length[OptionValue["Intensities"]] == 0,
        FuzzyRectangle[#, lineWidth, 0, height, colorFun[#]] &/@
    lines,
      Not[NumberQ[lineWidth]] && Length[OptionValue["Intensities"]]
    == 0,
        MapThread[FuzzyRectangle[#1, #2, 0, height, colorFun[#1]] &,
    {lines, lineWidth}],
      NumberQ[lineWidth] && Length[OptionValue["Intensities"]] > 0,
        MapThread[FuzzyRectangle[#1, lineWidth, 0, height, colorFun
    [#1], #2] &, {lines, OptionValue["Intensities"]}],
      Not[NumberQ[lineWidth]] && Length[OptionValue["Intensities"]] >
     0,
        MapThread[FuzzyRectangle[#1, #2, 0, height, colorFun[#1], #3]
     &, {lines, lineWidth, OptionValue["Intensities"]}]
    ];
    comments = Which[
      Length[OptionValue["Comments"]] > 0,
        MapThread[StringJoin[ToString[#1]<>" nm","\n",ToString[#2]]&,
        {lines, OptionValue["Comments"]}],
      Length[OptionValue["Comments"]] == 0,
        ToString[#] <>" nm" & /@ lines,
      True,
      {}
    ];
    If[OptionValue["Tooltips"],
      fuzzyLines = MapThread[Tooltip[#1, #2] &, {fuzzyLines, comments
    }];
    ];
    graphicsOpts = FilterRules[{opts}, Options[Graphics]];
    Graphics[fuzzyLines,
        graphicsOpts,
        Background -> Black,
        PlotRange -> {{minWave, maxWave}, {0, height}}]
    )
  ];

End[];

EndPackage[];
```

17.4 misc.m

This module includes a few functions useful for data-handling.

```
BeginPackage["misc`"];
Needs["MaTeX`"];

ArrayBlocker;
BlockAndIndex;
BlockArrayDimensionsArray;
BlockMatrixMultiply;
BlockTranspose;

EllipsoidBoundingBox;
EllipsoidBoundingBox2;
ExportToH5;
ExtractSymbolNames;
FirstOrderPerturbation;
FlattenBasis;
```

```
16
17 FlowMatching;
18 GetModificationDate;
19 GreedyMatching;
20 HamTeX;
21 HelperNotebook;
22
23 RecoverBasis;
24 RemoveTrailingDigits;
25 ReplaceDiagonal;
26 RobustMissingQ;
27 RobustMissingQ;
28
29 RoundToSignificantFigures;
30 RoundValueWithUncertainty;
31 SecondOrderPerturbation;
32 StochasticMatching;
33 SuperIdentity;
34
35 TextBasedProgressBar;
36 ToPythonSparseFunction;
37 ToPythonSymPyExpression;
38 TruncateBlockArray;
39
40 Begin["`Private`"];
41
42   RemoveTrailingDigits[s_String] := StringReplace[s,
      RegularExpression["\\d+$"] -> ""];
43
44   BlockTranspose[anArray_]:=(
45     Map[Transpose, Transpose[anArray], {2}]
46   );
47
48   BlockMatrixMultiply::usage="BlockMatrixMultiply[A,B] gives the
      matrix multiplication of A and B, with A and B having a compatible
       block structure that allows for matrix multiplication into a
      congruent block structure.";
49   BlockMatrixMultiply[Amat_,Bmat_]:=Module[{rowIdx,colIdx,sumIdx},
50   (
51     Table[
52       Sum[Amat[[rowIdx,sumIdx]].Bmat[[sumIdx,colIdx]],{sumIdx,1,
      Dimensions[Amat][[2]]}],
53     {rowIdx,1,Dimensions[Amat][[1]]},
54     {colIdx,1,Dimensions[Bmat][[2]]}
55     ]
56   )
57   ];
58
59   BlockAndIndex::usage="BlockAndIndex[blockSizes, index] takes a list
       of bin widths and index. The function return in which block the
      index would be, were the bins to be layed out from left to right.
      The function also returns the position within the bin in which it
      is accomodated. The function returns these two numbers as a list
      of two elements {blockIndex, blockSubIndex}";
60   BlockAndIndex[blockSizes_List, index_Integer]:=Module[{
      accumulatedBlockSize,blockIndex, blockSubIndex},
61   (
62     accumulatedBlockSize = Accumulate[blockSizes];
63     If[accumulatedBlockSize[[-1]]-index<0,
64       Print["Index out of bounds"];
65       Abort[]
66     ];
67     blockIndex    = Flatten[Position[accumulatedBlockSize-index,n_ /;
       n>=0]][[1]];
68     blockSubIndex = Mod[index-accumulatedBlockSize[[blockIndex]],
      blockSizes[[blockIndex]],1];
69     Return[{blockIndex,blockSubIndex}]
70   )
71   ];
72
73   TruncateBlockArray::usage="TruncateBlockArray[blockArray,
      truncationIndices, blockWidths] takes a an array of blocks and
      selects the columns and rows corresponding to truncationIndices.
      The indices being given in what would be the ArrayFlatten[
      blockArray] version of the array. They blocks in the given array
      may be SparseArray. This is equivalent to FlattenArray[blockArray
```

