A primer on the occupation representation for many-body theory

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For all students who struggle with this material as I once did.

Contents

Introduction: Keeping track of all those electrons

Nothing corrupts a man so deeply as writing a book. – *Nero Wolfe*

A friend once asked me if I understood superconductivity. I'm a nuclear physicist by training, but I allowed I grasped the basic concepts of superconductivity well enough. He then asked: How do you keep track of all those electrons?

I answered: We don't. Instead we just keep track of one or two electrons, and assume all the rest act the same.

This book is devoted to that principle, but with more math.

It is easier to write down an equation than to solve it. This is certainly true in many-body theory, which involve coupled multi-variable partial differential equations. But humans are really only good at solving ordinary differential equations, that is, differential equations with one independent variable, so that nearly all our techniques for solving multivariable equations boil down to rewriting the problem as a set of decoupled ordinary differential equations, either exactly or approximately.

For the quantum many-body system, the differential equations are linear, so we can rewrite them as a matrix equation. Alternately, one can approximate the linear many-body system by a non-linear one-body system, leading to mean-field theory and its various progeny, including quasiparticles and the Bardeen-Cooper-Schrieffer (BCS) model of superconductors.

I intend this book to help the reader master the topic of the occupation representation, and working with creation and annihilation operators from second quantization, in prepartion for many-body theory. The basic idea of the occupation representation is to build up the many-body system through convenient one-body states. From this starting point I will develop the mathematical machinery for recasting coupled linear differential equations as a matrix equation, the derivation of mean-field-based approximations, and so on.

The goal is to focus on technical skills, and not on specific physics. For example, in many texts on nuclear physics, one reads statements that one can compute cross-section or decay lifetimes via Fermi's Golden Rule, which involves a phase space factor and a transition matrix element $\langle\psi_f|\hat{\mathcal{O}}|\psi_i\rangle$. But

the texts give very little idea how to compute this matrix element, or even how the wavefunction $|\psi\rangle$ and the transition operator $\hat{\mathcal{O}}$ are constructed. In this book I will completely ignore Fermi's Golden Rule, phase space factors, and cross-sections. Instead I will teach you, in great detail, how to understand and compute $\langle\psi_f|\hat{\mathcal{O}}|\psi_i\rangle$ for a many-body system. For another example, although I discuss the mathematics of the BCS approximation, I do not discuss superconductivity, which is covered well enough in many other texts.

This book is most directly aimed at nuclear and atomic physics, so I also include a great deal of the rules of angular momentum coupling. Some of it will undoubtedly also be useful for students of condensed matter, although they will be less interested in issues of angular momentum.

Although I frequently give detailed derivations, I encourage you to work out steps that I have skipped over, and I have included some exercises at the ends of chapters. In several places I give detailed numerical examples. I strongly encourage you to develop your own codes to reproduce those results, using a platform such as Mathematica, Maple, or MatLab, or a compiled language such as C or Fortran. Eigensolvers for compiled languages can be found, for example, through sources such as *Numerical Recipes* or standard libraries such as LAPACK (www.netlib.org/lapack).

As for broad organization, the first part of the book gives a detailed pedagogical introduction to the occupation representation in terms of fermion and boson operators and their manipulation. The second part illustrates the use of the occupation representation through toy models and then several common applications, including mean-field theory which is central to so much of many-body physics. The third part goes even deeper by introducing the quantum theory of angular momentum and utilizing it in the calculation of matrix elements. Although the development is linear, and later chapters build upon the previous, I don't recommend reading through the book as if it were a novel. I find context helps. Get a project, either one assigned by someone else or dreamed up by yourself. Then read the book to learn how to tackle your project.

Although I use advanced, abstract representations, all methods discussed in this book are based upon the search for a wavefunction. Another approach, quite different in many aspects (although it does draw upon the formalism of second quantization) are Green function methods. Whenever you see a Feynmann diagram they are probably talking about a Green function approach even if they don't say so. While Green function methods are applicable to condensed matter and nuclear physics, and are the heart and soul of quantum field theory and modern particle physics, there are many fine books on Feynmann diagrams and Green function approaches, so I will not attempt a discussion here. At least not yet.

Part I

The foundations, brick by brick

Chapter 1

A review of quantum mechanics

> Do not worry about your difficulties in Mathematics. I can assure you mine are still greater. – *Albert Einstein*

I assume the reader has taken a standard course in nonrelativistic quantum mechanics, at the advanced undergraduate or basic graduate level. For convenience I briefly review the important points here. Ideally you should find the concepts familiar; if not, I recommend going back to your quantum textbook before going further.

Quantum mechanics is one of the great triumphs of twentieth-century physics. While it certainly seems odd, arbitrary, or even bizarre when first encountered, with sufficient practice one can develop a strong intuition for much of quantum mechanics.

Part of the problem with quantum mechanics is its stitched-up nature. The other great triumph of twentieth-century physics, relativity, has a simpler origin. Relativity sprang mostly from one person, Albert Einstein (though I do not mean to denigrate the important contributions by Poincare, Lorentz, Hilbert, and others who foresaw many elements or who contributed further developments), who laid the foundations for both the special and general theories with elegant, concrete statements about observations: for special relativity, that one cannot make an observation that determines absolute motion, and in particular that the speed of light is the same in all inertial frames; and for general relativity, that one cannot make an observation that distinguishes between acceleration and gravity. If you takes these axioms seriously and rigorously, and add in a lot of math, one can deduce length contraction and time dilation, the equivalence of matter and energy, gravitational redshift, the bending of the fabric of space-time, and so on.

There are no analogous starting axioms for quantum mechanics, or least none with the same simple clarity and comprehensibility . And unlike relativ-

ity, quantum mechanics has multiple fathers: Planck and Bohr and Schrödinger and Heisenberg and de Broglie and Born and many others, including Einstein himself. Even to this day quantum mechanics bears the scars of this chimeric heritage: under the standard classroom pedagogy, the Copenhagen interpretation, a quantum system can change in time in two very distinct ways, either evolving under the time-dependent Schödinger equation, or through the so-called collapse of the wavefunction at the moment a measurement is made. While there are alternate interpretations available, they are not used on a day-to-day basis because they typically make calculations, the bread and butter of a theoretical physicist, *more* difficult without adding accuracy.

I will not devote time to foundational issues, but instead will focus on technical points. And here, assuming one does not obsess too much on trying to cram our macroscopic intuition into the microscopic realm (the assumption that the universe at all length scales must be beholden to our paleolithic hominid brains is the height of arrogance), the math issues are straightforward, nearly all linear algebra. This review will not attempt to be comprehensive, but instead aimed at reminding the reader of the points most relevant to the subject at hand.

So let us begin.

1.1 Quantum mechanics and linear algebra

Quantum mechanics is a linear theory. The time-dependent Schrödinger equation for the time evolution of a system,

$$\hat{H}\Psi(t) = i\hbar\frac{\partial}{\partial t}\Psi(t), \tag{1.1}$$

is a linear differential equation. Therefore many of the fundamental tools of quantum mechanics are basic concepts in linear algebra: eigenvalue problems, vectors and matrices, and linear transformations.

Linear algebra occurs even in the uttermost bedrock of physics: measurement. Suppose you measure something in your laboratory: position, velocity, angular momentum, you name it. In quantum mechanics the measurement is represented by a linear operator $\hat{\mathcal{O}}$, and the only values that you can read on your laboratory equipment are the eigenvalues of that operator:

$$\hat{\mathcal{O}}\Phi_\lambda = \lambda\Phi_\lambda. \tag{1.2}$$

We assume the operator $\hat{\mathcal{O}}$ is Hermitian, because then the eigenvalues λ, and thus what is measured in the laboratory, is real-valued. For some operators λ is continuous-valued, but for others λ has discrete values, and it is this that makes quantum mechanics 'quantum.'

Further, we assume that any system is described by a wavefunction Ψ. Technically Ψ and the Φ_λ are members of a vector space, but for the moment I'll be cagey in describing that vector space, because the entire point of this book is to develop the tools to handle wavefunctions appropriate to the many-body

problem! But since you have seen such wavefunctions before, you should not be stumped by this statement.