```
  ][truncationIndices, truncationIndices] but may be more efficient
  blockArray is sparse.";
74 TruncateBlockArray[blockArray_,truncationIndices_,blockWidths_]:=
  Module[
75 {truncatedArray,blockCol,blockRow,blockSubCol,blockSubRow},(
76 truncatedArray = Table[
77   {blockCol,blockSubCol} = BlockAndIndex[blockWidths,fullColIndex];
78   {blockRow,blockSubRow} = BlockAndIndex[blockWidths,fullRowIndex];
79   blockArray[[blockRow,blockCol]][[blockSubRow,blockSubCol]],
80 {fullColIndex,truncationIndices},
81 {fullRowIndex,truncationIndices}
82 ];
83 Return[truncatedArray]
84 )
85 ];
86
87 BlockArrayDimensionsArray::usage="BlockArrayDimensionsArray[
  blockArray] returns the array of block sizes in a given blocked
  array.";
88 BlockArrayDimensionsArray[blockArray_]:=(
89   Map[Dimensions,blockArray,{2}]
90 );
91
92 ArrayBlocker::usage="ArrayBlocker[anArray, blockSizes] takes a flat
   2d array and a congruent 2D array of block sizes, and with them
  it returns the original array with the block structure imposed by
  blockSizes. The resulting array satisfies ArrayFlatten[
  blockedArray] == anArray, and also Map[Dimensions, blockedArray
  ,{2}] == blockSizes.";
93 ArrayBlocker[anArray_,blockSizes_]:=Module[{rowStart,colStart,
  colEnd,numBlocks,blockedArray,blockSize,rowEnd,aBlock,idxRow,
  idxCol},(
94   rowStart   = 1;
95   colStart   = 1;
96   colEnd     = 1;
97   numBlocks = Length[blockSizes];
98   blockedArray = Table[(
99     blockSize = blockSizes[[idxRow,idxCol]];
100    rowEnd    = rowStart+blockSize[[1]]-1;
101    colEnd    = colStart+blockSize[[2]]-1;
102    aBlock    = anArray[[rowStart;;rowEnd,colStart;;colEnd]];
103    colStart  = colEnd+1;
104    If[idxCol==numBlocks,
105      rowStart=rowEnd+1;
106      colStart=1;
107    ];
108    aBlock
109  ),
110  {idxRow,1,numBlocks},
111  {idxCol,1,numBlocks}
112  ];
113  Return[blockedArray]
114 )
115 ];
116
117 ReplaceDiagonal::usage =
118   "ReplaceDiagonal[matrix, repValue] replaces all the diagonal of
  the given array to the given value. The array is assumed to be
  square and the replacement value is assumed to be a number. The
  returned value is the array with the diagonal replaced. This
  function is useful for setting the diagonal of an array to a given
   value. The original array is not modified. The given array may be
   sparse.";
119 ReplaceDiagonal[matrix_, repValue_] :=
120   ReplacePart[matrix,
121     Table[{i, i} -> repValue, {i, 1, Length[matrix]}]];
122
123 Options[RoundValueWithUncertainty] = {"SetPrecision" -> False};
124 RoundValueWithUncertainty::usage = "RoundValueWithUncertainty[x,dx]
   given a number x together with an uncertainty dx this function
  rounds x to the first significant figure of dx and also rounds dx
  to have a single significant figure.
125 The returned value is a list with the form {roundedX, roundedDx}.
126 The option \"SetPrecision\" can be used to control whether the
  Mathematica precision of x and dx is also set accordingly to these
   rules, otherwise the rounded numbers still have the original
```

```
    precision of the input values.
127 If the position of the first significant figure of x is after the
    position of the first significant figure of dx, the function
    returns {0,dx} with dx rounded to one significant figure.";
128 RoundValueWithUncertainty[x_, dx_, OptionsPattern[]] := Module[
129   {xExpo, dxExpo, sigFigs, roundedX, roundedDx, returning},
130   (
131     xExpo   = RealDigits[x][[2]];
132     dxExpo  = RealDigits[dx][[2]];
133     sigFigs = (xExpo - dxExpo) + 1;
134     {roundedX, roundedDx} = If[sigFigs <= 0,
135       {0., N@RoundToSignificantFigures[dx, 1]},
136       N[
137       {
138         RoundToSignificantFigures[x, xExpo - dxExpo + 1],
139         RoundToSignificantFigures[dx, 1]}
140       ]
141       ];
142     returning = If[
143       OptionValue["SetPrecision"],
144       {SetPrecision[roundedX, Max[1, sigFigs]],
145       SetPrecision[roundedDx, 1]},
146       {roundedX, roundedDx}
147       ];
148     Return[returning]
149     )
150   ];
151
152 RoundToSignificantFigures::usage =
153   "RoundToSignificantFigures[x, sigFigs] rounds x so that it only
    has \
154 sigFigs significant figures.";
155 RoundToSignificantFigures[x_, sigFigs_] :=
156   Sign[x]*N[FromDigits[RealDigits[x, 10, sigFigs]]];
157
158 RobustMissingQ[expr_] := (FreeQ[expr, _Missing] === False);
159
160 TextBasedProgressBar[progress_, totalIterations_, prefix_:""] :=
    Module[
161     {progMessage},
162     progMessage = ToString[progress] <> "/" <> ToString[
    totalIterations];
163     If[progress < totalIterations,
164         WriteString["stdout", StringJoin[prefix, progMessage, "\r"
    ]],
165         WriteString["stdout", StringJoin[prefix, progMessage, "\n"
    ]]
166     ];
167 ];
168
169 FirstOrderPerturbation::usage="Given the eigenVectors of a matrix A
     (which doesn't need to be given) together with a corresponding
    perturbation matrix perMatrix, this function calculates the first
    derivative of the eigenvalues with respect to the scale factor of
    the perturbation matrix. In the sense that the eigenvalues of the
    matrix A + β perMatrix are to first order equal to \[Lambda] + \[
    Delta]_i β, where the \[Delta]_i are the returned values. This
    assuming that the eigenvalues are non-degenerate.";
170 FirstOrderPerturbation[eigenVectors_,
171   perMatrix_] := (Chop@Diagonal[
172   Conjugate@eigenVectors . perMatrix . Transpose[eigenVectors]])
173
174 SecondOrderPerturbation::usage="Given the eigenValues and
    eigenVectors of a matrix A (which doesn't need to be given)
    together with a corresponding perturbation matrix perMatrix, this
    function calculates the second derivative of the eigenvalues with
    respect to the scale factor of the perturbation matrix. In the
    sense that the eigenvalues of the matrix A + β perMatrix are to
    second order equal to \[Lambda] + \[Delta]_i β + \[Delta]_i^{(2)
    }/2 β^2, where the \[Delta]_i^{(2)} are the returned values. The
    eigenvalues and eigenvectors are assumed to be given in the same
    order, i.e. the ith eigenvalue corresponds to the ith eigenvector.
     This assuming that the eigenvalues are non-degenerate.";
175 SecondOrderPerturbation[eigenValues_, eigenVectors_, perMatrix_] :=
     (
176   dim = Length[perMatrix];
```