The Hermiticity of $\hat{\mathcal{O}}$ also means the eigenfunctions (or eigenvectors, I'm still being cagey) Φ_λ must span the space and are orthogonal, which means they form a convenient basis for the expansion of any wavefunction in:

$$\Psi = \sum_\lambda c_\lambda \Phi_\lambda. \tag{1.3}$$

As mentioned earlier, for any single experiment the only allowed values you can measure in the laboratory are the eigenvalues λ. But quantum mechanics is random, and so even with the same initial conditions, with the same starting wavefunction Ψ, one can have different outcomes. (The idea that somewhere there is unnoticed clockwork that deterministically determines the particular outcome is known as *hidden variables theory*. Bell's inequality has squashed the simplest and most appealing, at least, hidden variables theories. But no more on foundational issues.) The probability of measuring any particular value λ is given by $|c_\lambda|^2$.

In order to find the coefficient c_λ, called *amplitudes* in quantum mechanics, one needs to take a dot product, also known as an inner or scalar product. Novices get the idea that a dot product is between two vectors, but it isn't that simple. If you have two real-valued vectors, $\vec{v} = (v_1, v_2, v_3)$ and $\vec{w} = (w_1, w_2, w_3)$, one might write the dot product $\vec{v} \cdot \vec{w} = v_1 w_1 + v_2 w_2 + v_3 w_3$. But this definition is unsatisfactory for complex-value vectors, especially since we want the inner product to be positive definite (the inner product of any vector with itself to be a real, nonnegative number and is zero if and only if the vector itself is zero).

You're likely aware that the solution is to modify the dot product to be $v_1^* w_1 + v_2^* w_2 + v_3^* w_3$. This seems ad hoc at first, but mathematicians formalized the solution through the concept of *adjoint* vectors. The purpose of an adjoint vector is to map a vector onto a *scalar* (that is, a single real or complex number). A common way to denote the adjoint operation is through a raised 'dagger' or †. Thus if $\vec{v}$ is a vector, then $\vec{v}^\dagger$ is the adjoint.

Visually, it is helpful to represent vectors as column $(N \times 1)$ arrays, and adjoint vectors as row $(1 \times N)$ arrays:

$$\vec{v} = \begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix}, \quad \vec{v}^\dagger = \begin{pmatrix} v_1^* & v_2^* & v_3^* \end{pmatrix}, \tag{1.4}$$

where the complex conjugation in the adjoint guarantees that one has positive-definite magnitudes, that is, $\vec{v}^\dagger \cdot \vec{v}$ is real and positive if $\vec{v}$ is nonzero.

This convention for vectors and adjoint vectors is useful because it calls upon our notions of matrix multiplication: if $\mathbf{C} = \mathbf{AB}$, to get the i,jth element of $\mathbf{C}$ we multiply the ith row of $\mathbf{A}$ by the j column of $\mathbf{B}$. It also helps us because we can see immediately that

$$\vec{w}^\dagger \cdot \vec{v} = \left(\vec{v}^\dagger \cdot \vec{w}\right)^*, \tag{1.5}$$

an important technical requirement for inner products (consult a convenient linear algebra text, or a convenient mathematician, if you have questions about this).

While the concept of the adjoint clears up technical problems, notationally writing $\vec{w}$ and $\vec{v}^\dagger$ is difficult to distinguish, and writing out column and row vectors with their components is clunky. Therefore in the next section we bring up Dirac's clever notation.

1.2 Dirac's bra-ket notation

An alternate notional convention used by physicists (but not mathematicians) is Dirac's bra-ket notation. Rather than drawing an arrow over a vector $\vec{v}$, Dirac wrote it as a 'ket' $|v\rangle$. The adjoint vector $\vec{v}^\dagger$ he wrote as a 'bra' $\langle v|$. You should still think of kets as column vectors and bras as adjoint row vectors. But we now write the dot or inner product as $\langle v|w\rangle$ which, to my mind, is cleaner to see than $\vec{v}^\dagger \cdot \vec{w}$. For example, we can see that

$$\vec{v}^\dagger \vec{w} = \langle v|w\rangle = \begin{pmatrix} v_1^* & v_2^* & v_3^* \end{pmatrix} \begin{pmatrix} w_1 \\ w_2 \\ w_3 \end{pmatrix} = v_1^* w_1 + v_2^* w_2 + v_3^* w_3$$

correctly gives us the inner product, while

$$\begin{aligned} \vec{w}\vec{v}^\dagger = |w\rangle\langle v| &= \begin{pmatrix} w_1 \\ w_2 \\ w_3 \end{pmatrix} \begin{pmatrix} v_1^* & v_2^* & v_3^* \end{pmatrix} \\ &= \begin{pmatrix} v_1^* w_1 & v_2^* w_1 & v_3^* w_1 \\ v_1^* w_2 & v_2^* w_2 & v_3^* w_2 \\ v_1^* w_3 & v_2^* w_3 & v_3^* w_3 \end{pmatrix} \end{aligned} \tag{1.6}$$

does not.

We also write (1.5) as

$$\langle w|v\rangle = \langle v|w\rangle^*, \tag{1.7}$$

which we'll have frequent occasion to use.

So now given a set of orthonormal basis vector $\{|e_i\rangle\}$, we can easily write the orthonormality condition,

$$\langle e_i|e_j\rangle = \delta_{ij} \tag{1.8}$$

and the completeness identity

$$\sum_i |e_i\rangle\langle e_i| = \mathbf{1}, \tag{1.9}$$

where $\mathbf{1}$ is the unit matrix.

The Dirac notation allows us to easily distinguish between a representation-free vector, $|v\rangle$, and its components in some basis $\{|e_i\rangle\}$ given by $v_i = \langle e_i|v\rangle$. Indeed, the notation allows us to visually distinguish between a vector '$|something\rangle$' and a scalar '$c = \langle something|something\,else\rangle$', and draws out attention that the way we get a scalar from a vector is to take the inner product with an adjoint vector.

When I first aspired to be a physicist, but had no physics or mathematics, I saw the time-independent Schrödinger equation written as

$$H\Psi = E\Psi \tag{1.10}$$

which of course shed no light on the topic whatsoever. Nowadays I write the Schrödinger equation instead as

$$\hat{H}|\Psi\rangle = E|\Psi\rangle \tag{1.11}$$

where the notation clearly distinguishes between an operator $\hat{H}$, a vector $|\Psi\rangle$, and a scalar E.

Along with the Schrödinger equation we can rewrite our eigenvalue equation:

$$\hat{\mathcal{O}}|\Phi_\lambda\rangle = \lambda|\Phi_\lambda\rangle. \tag{1.12}$$

If the $\{|\Phi_\lambda\rangle\}$ form an orthonormal set, we write

$$\langle\Phi_\lambda|\Phi_{\lambda'}\rangle = \delta_{\lambda\lambda'} \tag{1.13}$$

and we can expand any vector in this orthonormal basis set

$$|\Psi\rangle = \sum_\lambda c_\lambda|\Phi_\lambda\rangle, \tag{1.14}$$

where the amplitudes c_λ are found through the inner product

$$c_\lambda = \langle\Phi_\lambda|\Psi\rangle. \tag{1.15}$$

As the probability to measure the value λ is $|c_\lambda|^2$ then after many measurements the average value of λ is

$$\begin{aligned}\sum_\lambda \lambda|c_\lambda|^2 &= \sum_\lambda \lambda c_\lambda^* c_\lambda = \sum_\lambda \lambda\langle\Psi|\Phi_\lambda\rangle\langle\Phi_\lambda|\Psi\rangle \\ &= \sum_\lambda \langle\Psi|\hat{\mathcal{O}}|\Phi_\lambda\rangle\langle\Phi_\lambda|\Psi\rangle = \langle\Psi|\hat{\mathcal{O}}|\Psi\rangle\end{aligned} \tag{1.16}$$

where I've used $\langle\alpha|\beta\rangle* = \langle\beta|\alpha\rangle$, the eigenvalue equation (1.12) and the completeness relation (1.9). The final result $\langle\Psi|\hat{\mathcal{O}}|\Psi\rangle$ is called the expectation value, a misleading name–it is it is not the most expected value, but simply the average. Hence it is sometimes written simply as $\langle\hat{\mathcal{O}}\rangle$, which indicates the average. It is this bracket notation for the average which inspired Dirac to invent his bra-ket, or bracket, notation for vectors.