```
177     eigenBras = Conjugate[eigenVectors];
178     eigenKets = eigenVectors;
179     matV = Abs[eigenBras . perMatrix . Transpose[eigenKets]]^2;
180     OneOver[x_, y_] := If[x == y, 0, 1/(x - y)];
181     eigenDiffs = Outer[OneOver, eigenValues, eigenValues, 1];
182     pProduct = Transpose[eigenDiffs]*matV;
183     Return[2*(Total /@ Transpose[pProduct])];
184     )
185
186   SuperIdentity::usage="SuperIdentity[args] returns the arguments
        passed to it. This is useful for defining a function that does
        nothing, but that can be used in a composition.";
187   SuperIdentity[args___] := {args};
188
189   FlattenBasis::usage="FlattenBasis[basis] takes a basis in the
        standard representation and separates out the strings that
        describe the LS part of the labels and the additional numbers that
         define the values of J MJ and MI. It returns a list with two
        elements {flatbasisLS, flatbasisNums}. This is useful for saving
        the basis to an h5 file where the strings and numbers need to be
        separated.";
190   FlattenBasis[basis_] := Module[{flatbasis, flatbasisLS,
        flatbasisNums},
191     (
192       flatbasis = Flatten[basis];
193       flatbasisLS = flatbasis[[1 ;; ;; 4]];
194       flatbasisNums = Select[flatbasis, Not[StringQ[#]] &];
195       Return[{flatbasisLS, flatbasisNums}]
196       )
197     ];
198
199   RecoverBasis::usage="RecoverBasis[{flatBasisLS, flatbasisNums}]
        takes the output of FlattenBasis and returns the original basis.
        The input is a list with two elements {flatbasisLS, flatbasisNums
        }.";
200   RecoverBasis[{flatbasisLS_, flatbasisNums_}] := Module[{recBasis},
201     (
202     recBasis = {{{#[[1]], #[[2]]}, #[[3]]}, #[[4]]} & /@ (Flatten /@
203         Transpose[{flatbasisLS,
204           Partition[Round[2*#]/2 & /@ flatbasisNums, 3]}]);
205     Return[recBasis];
206     )
207     ]
208
209   ExtractSymbolNames[expr_Hold] := Module[
210     {strSymbols},
211     strSymbols = ToString[expr, InputForm];
212     StringCases[strSymbols, RegularExpression["\\w+"]][[2 ;;]]
213     ]
214
215   ExportToH5::usage =
216     "ExportToH5[fname, Hold[{symbol1, symbol2, ...}]] takes an .h5
        filename and a held list of symbols and export to the .h5 file the
         values of the symbols with keys equal the symbol names. The
        values of the symbols cannot be arbitrary, for instance a list
        with mixes numbers and string will fail, but an Association with
        mixed values exports ok. Do give it a try.
217     If the file is already present in disk, this function will
        overwrite it by default. If the value of a given symbol contains
        symbolic numbers, e.g. \[Pi], these will be converted to floats in
         the exported file.";
218   Options[ExportToH5] = {"Overwrite" -> True};
219   ExportToH5[fname_String, symbols_Hold, OptionsPattern[]] := (
220     If[And[FileExistsQ[fname], OptionValue["Overwrite"]],
221     (
222       Print["File already exists, overwriting ..."];
223       DeleteFile[fname];
224       )
225     ];
226     symbolNames = ExtractSymbolNames[symbols];
227     Do[(Print[symbolName];
228       Export[fname, ToExpression[symbolName], {"Datasets", symbolName
      },
229       OverwriteTarget -> "Append"]
230       ), {symbolName, symbolNames}]
231     )
```

```
232
233  GreedyMatching::usage="GreedyMatching[aList, bList] returns a list
       of pairs of elements from aList and bList that are closest to each
        other, this is returned in a list together with a mapping of
       indices from the aList to those in bList to which they were
       matched. The option \"alistLabels\" can be used to specify labels
       for the elements in aList. The option \"blistLabels\" can be used
       to specify labels for the elements in bList. If these options are
       used, the function returns a list with three elements the pairs of
        matched elements, the pairs of corresponding matched labels, and
       the mapping of indices.";
234  Options[GreedyMatching] = {
235      "alistLabels" -> {},
236      "blistLabels" -> {}};
237  GreedyMatching[aValues0_, bValues0_, OptionsPattern[]] := Module[{
238    aValues = aValues0,
239    bValues = bValues0,
240    bValuesOriginal = bValues0,
241    bestLabels, bestMatches,
242    bestLabel, aElement, givenLabels,
243    aLabels, aLabel,
244    diffs, minDiff,
245    bLabels,
246    minDiffPosition, bestMatch},
247    (
248    aLabels     = OptionValue["alistLabels"];
249    bLabels     = OptionValue["blistLabels"];
250    bestMatches = {};
251    bestLabels  = {};
252    givenLabels = (Length[aLabels] > 0);
253    Do[
254      (
255      aElement        = aValues[[idx]];
256      diffs           = Abs[bValues - aElement];
257      minDiff         = Min[diffs];
258      minDiffPosition = Position[diffs, minDiff][[1, 1]];
259      bestMatch       = bValues[[minDiffPosition]];
260      bestMatches     = Append[bestMatches, {aElement, bestMatch}];
261      If[givenLabels,
262        (
263        aLabel     = aLabels[[idx]];
264        bestLabel  = bLabels[[minDiffPosition]];
265        bestLabels = Append[bestLabels, {aLabel, bestLabel}];
266        bLabels    = Drop[bLabels, {minDiffPosition}];
267        )
268        ];
269      bValues = Drop[bValues, {minDiffPosition}];
270      If[Length[bValues] == 0, Break[]];
271      ),
272      {idx, 1, Length[aValues]}
273      ];
274    pairedIndices = MapIndexed[{#2[[1]], Position[bValuesOriginal,
       #1[[2]]][[1, 1]]} &, bestMatches];
275    If[givenLabels,
276      Return[{bestMatches, bestLabels, pairedIndices}],
277      Return[{bestMatches, pairedIndices}]
278      ]
279    )
280    ]
281
282  StochasticMatching::usage="StochasticMatching[aValues, bValues]
       finds a better assignment by randomly shuffling the elements of
       aValues and then applying the greedy assignment algorithm. The
       function prints what is the range of total absolute differences
       found during shuffling, the standard deviation of all of them, and
        the number of shuffles that were attempted. The option \"
       alistLabels\" can be used to specify labels for the elements in
       aValues. The option \"blistLabels\" can be used to specify labels
       for the elements in bValues. If these options are used, the
       function returns a list with three elements the pairs of matched
       elements, the pairs of corresponding matched labels, and the
       mapping of indices.";
283  Options[StochasticMatching] = {"alistLabels" -> {},
284    "blistLabels" -> {}};
285  StochasticMatching[aValues0_, bValues0_, numShuffles_ : 200,
       OptionsPattern[]] := Module[{
```