Although the time-evolution of a quantum system will not be a major concern for us, it is an instructive topic to review. Starting from the time-independent Schrödinger equation,

$$\hat{H}|\psi_n\rangle = E_n|\psi_n\rangle, \tag{1.17}$$

one writes the general solution of the time-dependent equation

$$i\hbar\frac{\partial}{\partial t}|\Psi(t)\rangle = \hat{H}|\Psi(t)\rangle \tag{1.18}$$

by expanding, as usual, in the eigenstates:

$$|\Psi(t)\rangle = \sum_n c_n e^{iE_n t/\hbar}|\psi_n\rangle, \tag{1.19}$$

where one finds the coefficient c_n from the initial condition:

$$c_n = \langle\psi_n|\Psi(0)\rangle. \tag{1.20}$$

When students first learn about vectors, they commonly of them as simple lists (or a one-dimensional array) of numbers $\vec{v} = (v_1, v_2, v_3)$. But this is not the vector itself; this is a *representation* of a vector through its components v_i, which are complex numbers or *scalars*, in a particular basis. If we choose a different basis, the components change, though the vector itself does not.

The Dirac notation helps us to remember this distinction. $|v\rangle$ is the physical, *representation-free* vector. It is only when we choose a basis $\{|e_i\rangle\}$ that we can find the components $v_i = \langle e_i|v\rangle$.

Now the components of a vector are a necessarily evil, because we humans and our numerical servants computers can really only compute with scalars. But by making clear the distinction between a vector and its components in a particular basis, it helps to free us to choose a different basis, and to transform one from basis to another.

So: suppose we start with the components of a vector $|v\rangle$ in some basis $\{|e_i\rangle\}$, that is $v_i = \langle e_i|v\rangle$. Further suppose we have a second basis, $\{|f_\alpha\rangle\}$, which yields different components $v'_\alpha = \langle f_\alpha|v\rangle$. (Note: one can and should employ notation to emphasize and clarify ideas; for example, as here, using lower-case latin letters $i, j, \ldots$ for the first basis and lower-case greek letters $\alpha, \beta, \ldots$ for the second. You'll see this strategy several more times in this book.) We assume all bases are orthonormal (see the exercises for hints on how to deal with non-orthonormal bases), so that the standard completeness relation (1.9) also holds. We easily derive the unitary transformation from one basis to another by inserting the completeness relation:

$$v'_\alpha = \langle f_\alpha|v\rangle = \langle f_\alpha|\left(\sum_i |e_i\rangle\langle e_i|\right)|v\rangle = \sum_i \langle f_\alpha|e_i\rangle\langle e_i|v\rangle = \sum_i U_{\alpha i} v_i, \tag{1.21}$$

where

$$U_{\alpha i} = \langle f_\alpha|e_i\rangle \tag{1.22}$$

is the unitary transformation that takes us from one basis to another. You may remember that the columns, and separately the rows, of a unitary matrix form an orthonormal set of vectors. A useful interpretation of the elements of a unitary matrix are the components of a set of (basis) vectors $\{|e_i\rangle\}$ in another basis $\{|f_\alpha\rangle\}$; this is exactly what (1.22) means.

With the Dirac notation in hand, we can easily accomplish many important tasks.

Example. Given an orthonormal basis that satisfies the completeness relation, the unitarity of (1.22) becomes nearly tautological:

$$\begin{aligned}\left(\mathbf{U}\mathbf{U}^\dagger\right)_{\alpha\beta} &= \sum_i U_{\alpha i}U^*_{\beta i} = \sum_i \langle f_\alpha|e_i\rangle\langle f_\beta|e_i\rangle^* \\ &= \sum_i \langle f_\alpha|e_i\rangle\langle e_i|f_\beta\rangle = \langle f_\alpha|f_\beta\rangle = \delta_{\alpha\beta}. \end{aligned} \tag{1.23}$$

Example. We can derive a lemma: *Inner products are independent of basis.* Although we write $\langle v|w\rangle$ for an inner product, in practice we need to carry it out in a basis, which we becomes obvious by inserting a completeness relation:

$$\langle v|w\rangle = \sum_i \langle v|e_i\rangle\langle e_i|w\rangle = \sum_i v_i^* w_i. \tag{1.24}$$

But now let's insert two more completeness relations:

$$\begin{aligned}\langle v|w\rangle &= \sum_i \langle v| \sum_\alpha |f_\alpha\rangle\langle f_\alpha|e_i\rangle\langle e_i| \sum_\beta |f_\beta\rangle\langle f_\beta|w\rangle \\ = \sum_\alpha \langle v|f_\alpha\rangle \sum_\beta \sum_i \langle f_\alpha|e_i\rangle\langle e_i|f_\beta\rangle\langle f_\beta|w\rangle &= \sum_\alpha v'^*_\alpha U_{\alpha i}U^*_{\beta i}w'_\beta \\ &= \sum_{\alpha\beta} v'^*_\alpha \delta_{\alpha\beta} w'_\beta = \sum_\alpha v'^*_\alpha w'_\alpha, \end{aligned} \tag{1.25}$$

where I used the unitaritary of $\mathbf{U}$. Hence we see we can take the inner product in any basis and get the same answer. A fancy phrase is the inner product is *invariant* under a change of basis.

1.3 The matrix formulation of quantum mechanics

By realizing that the 'real' vector is $|v\rangle$ and not its components helps us to an important insight in quantum mechanics. In introductory quantum mechanics we learn the Born probabilistic interpretation of the wavefunction, that $|\Psi(x)|^2$ is the probability to find a particle at point x (more technically, it is the probability density, and $|\Psi(x)|^2 dx$ is the probability to find a particle in a range dx about x).

But the wavefunction is $|\Psi\rangle$ and its *representation* in coordinate space is $\Psi(x) = \langle x|\Psi\rangle$. This is a difficult point, because it is difficult to grasp what

the basis vectors $|x\rangle$ are. (In fact, we can't really grasp them, because they are vectors, and to represent them means choosing a basis...) The most accurate description is that the $\{|x\rangle\}$ are the eigenfunctions of the position operator $\hat{x}$, that is, $\hat{x}|x\rangle = x|x\rangle$. Because they are continuous-valued states, their orthonormality relation is given not by the Kronecker δ but by the Dirac δ-distribution: $\langle x|x'\rangle = \delta(x - x')$.

There are two very important ideas that come out this, so pay attention. The first is critical to a broader understanding of quantum mechanics (although not so much to the topic of this book); the second is absolutely critical to understanding the occupation representation.

The first idea is the *generalized statistical interpretation*. Under the Born interpretation, $|\Psi(x)|^2 = |\langle x|\Psi\rangle|^2$ is the probability to find the particle with wavefunction $|\Psi\rangle$ in the state $|x\rangle$, which we colloquially state as 'the probability to find the particle at position x.' But this is true for any basis state $|\phi\rangle$, so that $|\langle\phi|\Psi\rangle|^2$ is the probability to find the particle with wavefunction $|\Psi\rangle$ in the state $|\phi\rangle$. In particular, if $|\phi\rangle$ is an eigenstate of a operator representing a measurement, then this is also the probability to obtain the eigenvalue (measurement) corresponding to $|\phi\rangle$.

The second idea is to emphasize, once again, that $\Psi(x)$ is not the real wavefunction, but that $|\Psi\rangle$ is, and that we can write the components of $|\Psi\rangle$ in any useful basis set, $\{\phi_\lambda\}$, and that the representation of the wavefunction in this basis,

$$|\Psi\rangle = \sum_\lambda |\phi_\lambda\rangle\langle\phi_\lambda|\Psi\rangle = \sum_\lambda c_\lambda|\phi_\lambda\rangle \tag{1.26}$$

is just as *real* as the coordinate space representation.

So, so example, the Fourier transform of a wavefunction,

$$\tilde{\Psi}(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{ikx}\Psi(x)dx \tag{1.27}$$

is really just a unitary transformation from coordinate space to wavenumber space. We can write this as

$$\tilde{\Psi}(k) = \langle k|\Psi\rangle = \sum_x \langle k|x\rangle\langle x|\Psi\rangle \tag{1.28}$$

where I treat the integral over x the same as a sum "$\sum_x$." (In an abstract sense, one can treat states with continuous labels, such as $|x\rangle$, and states with discrete labels, $|\phi_n\rangle$, in nearly the same fashion. There are of course important technical differences; you sum over the latter and integrate over the former; the latter's orthonormality is given by a Kronecker-δ and the former by a Dirac-δ. Consult an advanced quantum textbook for more details.)