```
    aValues = aValues0,
    bValues = bValues0,
    matchingLabels, ranger, matches, noShuff, bestMatch, highestCost,
     lowestCost, dev, sorter, bestValues,
    pairedIndices, bestLabels, matchedIndices, shuffler
    },
    (
    matchingLabels = (Length[OptionValue["alistLabels"]] > 0);
    ranger = Range[1, Length[aValues]];
    matches = If[Not[matchingLabels], (
        Table[(
          shuffler = If[i == 1, ranger, RandomSample[ranger]];
          {bestValues, matchedIndices} =
          GreedyMatching[aValues[[shuffler]], bValues];
          cost = Total[Abs[#[[1]] - #[[2]]] & /@ bestValues];
          {cost, {bestValues, matchedIndices}}
          ), {i, 1, numShuffles}]
        ),
      Table[(
        shuffler = If[i == 1, ranger, RandomSample[ranger]];
        {bestValues, bestLabels, matchedIndices} =
          GreedyMatching[aValues[[shuffler]], bValues,
          "alistLabels" -> OptionValue["alistLabels"][[shuffler]],
          "blistLabels" -> OptionValue["blistLabels"]];
        cost = Total[Abs[#[[1]] - #[[2]]] & /@ bestValues];
        {cost, {bestValues, bestLabels, matchedIndices}}
        ), {i, 1, numShuffles}]
      ];
    noShuff = matches[[1, 1]];
    matches = SortBy[matches, First];
    bestMatch = matches[[1, 2]];
    highestCost = matches[[-1, 1]];
    lowestCost = matches[[1, 1]];
    dev = StandardDeviation[First /@ matches];
    Print[lowestCost, " <-> ", highestCost, " | \[Sigma]=", dev,
      " | N=", numShuffles, " | null=", noShuff];
    If[matchingLabels,
      (
      {bestValues, bestLabels, matchedIndices} = bestMatch;
      sorter = Ordering[First /@ bestValues];
      bestValues = bestValues[[sorter]];
      bestLabels = bestLabels[[sorter]];
      pairedIndices =
        MapIndexed[{#2[[1]], Position[bValues, #1[[2]]][[1, 1]]} &,
        bestValues];
      Return[{bestValues, bestLabels, pairedIndices}]
      ),
      (
      {bestValues, matchedIndices} = bestMatch;
      sorter = Ordering[First /@ bestValues];
      bestValues = bestValues[[sorter]];
      pairedIndices =
        MapIndexed[{#2[[1]], Position[bValues, #1[[2]]][[1, 1]]} &,
        bestValues];
      Return[{bestValues, pairedIndices}]
      )
      ];
    )
    ]

  FlowMatching::usage="FlowMatching[aList, bList] returns a list of
    pairs of elements from aList and bList that are closest to each
    other, this is returned in a list together with a mapping of
    indices from the aList to those in bList to which they were
    matched. The option \"alistLabels\" can be used to specify labels
    for the elements in aList. The option \"blistLabels\" can be used
    to specify labels for the elements in bList. If these options are
    used, the function returns a list with three elements the pairs of
     matched elements, the pairs of corresponding matched labels, and
    the mapping of indices. This is basically a wrapper around
    Mathematica's FindMinimumCostFlow function. By default the option
    \"notMatched\" is zero, and this means that all elements of aList
    must be matched to elements of bList. If this is not the case, the
     option \"notMatched\" can be used to specify how many elements of
     aList can be left unmatched. By default the cost function is Abs
    [#1-#2]&, but this can be changed with the option \"CostFun\",
```

```
    this function needs to take two arguments.";
346 Options[FlowMatching] = {"alistLabels" -> {}, "blistLabels" -> {},
    "notMatched" -> 0, "CostFun"-> (Abs[#1-#2] &)};
347 FlowMatching[aValues0_, bValues0_, OptionsPattern[]] := Module[{
348   aValues = aValues0, bValues = bValues0, edgesSourceToA,
    capacitySourceToA, nA, nB,
349   costSourceToA, midLayer, midLayerEdges, midCapacities,
350   midCosts, edgesBtoSink, capacityBtoSink, costBtoSink,
351   allCapacities, allCosts, allEdges, graph,
352   flow, bestValues, bestLabels, cFun,
353   aLabels, bLabels, pairedIndices, matchingLabels},
354   (
355   matchingLabels = (Length[OptionValue["alistLabels"]] > 0);
356   aLabels = OptionValue["alistLabels"];
357   bLabels = OptionValue["blistLabels"];
358   cFun    = OptionValue["CostFun"];
359   nA      = Length[aValues];
360   nB      = Length[bValues];
361   (*Build up the edges costs and capacities*)
362   (*From source to the nodes representing the values of the first \
363 list*)
364   edgesSourceToA    = ("source" \[DirectedEdge] {"A", #}) & /@
    Range[1, nA];
365   capacitySourceToA = ConstantArray[1, nA];
366   costSourceToA     = ConstantArray[0, nA];
367
368   (*From all the elements of A to all the elements of B*)
369   midLayer = Table[{{"A", i} \[DirectedEdge] ({"B", j}), 1, cFun[
    aValues[[i]], bValues[[j]]]}, {i, 1, nA}, {j, 1, nB}];
370   midLayer = Flatten[midLayer, 1];
371   {midLayerEdges, midCapacities, midCosts} = Transpose[midLayer];
372
373   (*From the elements of B to the sink*)
374   edgesBtoSink    = ({"B", #} \[DirectedEdge] "sink") & /@ Range[1,
    nB];
375   capacityBtoSink = ConstantArray[1, nB];
376   costBtoSink     = ConstantArray[0, nB];
377
378   (*Put it all together*)
379   allCapacities = Join[capacitySourceToA, midCapacities,
    capacityBtoSink];
380   allCosts      = Join[costSourceToA, midCosts, costBtoSink];
381   allEdges      = Join[edgesSourceToA, midLayerEdges, edgesBtoSink
    ];
382   graph         = Graph[allEdges, EdgeCapacity -> allCapacities,
383     EdgeCost -> allCosts];
384
385   (*Solve it*)
386   flow          = FindMinimumCostFlow[graph, "source", "sink", nA -
    OptionValue["notMatched"], "OptimumFlowData"];
387   (*Collect the pairs of matched indices*)
388   pairedIndices = Select[flow["EdgeList"], And[Not[#[[1]] === "
    source"], Not[#[[2]] === "sink"]] &];
389   pairedIndices = {#[[1, 2]], #[[2, 2]]} & /@ pairedIndices;
390   (*Collect the pairs of matched values*)
391   bestValues    = {aValues[[#[[1]]]], bValues[[#[[2]]]]} & /@
    pairedIndices;
392   (*Account for having been given labels*)
393   If[matchingLabels,
394     (
395     bestLabels = {aLabels[[#[[1]]]], bLabels[[#[[2]]]]} & /@
    pairedIndices;
396     Return[{bestValues, bestLabels, pairedIndices}]
397     ),
398     (
399     Return[{bestValues, pairedIndices}]
400     )
401     ];
402   )
403   ]
404
405 HelperNotebook::usage="HelperNotebook[nbName] creates a separate
    notebook and returns a function that can be used to print to the
    bottom of it. The name of the notebook, nbName, is optional and
    defaults to OUT.";
406 HelperNotebook[nbName_:"OUT"] :=
```

```
Module[{screenDims, screenWidth, screenHeight, nbWidth, leftMargin,
  PrintToOutputNb}, (
  screenDims =
    SystemInformation["Devices", "ScreenInformation"][[1, 2, 2]];
  screenWidth = screenDims[[1, 2]];
  screenHeight = screenDims[[2, 2]];
  nbWidth = Round[screenWidth/3];
  leftMargin = screenWidth - nbWidth;
  outputNb = CreateDocument[{}, WindowTitle -> nbName,
    WindowMargins -> {{leftMargin, Automatic}, {Automatic,
        Automatic}}, WindowSize -> {nbWidth, screenHeight}];
  PrintToOutputNb[text_] :=
    (
        SelectionMove[outputNb, After, Notebook];
        NotebookWrite[outputNb, Cell[BoxData[ToBoxes[text]], "
  Output"]];
    );
  Return[PrintToOutputNb]
  )
  ]

GetModificationDate::usage="GetModificationDate[fname] returns the
  modification date of the given file.";
GetModificationDate[theFileName_] := FileDate[theFileName, "
  Modification"];