You can see that the element of the unitary transformation is $\langle k|x\rangle = \exp(ikx)/\sqrt{2\pi}$. More importantly, however, the Fourier transformed wavefunction $\tilde{\Psi}(k)$ is just as 'true' and no less original than the coordinate space wavefunction $\Psi(x)$.

I emphasize this point because this text revolves around an even more abstract representations of wavefunctions, one that nonetheless is just as 'true' as the coordinate-space representation.

We can now turn to the idea of a *function space*. We can treat functions as vectors in an infinite-dimensional vector space. The concept of an infinite-dimensional space, to say nothing of functions as vectors is nonintuitive and even overwhelming at first, but if one pays attention to the rigorous mathematical definition of an abstract vector space, then functions can indeed act as vectors. I won't go into rigorous details, but the important idea is that a linear combination of vectors $\alpha\vec{v} + \beta\vec{w}$ is also a vector–and a linear combination of functions $\alpha f(x) + \beta g(x)$ is also a function.

We also can introduce an inner product for functions:

$$\langle f|g\rangle = \int f^*(x)g(x)dx. \tag{1.29}$$

An inner product must have certain properties (linearity, positive-definitiveness, and so on) which this definition satisfies. But it also makes intuitive sense; in particular, if you have any experience with numerical quadrature (calculation of definite integrals), then you know that one discretizes a function $f(x)$ as an array $f(x_i)$ and the integral (1.29) is approximately

$$\int f^*(x)g(x)dx \approx \sum_i f^*(x_i)g(x_i)\Delta x. \tag{1.30}$$

Aside from the lattice spacing Δx, this is very reminiscent of the standard dot product for finite vectors. We can also arrive at this definition by simply using the completeness relation

$$\langle f|g\rangle = \sum_x \langle f|x\rangle\langle x|g\rangle \tag{1.31}$$

and noting that for a continuous variable like x we replace the sum by an integral, and remembering that $\langle f|x\rangle = \langle x|f\rangle^* = f^*(x)$, we arrive at (1.29).

Now let's go back and look again at expanding a wavefunction $|\Psi\rangle$ in a set of discrete basis functions ϕ_λ. We wrote this down formally before, but now we can see how to evaluate the inner products:

$$\langle\phi_\lambda|\Psi\rangle = \sum_x \langle\phi|x\rangle\langle x|\Psi\rangle = \int \phi_\lambda^*(x)\Psi(x)dx. \tag{1.32}$$

Of course, we could evaluate this equally well in Fourier space

$$\langle\phi_\lambda|\Psi\rangle = \sum_k \langle\phi|k\rangle\langle k|\Psi\rangle = \int \tilde{\phi}_\lambda^*(k)\tilde{\Psi}(k)dk \tag{1.33}$$

which might be more convenient in some cases.

With this experience under our belts, let us also return to the time-independent Schrödinger equation:

$$\hat{H}|\Psi\rangle = E|\Psi\rangle. \tag{1.34}$$

While this now makes mathematical sense, as written it does not illuminate any method of solution. Again, this is because as humans we are not very good with vectors and operators; we are better with scalars (numbers); computers are even more dependent on scalars. To convert to scalars, we take the inner product with an convenient basis vector $|\phi_\lambda\rangle$ (which might even be the coordinate basis vector $|x\rangle$:

$$\langle\phi_\lambda|\hat{H}|\Psi\rangle = E\langle\phi_\lambda|\Psi\rangle. \tag{1.35}$$

To go further, we strategically insert a completeness relation:

$$\sum_\mu \langle\phi_\lambda|\hat{H}|\phi_\mu\rangle\langle\phi_\mu|\Psi\rangle = E\langle\phi_\lambda|\Psi\rangle. \tag{1.36}$$

Now everything here has been converted to scalars. We can define

$$H_{\lambda\mu} = \langle\phi_\lambda|\hat{H}|\phi_\mu\rangle, \tag{1.37}$$

which is the *matrix element* of the operator $\hat{H}$ in the basis $\{|\phi_\lambda\}$. Matrix elements are very important in quantum mechanics–among other things they allow us to carry out actual and not just formal calculations–and computing them will be a central concern to us.

Why do we call $H_{\lambda\mu}$ a matrix elements? Recalling that we expand

$$|\Psi\rangle = \sum_\lambda c_\lambda|\phi_\lambda\rangle, \tag{1.38}$$

with $c_\lambda = \langle\phi_\lambda|\Psi\rangle$, we now have turned the abstract Schrödinger equation into a matrix equation:

$$\sum_\mu H_{\lambda\mu}c_\mu = Ec_\lambda, \tag{1.39}$$

a formulation suitable for numerical solution by a computer.

Back at the dawn of quantum mechanics, Schrödinger developed his wave mechanics and Heisenberg his matrix mechanics. It was our friend Dirac who showed the two were equivalent. If $\hat{H}$ started life as a differential operator, it can be converted to matrix form by (1.37). Specifically, we can even write this in integral form:

$$\begin{aligned} H_{\lambda\mu} = \langle\phi_\lambda|\hat{H}|\phi_\mu\rangle &= \sum_x\sum_{x'}\langle\phi_\lambda|x\rangle\langle x|\hat{H}|x'\rangle\langle x'|\phi_\mu\rangle \\ &= \int\int \phi^*_\lambda(x)H(x,x')\phi_\mu(x')dx\,dx'. \end{aligned} \tag{1.40}$$

If, as so often is the case, $\hat{H}$ is a *local* operator (just functions of x and low derivatives of x), we just write this in familiar form

$$H_{\lambda\mu} = \int \phi^*_\lambda(x)\hat{H}\phi_\mu(x)dx, \tag{1.41}$$

with the implicit assumption $\hat{H}$ is a (local) operator in coordinate space.

I cannot stress enough the importance to our topic the concept of expanding a wavefunction in basis functions, and rewriting any differential equation as a matrix equation.

In the same way we could explicitly expand any vector in a basis, we can also expand any operator in a basis:

$$\hat{A} = \sum_{i,j} |e_i\rangle\langle e_i|\hat{A}|e_j\rangle\langle e_j| = \sum_{i,j} |e_i\rangle A_{ij}\langle e_j|. \tag{1.42}$$

The orientation of the bra and ket vectors help us see this is an operator.

Example. Given the unitary transformation (1.22) of a vector from one basis to another, we can easily derive the equivalent transformation of the matrix elements of an operator, that is, the unitary transformation of a matrix. For some operator $\hat{A}$, the matrix elements in the final basis are $A'_{\alpha\beta} = \langle f_\alpha|\hat{A}|f_\beta\rangle$ (here is another case where notation is important: I use primed quantities and Greek indices for objects in the final basis, and unprimed quantities and lowercase Latin indices for the initial basis) and inserting the completeness relation twice

$$A'_{\alpha\beta} = \langle f_\alpha| \sum_i |e_i\rangle\langle e_i|\hat{A} \sum_j |e_j\rangle\langle e_j|f_\beta\rangle = \sum_{ij} U_{\alpha i} A_{ij} U^*_{\beta j} \tag{1.43}$$

or in more compact matrix notation

$$\mathbf{A}' = \mathbf{U}\mathbf{A}\mathbf{U}^\dagger. \tag{1.44}$$

Example. We can prove that the trace of an operator is independent of the (orthonormal) basis, that is, the trace is *invariant* under a unitary transformation. Given an operator $\hat{A}$, for some orthonormal basis $\{|e_i\rangle\}$ the matrix elements are $A_{ij} = \langle e_i|\hat{A}|e_j\rangle$, and the trace is

$$\mathrm{tr}\mathbf{A} = \sum_i A_{ii} = \sum_i \langle e_i|\hat{A}|e_i\rangle. \tag{1.45}$$

Now suppose we are in a different basis, $\{|f_\alpha\rangle\}$. We can insert twice the completeness relation:

$$\mathrm{tr}\mathbf{A} = \sum_i \langle e_i| \sum_\alpha |f_\alpha\rangle\langle f_\alpha|\hat{A} \sum_\beta |f_\alpha\rangle\langle f_\alpha|e_i\rangle$$

$$= \sum_i \sum_{\alpha,\beta} \langle e_i|f_\alpha\rangle A'_{\alpha\beta}\langle f_\beta|e_i\rangle = \sum_i \sum_{\alpha,\beta} \langle f_\beta|e_i\rangle\langle e_i|f_\alpha\rangle A'_{\alpha\beta} \tag{1.46}$$

$$= \sum_{\alpha,\beta} \langle f_\beta|f_\alpha\rangle A'_{\alpha\beta} = \sum_{\alpha,\beta} \delta_{\alpha\beta} A'_{\alpha\beta} = \sum_\alpha A'_{\alpha\alpha} = \mathrm{tr}\mathbf{A}'. \tag{1.47}$$

You will have a chance to practice these kinds of derivations in the exercises at the end of the chapter.