(*Helper function to convert Mathematica expressions to standard
  form*)
StandardFormExpression[expr0_] := Module[{expr=expr0}, ToString[
  expr, InputForm]];

(*Helper function to translate to Python/SymPy expressions*)
ToPythonSymPyExpression::usage="ToPythonSymPyExpression[expr]
  converts a Mathematica expression to a SymPy expression. This is a
   little iffy and might break if the expression includes
  Mathematica functions that haven't been given a SymPy equivalent."
  ;
ToPythonSymPyExpression[expr0_] := Module[{standardForm, expr=expr0
  },
  standardForm = StandardFormExpression[expr];
  StringReplace[standardForm, {
    "Power[" -> "Pow(",
    "Sqrt[" -> "sqrt(",
    "[" -> "(",
    "]" -> ")",
    "\\" -> "",
    "I" -> "1j",
    (*Remove special Mathematica backslashes*)
    "/" -> "/" (*Ensure division is represented with a slash*)}]];

ToPythonSparseFunction[sparseArray_SparseArray, funName_] :=
  Module[{data, rowPointers, columnIndices, dimensions, pyCode,
  vars,
    varList, dataPyList,
    colIndicesPyList},(*Extract unique symbolic variables from the
  \
SparseArray*)
  vars = Union[Cases[Normal[sparseArray], _Symbol, Infinity]];
  varList = StringRiffle[ToString /@ vars, ", "];
  (*varList=ToPythonSymPyExpression/@varList;*)
  (*Convert data to SymPy compatible strings*)
  dataPyList =
    StringRiffle[
    ToPythonSymPyExpression /@ Normal[sparseArray["NonzeroValues"
  ]],
    ", "];
  colIndicesPyList =
    StringRiffle[
    ToPythonSymPyExpression /@ (Flatten[
        Normal[sparseArray["ColumnIndices"]] - 1]), ", "];
  (*Extract sparse array properties*)
  rowPointers = Normal[sparseArray["RowPointers"]];
  dimensions = Dimensions[sparseArray];
  (*Create Python code string*)pyCode = StringJoin[
    "#!/usr/bin/env python3\n\n",
    "from scipy.sparse import csr_matrix\n",
```

```
      "from sympy import *\n",
      "import numpy as np\n",
      "\n",
      "sqrt = np.sqrt\n",
      "\n",
      "def ", funName, "(",
      varList,
      "):\n",
      "    data = np.array([", dataPyList, "])\n",
      "    indices = np.array([",
      colIndicesPyList,
      "])\n",
      "    indptr = np.array([",
      StringRiffle[ToString /@ rowPointers, ", "], "])\n",
      "    shape = (", StringRiffle[ToString /@ dimensions, ", "],
      ")\n",
      "    return csr_matrix((data, indices, indptr), shape=shape)"];
    pyCode
    ];