1.4 Example: Diagonalization in a basis

The idea that solving a differential eigenvalue equation is equivalent to diagonalizing a matrix is a key concept. Therefore I'll work out an example in detail. Actually, I'll work out examples throughout the text, as we develop more and more technology.

For now let us consider a problem in one-dimensional quantum mechanics, the delta-function potential:

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} - \lambda\delta(x). \tag{1.48}$$

This is a standard problem in introductory quantum mechanics and can be solved analytically; it has one bound state with an energy $E = -m\lambda^2/2\hbar^2$ and an value $\langle x^2\rangle = \hbar^2/m\lambda$.

But we are going to find approximate solutions by diagonalizing. To do this we choose a basis $\{|n\rangle\}$ and compute matrix elements of the Hamiltonian, $H_{mn} = \langle m|\hat{H}|n\rangle$. We then find the eigenvalues and eigenvectors of $\mathbf{H}$. Because a function space is infinite-dimensional, one must truncate the basis and thus the Hamiltonian matrix. From the variational theorem, see section 1.7, such a truncation is guaranteed to be an upper bound.

Almost always a basis is found by using the eigenstates of some other, simpler Hamiltonian. For this particular example we'll use a particle in a box between $x = -L/2$ and $x = L/2$. The basis eigenstates are sine and cosine functions; the ones that interest us here are the even functions $\phi_n(x) = \langle x|n\rangle = \sqrt{2/L}\cos((2n+1)\pi x/L), n = 0, 1, 2, \ldots$, which vanish at the walls of the box. (For this box there are also sine eigenfunctions, but they vanish at the origin and so do not "see" the potential.) The matrix elements of the kinetic energy are diagonal in the basis of sines and cosines (which is why I choose it; for a general basis the kinetic energy matrix elements will *not* be diagonal):

$$\left\langle m \left| -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} \right| n \right\rangle = \delta_{mn}\frac{\hbar^2\pi^2(2n+1)^2}{2mL^2}. \tag{1.49}$$

The matrix element of the delta-function potential between any two of these is simple:

$$\langle m\,|-\lambda\delta(x)|\,n\rangle = -\lambda\frac{2}{L}, \tag{1.50}$$

independent of m and n.

(At the risk of repeating myself, let me emphasize that these matrix elements depend on the choice of basis; later on, in section 3.4 I'll give the matrix elements of the kinetic energy and δ-potential but in a basis of harmonic oscillator eigenfunctions, with very different individual values. Nonetheless, in the limit of large basis dimension, the ground state energy and other quantities converge to the same result.)

To further simplify things, dimensional analysis tells us that the basic unit of length is $\hbar/m\lambda$ and the basic unit of energy is $m\lambda^2/\hbar^2$. Therefore let

$$L = L_0 \frac{\hbar^2}{m\lambda} \tag{1.51}$$

where L_0 is a dimensionless parameter.

Then the matrix element is

$$H_{mn} = \frac{m\lambda^2}{\hbar^2} \times \left(-\frac{2}{L_0} + \delta_{mn} \frac{\pi^2}{2L_0^2} (2n+1)^2 \right). \tag{1.52}$$

Now you can have fun: choose some value of L_0. For practical reasons, you have to truncate and choose a maximal value of n. With this truncated Hamiltonian in hand, you can run it through an eigensolver, for example in Mathematica, MatLab, Fortran or C.

I'll choose a couple of cases. To begin with, I'll let $L_0 = \pi^2/2$; as we'll see later on, this is motivated by variational theory.

If we take only the lowest state, $n = 0$, then $E \approx H_{00} = -(2/\pi^2) m\lambda^2/\hbar^2 = -0.2026 m\lambda^2/\hbar^2$, a mediocre approximation to the exact ground state of $-0.5 m\lambda^2/\hbar^2$. Now let's take $n = 0, 1$. The matrix is now

$$\frac{2}{\pi^2} \frac{m\lambda^2}{\hbar^2} \begin{pmatrix} -1 & -2 \\ -2 & 7 \end{pmatrix}, \tag{1.53}$$

and the ground state energy is $(-6 + 4\sqrt{5})/\pi^2 \times (m\lambda^2/\hbar^2) = -0.2983 m\lambda^2/\hbar^2$, not a vast improvement, but an improvement nonetheless.

We can continue numerically by including more states. Figure 1.1 show the results of finding the ground state energy as one increases the number of basis states from 1 to 500. In order to better examine the convergence, Figure 1.2 is a log-log plot of the difference ΔE between the numerical energy and the exact ground state energy as a function of the size of the basis. Also shown are different box sizes L_0. Notice that as the box size increases from $5 (\approx \pi^2/2)$ the energy starts out higher for one state, but then becomes lower. Thus Fig. 1.1 , 1.2 illustrate how complicated convergence can be. Depending on the basis chosen, one can start at a lower value, but may not ultimately converge to the correct result.

By diagonalizing we get not only information about the energies, but also the eigenstates themselves. By solving

$$\sum_n H_{mn} v_n = E v_n,$$

we can expand the wavefunction in coordinate space:

$$\psi(x) = \langle x|\psi\rangle = \sum_n v_n \langle x|n\rangle = \sum_{n=0}^{n_{\max}} v_n \sqrt{\frac{2}{L}} \cos\left(\frac{(2n+1)\pi x}{L} \right). \tag{1.54}$$

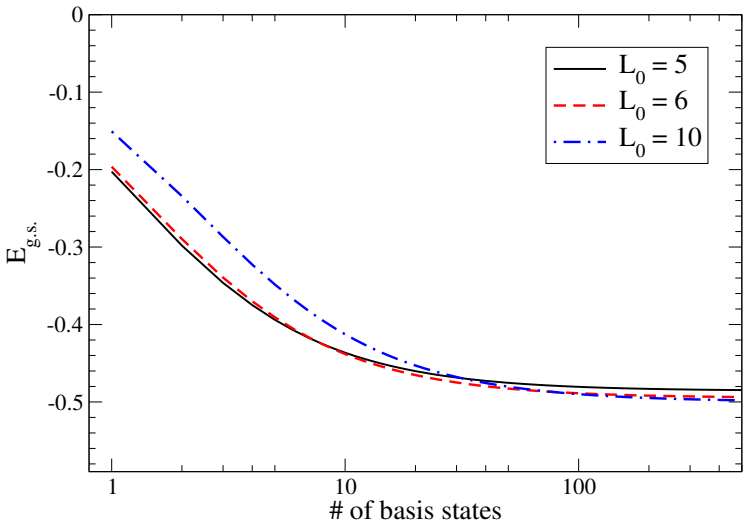

Figure 1.1: Convergence of the ground state energy for the δ-potential as a function of the number of basis states and of the size of the box L_0 (in units of $\hbar^2/m\lambda$.

This I illustrate in Figure 1.3, where for a box of size $L_0 = 7$, I show the approximate ground state wavefunctions for 1, 10, and 100 basis states. For comparison I also show the exact ground state wavefunction, $\psi(x) = (\sqrt{m\lambda}/\hbar)\exp(-m\lambda|x|/\hbar^2)$. By the time we get to 100 basis states, the cusp at $x = 0$ is well reproduced, and the only deviation from the exact answer is at the tails: the numerical wavefunction must vanish at the box boundaries.

1.5 Copenhagen, commutators, and conservation laws

You undoubtedly have heard the statement 'it is impossible to know simultaneously the position and momentum of a particle' as a fundamental principle of quantum mechanics. But what does that mean in terms of our mathematical framework?

Suppose we have a particle with a wavefunction $|\Psi\rangle$. If we measure its position, that measurement is represented by the position operator $\hat{x}$ with eigenvalue equation $\hat{x}|x\rangle = x|x\rangle$, and the probability to find the particle at position x is given by $|\langle x|\Psi\rangle|^2$. *Immediately thereafter* the particle is now found in a new state $|\Psi'\rangle = |x\rangle$. In the Copenhagen interpretation of quantum mechanics one says the wavefunction has 'collapsed' from $|\Psi\rangle$ to $|x\rangle$. If you don't like this idea, and you aren't alone in this, you can think of the Copenhagen interpretation as shorthard for some other, subtler process, such as decoherence.

What does it mean to say the particle is in the state $|x\rangle$? It means that

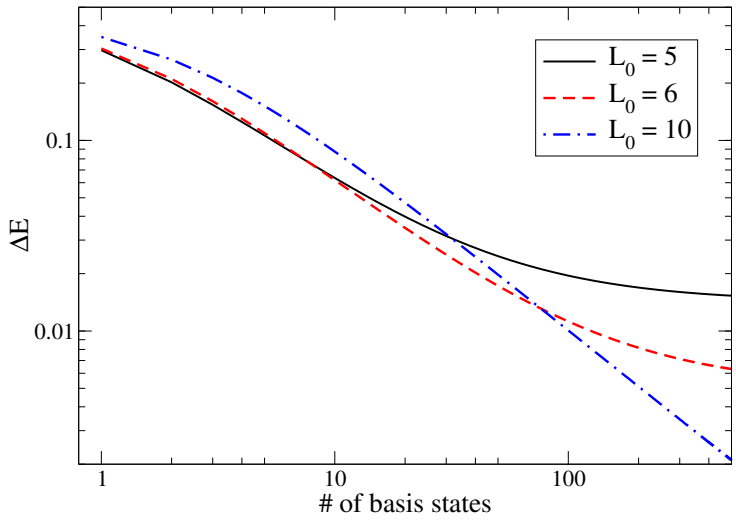

Figure 1.2: Error of the numerical ground state energy for the δ-potential as a function of the number of basis states and of the size of the box L_0 (in units of $\hbar^2/m\lambda$. ΔE is $E_{\text{numerical}} - E_{\text{exact}}$.

if you measure the position immediately again, you will find the particle still at position x and not some other position x'; quantum mechanics is weird, but not *that* weird. A little more formally, the probability to find the particle at position x' is $|\langle x'|\Psi'\rangle|^2 = |\langle x'|x\rangle|^2$ which is zero unless $x' = x$.

(Even more formally: $|\langle x'|\Psi'\rangle|^2 = |\delta(x'-x)|^2$ and one needs to integrate over x and x' to make everything finite. It's unfortunate that in quantum mechanics some of the most intuitive situations, such as measuring position and momentum, have such mathematical complications. I take it as more evidence that our Olduvai-honed intuition is not trustworthy when it comes to the subatomic world.)

So, once you have made a measurement and collapsed a state into an eigenstate of a measurement operator, you can measure over and over and you will now get 100% of the time the same eigenvalue–which is another way of saying the uncertainty of the measurement is zero.

(Comment: one has to make the measurement immediately, which here means such a short period of time the wavefunction has not had time to evolve under the time-dependent Schrödinger equation.)

If you finally get tired of measuring the position over and over again, you might switch to measuring the momentum with operator $\hat{p}$ and eigenvalues p and eigenstates $|p\rangle$. The same procedure applies: the probability to measure p is $|\langle p|\Psi'\rangle|^2$. But since we are in the eigenstate $|x\rangle$ from the previous measurement, this is $|\langle p|x\rangle|^2$, which because $\langle p|x\rangle \approx \exp(ipx/\hbar)$, is constant and independent of p. In other words, you can take on any momentum value, and the uncertainty is the largest possible.

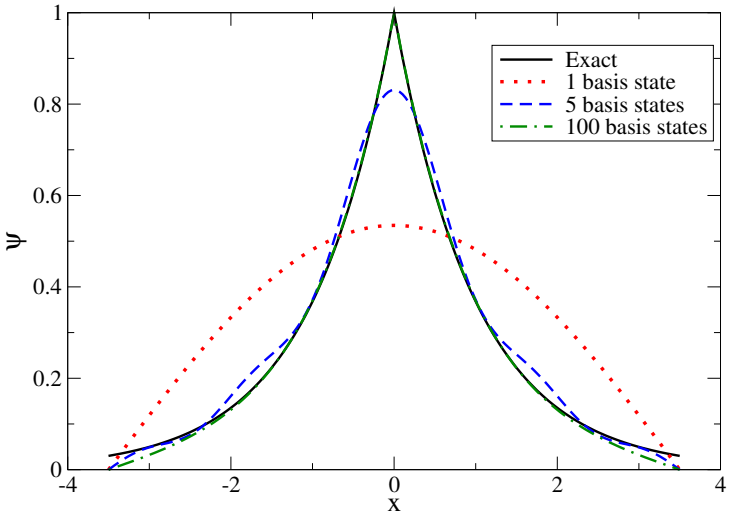

Figure 1.3: Convergence of the ground state wavefunction for the δ-potential, for a box size $L_0 = 7$, including 1, 5, and 100 states. Also shown is the exact ground state wavefunction.

You are now in the state $|\Psi''\rangle = |p\rangle$. You can measure momentum over and over and you will now always get the same value p, etc. .

If you measure position, again, however, the probability to measure any x' will be $|\langle x'|\Psi''\rangle|^2 = |\langle x'|p\rangle|^2$, which means now that you could find yourself at *any* x' independent of your original x. And now if you measure position over and over again you will get over and over again the same value x'.

And so on.

The reason all this happens is because it is impossible to have a state $|\Psi\rangle$ that is a *simultaneous eigenstate* of both the position operator $\hat{x}$ and the momentum operator $\hat{p}$. And it is impossible because $\hat{x}$ and $\hat{p}$ are not simultaneously diagonalizable: there is no basis in which both $\hat{x}$ and $\hat{p}$ are both diagonal.

How do we know this? Because the commutator of $\hat{x}$ and $\hat{p}$:

$$[\hat{x}, \hat{p}] = \hat{x}\hat{p} - \hat{p}\hat{x} = i\hbar \tag{1.55}$$

is nonzero. (You prove: if two operators are both diagonal, then they commute.) Although the commutator appears to be an abstract and even spurious construct, we'll later see that commutator play a central role in the occupation representation, so pay attention!

Theorem (which I won't prove here): If two operators commute (i.e., their commutator vanishes), then it is possible to have simultaneous eigenfunctions.

This leads to Noether's theorem. Classically, if the Hamiltonian of a system is invariant under some operation, such as translation in time or space, or rotation, then there is some conserved quantity. So: if the Hamiltonian is constant (invariant) in time, then energy is conserved; if it is translationally

invariant, then linear momentum is conserved; if rotationally invariant, then angular mometum conserved; and so on.

For the quantum version of Noether's theorem, consider an operator $\hat{A}$ which commutes with the Hamiltonian $\hat{H}$. In that case, it is possible to have a state $|E, a\rangle$ that is a simultaneous eigenstate of both $\hat{H}$ and $\hat{A}$. Then, even as this wavefunction evolves under the time-dependent Schrödinger equation, it will always remain 100% with eigenvalue a. Often we call a conserved quantity such as a a *quantum number*. This is especially true when it is indexed by a simple number such as integers. The examples that will concern us most are parity π, total angular momentum J, and the z-component of angular momentum $J_z = M$.

Some quantum numbers are only partially conserved. For example, in nuclear physics, isospin is approximately conserved, but is broken at the level of a few percent. Parity is broken at only a part in a million. If a quantum number is only partially conserved, it is often still a useful concept.

1.6 Quantum mechanics in three dimensions

While one can easily write down a Hamiltonian for one particle in three dimensions,

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(x, y, z), \tag{1.56}$$

in general the differential equations are coupled and intractable.

The only cases we can solve analytically are those where we can–you may have guessed it–reduce the problem to a set of three one-dimensional problems. These cases are of particular importance because they will provide important examples, or paradigms, for the occupation representation.