  Options[HamTeX] = {"T2" -> False};
  HamTeX::usage="HamTeX[numE] returns an image with parsed LaTeX code
     for the Hamiltonian of the given number of electrons. The option
    \"T2\" can be used to specify whether the T2 term should be
    included in the Hamiltonian for the f^12 configuration. The
    default is False and the option is ignored if the number of
    electrons is not 12. The function requires the MaTeX package.";
  HamTeX[nE_, OptionsPattern[]] := (
    tex = Which[
      MemberQ[{1, 13}, nE],
        "\\zeta \\sum_{i=1}^{n}\\left(\\hat{s}_i \\cdot \
    \\hat{l}_i\\right) \
    +\\sum_{i=1}^n\\sum_{k=2,4,6}\\sum_{q=-k}^{k}B_q^{(k)}\\mathcal{C
    }(i)_\
    q^{(k)} + \\epsilon",
      nE == 2,
        "\\hat{H}&=\\sum_{k=2,4,6}F^{(k)}\\hat{f}_k
    +\\alpha \\hat{L}^2
    +\\beta \\,\\mathcal{C}\\left(\\mathcal{G}(2)\\right)
    +\\gamma \\,\\mathcal{C}\\left(\\mathcal{SO}(7)\\right)\\\\
    &\\quad + \\zeta \\sum_{i=1}^{n}\\left(\\hat{s}_i \\cdot \
    \\hat{l}_i\\right)
    +\\sum_{k=0,2,4}M^{(k)}\\hat{m}_k
    +\\sum_{k=2,4,6}P^{(k)}\\hat{p}_k \\\\
    &\\quad\\quad\\quad\\quad\\quad+\\sum_{i=1}^n\\sum_{k=2,4,6}\\
    sum_{q=-\
    k}^{k}B_q^{(k)}\\mathcal{C}(i)_q^{(k)} + \\epsilon",
      And[nE == 12, OptionValue["T2"]],
        "\\hat{H}&=\\sum_{k=2,4,6}F^{(k)}\\hat{f}_k
        +T^{(2)}\\hat{t}_2
        +\\alpha \\hat{L}^2
        +\\beta \\,\\mathcal{C}\\left(\\mathcal{G}(2)\\right)
        +\\gamma \\,\\mathcal{C}\\left(\\mathcal{SO}(7)\\right)\\\\
        &\\quad\\quad\\quad + \\zeta \\sum_{i=1}^{n}\\left(\\hat{s}_i
     \\cdot \
        \\hat{l}_i\\right)
        +\\sum_{k=0,2,4}M^{(k)}\\hat{m}_k
        +\\sum_{k=2,4,6}P^{(k)}\\hat{p}_k \\\\
        &\\quad\\quad\\quad\\quad\\quad\\quad\\quad+\\sum_{i=1}^n\\
    sum_{k=2,4,\
        6}\\sum_{q=-k}^{k}B_q^{(k)}\\mathcal{C}(i)_q^{(k)} + \\
    epsilon",
      And[nE == 12, Not@OptionValue["T2"]],
        "\\hat{H}&=\\sum_{k=2,4,6}F^{(k)}\\hat{f}_k
        +\\alpha \\hat{L}^2
        +\\beta \\,\\mathcal{C}\\left(\\mathcal{G}(2)\\right)
        +\\gamma \\,\\mathcal{C}\\left(\\mathcal{SO}(7)\\right)\\\\
        &\\quad + \\zeta \\sum_{i=1}^{n}\\left(\\hat{s}_i \\cdot \
        \\hat{l}_i\\right)
        +\\sum_{k=0,2,4}M^{(k)}\\hat{m}_k
        +\\sum_{k=2,4,6}P^{(k)}\\hat{p}_k \\\\
        &\\quad\\quad\\quad+\\sum_{i=1}^n\\sum_{k=2,4,6}\\sum_{q=-k
    }^{k}B_q^{(\
    k)}\\mathcal{C}(i)_q^{(k)} + \\epsilon",
      True,
        "\\hat{H}&=\\sum_{k=2,4,6}F^{(k)}\\hat{f}_k
```

```
535         +\\sum_{k=2,3,4,6,7,8}T^{(k)}\\hat{t}_k
536         +\\alpha \\hat{L}^2
537         +\\beta \\,\\mathcal{C}\\left(\\mathcal{G}(2)\\right)
538         +\\gamma \\,\\mathcal{C}\\left(\\mathcal{SO}(7)\\right)\\\\
539         &\\quad\\quad\\quad\\quad + \\zeta \\sum_{i=1}^{n}\\left(\\
    hat{s}_i \
540         \\cdot \\hat{l}_i\\right)
541         +\\sum_{k=0,2,4}M^{(k)}\\hat{m}_k
542         +\\sum_{k=2,4,6}P^{(k)}\\hat{p}_k \\\\
543         &\\quad\\quad\\quad\\quad\\quad\\quad\\quad\\quad+\\sum_{i
    =1}^n\\sum_{\
544         k=2,4,6}\\sum_{q=-k}^{k}B_q^{(k)}\\mathcal{C}(i)_q^{(k)} + \\
    epsilon"
545       ];
546     MaTeX[StringJoin[{"\\begin{aligned}\n", tex, "\n\\end{aligned}"
    }]]
547     )
548
549   EllipsoidBoundingBox::usage = "EllipsoidBoundingBox[A,\[Kappa]]
      gives the coordinate intervals that contain the ellipsoid
      determined by r^T.A.r==\[Kappa]^2. The matrix A must be square NxN
      , symmetric, and positive definite. The function returns a list
      with N pairs of numbers, each pair being of the form {-x_i, x_i}."
      ;
550   EllipsoidBoundingBox[Amat_,\[Kappa]_]:=Module[
551     {invAmat, stretchFactors, boundingPlanes, quad},
552       (
553       invAmat = Inverse[Amat];
554       stretchFactors = Sqrt[1/Diagonal[invAmat]];
555       boundingPlanes = DiagonalMatrix[stretchFactors].invAmat;
556       (* The solution is proportional to \[Kappa] *)
557       boundingPlanes = \[Kappa] * boundingPlanes;
558       boundingPlanes = Max /@ Transpose[boundingPlanes];
559       Return[{-#,#}& /@ boundingPlanes]
560     )
561   ];
562
563 End[];
564 EndPackage[];
```

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