Let's start with a special case: the spherically symmetric harmonic oscillator. In cartesian coordinates, the Hamiltonian is

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) + \frac{1}{2}m\omega^2\left(x^2 + y^2 + z^2\right) \tag{1.57}$$

which we rearrange as

$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega^2 x^2\right) + \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial y^2} + \frac{1}{2}m\omega^2 y^2\right) + \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial z^2} + \frac{1}{2}m\omega^2 z^2\right) = \hat{H}_x + \hat{H}_y + \hat{H}_z. \tag{1.58}$$

Now we invoke separation of variables and assume a *product wavefunction*:

$$\Psi(x, y, z) = \psi_1(x)\psi_2(y)\psi_3(z). \tag{1.59}$$

Separation of variables means that we reduce the original problem in three variables

$$\left(\hat{H}_x + \hat{H}_y + \hat{H}_z\right)\psi_1(x)\psi_2(y)\psi_3(z) = E\psi_1(x)\psi_2(y)\psi_3(z) \tag{1.60}$$

to three independent problems each with one variable:

$$\begin{aligned} \hat{H}_x\psi_1(x) &= E_x\psi_1(x); \\ \hat{H}_y\psi_2(y) &= E_y\psi_2(y); \\ \hat{H}_z\psi_3(z) &= E_z\psi_3(z). \end{aligned} \tag{1.61}$$

Each of ψ_1, ψ_2, ψ_3 are the well-known 1-D harmonic oscillator eigensolutions, and the energies $E_x = \hbar\omega(n_x + 1/2)$, etc, so that the total energy is $E = \hbar\omega(N + 3/2)$, $N = n_x + n_y + n_z = 0, 1, 2, \ldots$. What we want to take away from this is not the particular solution, however, but how the 3-D wavefunction is a product of one-variable functions.

Luckily for us, the same principle continues to hold for the general case when the potential is rotationally invariant, that is, when we go from cartesian x, y, z coordinates to spherical r, θ, ϕ coordinates and the potential $V(r, \theta, \phi) = V(r)$ only. Although the details are slightly messier, and so I skip over them, we can apply separation of variables again

Because we know what the answer will be, we write a separable *ansatz* for the wavefunction in spherical coordinates:

$$\psi(r, \theta, \phi) = R(r)Y_{\ell m}(\theta, \phi) \tag{1.62}$$

where $Y_{\ell m}$ is of course the spherical harmonic. (For a marginally less brief discussion, see the Appendix.) Then

$$\nabla^2\psi = \nabla^2 R(r)Y_{\ell m}(\theta, \phi) = \left(\frac{1}{r}\frac{\partial}{\partial r}r\frac{\partial}{\partial r}R(r)\right)Y_{\ell m}(\theta, \phi) - R(r)\frac{\ell(\ell+1)}{r^2}Y_{\ell m}(\theta, \phi). \tag{1.63}$$

With this in hand we can factor out the $Y_{\ell m}$ leaving the Schrödinger equation for the radial part,

$$-\frac{\hbar^2}{2m}\frac{1}{r}\frac{\partial}{\partial r}r\frac{\partial}{\partial r}R(r) + \frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{r^2}R(r) + V(r)R(r) = ER(r), \tag{1.64}$$

or, if as usual, we make the substitution $R(r) = u(r)/r$, we get the standard radial Schrödinger equation,

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial r^2}u(r) + \frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{r^2}u(r) + V(r)u(r) = Eu(r). \tag{1.65}$$

We've successfully reduced a three-dimensional differential equation to a one-dimensional differential equation. Almost. There is a price to be paid: we must solve this equation separately for each value of $\ell = 0, 1, 2, \ldots$, so what we have done is to replace a single three-dimensional differential equation with an infinite number of different one-dimensional differential equations.

For some analytic cases such as the hydrogen atoms this poses no problem, but for a general potential (1.65) must be solved numerically, and solved numerically for each value of ℓ. Many times, however, one is only interested in a few low values of ℓ and so the price is a reasonable one to pay.

Sadly, we cannot always count on separation of variables to save us. Or, rather, a *single* product of one-variable (or even one-body) functions will not always yield exactly decoupled equations. Nonetheless nearly all of our approaches in many-body physics flow from this idea. We will either expand our solutions as *sums* of product wavefunctions, as we'll see in configuration-interaction calculations, or else choose a single product wavefunction as an approximate solution, which leads to mean-field approaches such as the Hartree-Fock and Gross-Pitaevskii approximations. These mean-field equations are effectively one-body problems but are nonlinear and must be solved iteratively, a different kind of price to pay for simplification. We will discuss such approaches in detail later on.

1.7 The variational theorem

Most quantum mechanical problems cannot be solved exactly, even with powerful computers. Therefore we must turn to approximate solutions. The two most powerful tools for dealing with approximations are perturbation theory (which we will not use here) and the variational theorem.

The Raleigh-Ritz variational theorem is: *Let $\hat{H}$ be some Hamiltonian with ground state energy E_0. Then for any wavefunction $|\Psi\rangle$,*

$$E = \frac{\langle\Psi|\hat{H}|\Psi\rangle}{\langle\Psi|\Psi\rangle} \geq E_0. \tag{1.66}$$

This theorem is quite easy to prove. (Do so.) It is also extremely useful when trying to find an approximate solution. Even if you don't know the ground state energy– or *especially* when you don't know the ground state energy–you can place an upper bound on it. If you have two wavefunctions, $|\Psi\rangle$ with energy E from (1.66) and $|\Psi'\rangle$ with energy E', whichever energy is lower is unequivocably better and whichever wavefunction gives the lower energy is better.

We can sharpen up this discussion. Suppose you have a trial wavefunction, often called an *ansatz*, which depends on a parameter, $|\Psi(\alpha)\rangle$. Then compute

$$E(\alpha) = \frac{\langle\Psi(\alpha)|\hat{H}|\Psi(\alpha)\rangle}{\langle\Psi(\alpha)|\Psi(\alpha)\rangle}. \tag{1.67}$$

The best choice of α minimizes the energy, which in turn leads to the variational condition

$$\frac{\partial}{\partial\alpha}E(\alpha) = 0. \tag{1.68}$$

One can of course generalize to multiple parameters and this will allow us to derive the Hartree-Fock approximation.

To illustrate, let me take a couple of examples in one dimension. The first relates to one we have already addressed: the δ-potential (1.48). We choose a gaussian *ansatz*:

$$\psi(x,\alpha) = \left(\frac{\alpha}{2\pi}\right)^{1/4} \exp\left(-\frac{1}{2}\alpha x^2\right) \tag{1.69}$$

which is always normalized. Then the trial energy $E(\alpha) = \langle \hat{H} \rangle$ is

$$E(\alpha) = \langle \hat{H} \rangle = \frac{\hbar^2 \alpha}{2m} - \lambda \sqrt{\frac{\alpha}{\pi}}. \tag{1.70}$$

Next, finding the extremum

$$\frac{\partial E(\alpha)}{\partial \alpha} = \frac{\hbar^2}{4m} - \frac{\lambda}{2} \frac{1}{\sqrt{\pi \alpha}} = 0 \tag{1.71}$$

one gets

$$\alpha_{\min} = \frac{4\lambda^2 m^2}{\hbar^4 \pi} \tag{1.72}$$

and

$$E(\alpha_{\min}) = -\frac{m\lambda^2}{\pi \hbar^2} \tag{1.73}$$

which is slightly greater than the exact ground state energy $-m\lambda^2/2\hbar^2$. Furthermore, the exact variance (square of the width) of the ground state is $\langle x^2 \rangle_{\text{exact}} = \hbar^4/2m^2\lambda^2$, but from our variational solution the variance is

$$\langle x^2 \rangle = \frac{1}{2\alpha_{\min}} = \frac{\pi \hbar^2}{8m^2\lambda^2} = \frac{\pi}{4} \langle x^2 \rangle_{\text{exact}}. \tag{1.74}$$

For a second example, consider a particle in one dimension with a quartic potential:

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{6} \lambda x^4. \tag{1.75}$$

This equation can be easily solved in coordinate space numerically, but we will tackle it variationally.

We assume a gaussian ansatz (1.69) and compute

$$E(\alpha) = \frac{\hbar^2 \alpha}{4m} + \lambda \frac{1}{8\alpha^2}. \tag{1.76}$$

Then taking the first derivative

$$\frac{\partial}{\partial \alpha} E(\alpha) = \frac{\hbar^2}{4m} - \lambda \frac{1}{4\alpha^3} = 0 \tag{1.77}$$

we find the extremum at a value

$$\alpha_{\min} = \left(\frac{\lambda m}{\hbar^2} \right)^{1/3} \tag{1.78}$$

and then

$$\frac{3}{8} \left(\frac{\hbar^4 \lambda}{m^2} \right)^{1/3}. \tag{1.79}$$

Numerically, the actually ground energy is $0.3676\hbar^{4/3}\lambda^{1/3}/m^{2/3}$. Furthermore, we can compute the ground state variance as

$$\langle x^2 \rangle = 0.5 \frac{\hbar^{2/3}}{\lambda^{1/3} m^{1/3}}, \tag{1.80}$$

while the numerically exact value is $0.522\hbar^{2/3}\lambda^{1/3}m^{1/3}$.

We will return to both the δ-potential and the quartic potential in Chapter 3.

1.8 Summary

What you should get from this chapter:

• The theory of quantum mechanics is worked out in a linear vector space; what we call *wavefunctions* should be thought of as abstract vectors, $|\psi\rangle$, where Dirac's bra-ket notation is a useful convention., particularly for inner products.

• The usual coordinate-space representation of a wavefunction is found by projecting onto a basis, $\psi(x) = \langle x|\psi\rangle$. But projection onto *any* basis is just as valid. This includes projection onto a linear function space spanned by (typically orthonormal) basis functions, $|\phi_n\rangle$, so that $\psi_n = \langle \phi_n|\psi\rangle$.

• Projection of vectors onto a discrete basis allows one to develop the matrix formulation of quantum mechanics. Solving the time-independent Schrödinger equation is now equivalent to diagonalizing (finding the eigenvalues and eigenvectors) of a matrix. Other important quantities, such as expectation values and transition amplitudes, can also be recast in terms of matrix elements. The computation of matrix elements is a fundamental topic in many-body theory.

• The variational principle is a useful tool for approximation in quantum mechanics.

• Another useful concept in quantum mechanics is, whenever possible, to break a multi-dimensional problem into separate one-dimensional problems, for example using a product *ansatz*. Sometimes, for example in three-dimensional quantum mechanics with a rotationally invariant potential, this can be done exactly. In future work we won't be able to do this exactly, but we will still find product wavefunctions a powerful guiding principle.

1.9 Exercises

(1.1) Prove for any two operators $\hat{A}, \hat{B}$ that trace $(\hat{A}\hat{B})$ = trace $(\hat{B}\hat{A})$.

(1.2) Prove that the trace of an operator is the sum of its eigenvalues and the determinant of an operator is the product of its eigenvalues. (Assume the operator is, if not Hermitian, diagonalizable).

(1.3) Show that it is plausible, at least, that

$$\mathrm{tr} \ln \hat{A} = \ln \det \hat{A}. \tag{1.81}$$

Hint: assume $\hat{A}$ is diagonalizable. In an advanced chapter we'll have use for this identity.

(1.4) Derive the matrix eigenvalue equation from a variational principle. Hint: For an operator $\hat{A}$, we want to find a vector $|\psi\rangle$ that is an extremum. To do so, we expand in an orthonormal basis $\{|n\rangle\}$, that is, $|\psi\rangle = \sum_n v_n|n\rangle$. Assume the v_n are real. Compute $\langle\psi|\psi\rangle$ and $\langle\psi|\hat{H}|\psi\rangle$ in terms of the components v_n and the matrix elements $H_{mn} = \langle m|H|n\rangle$. Note that even though the basis is orthonormal, we cannot assume that $|\psi\rangle$ is normalized. Therefore we cannot just minimize $\langle\psi|\hat{H}|\psi\rangle$; instead we have to add $\langle\psi|\psi\rangle = 1$ as a constraint. The way we do this is through Lagrange multipliers (consult a suitable mathematical methods text if you are unfamiliar with this concept) and so minimize $\langle\psi|\hat{H}|\psi\rangle - E\langle\psi|\psi\rangle$ with respect to v_n. You should regain the matrix eigenvalue equation with the Lagrange multiplier E now becoming the energy. We will use a similar method later on deriving the Hartree-Fock equations.

(1.5) Now consider an nonorthogonal basis, that is a basis $\{|\mu\rangle\}$ such that $\langle\mu|\nu\rangle = S_{\mu\nu}$ which is not the unit matrix. As long as the basis space spans the space $\mathbf{S}$ will be invertible. Now let's tackle some related problems:

(a) Prove that all the eigenvalues of $\mathbf{S}$ are real and positive, that is, $\mathbf{S}$ is positive definite. To do this you only have to show that for any set of components v_μ, that

$$\sum_{\mu\nu} v_\mu^* S_{\mu\nu} v_\nu > 0.$$

(b) Suppose we want to expand a vector in this basis, $|\psi\rangle = \sum_\nu v_\nu|\nu\rangle$. Deduce how to find the coefficients v_ν from the overlaps $\langle\mu|\psi\rangle$.

(c) To find the eigenvalues and eigenstates in this nonorthgonal basis, derive the generalized eigenvalue equation

$$\sum_\nu H_{\mu\nu} v_\nu = E \sum_\nu S_{\mu\nu} v_\nu \tag{1.82}$$

(1.6) Consider the δ-potential, with the Hamiltonian matrix elements given in (1.52). Show that for $m = n = 0$, this is minimized by $L_0 = \pi^2/2$.

(1.7) For the 3-D simple harmonic oscillator, the radial Schrödinger equation is

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + \frac{\hbar^2\ell(\ell+1)}{2mr^2} + \frac{1}{2}m\omega^2 r^2\right) u(r) = Eu(r). \tag{1.83}$$

It is well known that, for a given angular momentum ℓ the lower energy is $(\ell + 3/2)\hbar\omega$. Now make a variational estimate, using the exponential ansatz

$$\psi(r) = \sqrt{\alpha^3/2}r \exp\left(-\frac{\alpha}{2}r\right). \tag{1.84}$$

This are normalized by

$$\int_0^\infty u^2(r)dr = 1, \tag{1.85}$$

though of course you should check this yourself. Use this to find an upper bounds for the lowest energy for each ℓ.

For further work, try

$$\psi(r) = Cr^{\ell+1} \exp\left(-\frac{\alpha}{2}r\right), \tag{1.86}$$

for angular momentum ℓ; normalize and find the variational energy. Is it better than (1.84)?

(1.8) Diagonalize the simple harmonic oscillator Hamiltonian,

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2,$$

in the same basis we used for the δ-potential in section 1.4, that is, cosines and sines between $x = -L/2$ and $x = L/2$. For even functions this is $|n\rangle = \sqrt{2/L}\cos(2n+1)\pi x/L), n = 0, 1, 2, \ldots$. The matrix elements for the kinetic energy are easy, while the matrix elements $\langle m|x^2|n\rangle$ are tractable but more complicated integrals. As we did for the δ-potential, I recommend you rewrite $L = L_0 b$, where $b = \sqrt{\hbar/m\omega}$ is the oscillator length and L_0 is a dimensionless parameter. What value of L_0 gives you the minimum for the ground state energy, using just the $n = 0$ basis state? Now diagonalize numerically, truncating at some $n_{\max}$, and plot the convergence of the ground state energy as a function of the truncation. Try this for different values of L_0. As we did for the δ-potential, you should find that for larger L_0, the convergence is slower, but ultimately yields a better approximation to the 'exact' answer.

Look at the excited state energies as well. Try a scatter plot: the numerical energies versus the exact harmonic oscillator energies. You will get almost a straight line for a while, then a deviation. What happens at the deviation? Later in Chapter 3 we'll find that the rms width of the Nth excited state is $b\sqrt{N+1/2}$, so it makes sense that when the state starts touching the wall, that is when $L_0/2 \sim \sqrt{N}$, you'll get distortion, although keep in mind this is not an equality. Look at different values of L_0 and see if you have evidence for this behavior.

While you're at it, take the eigenvectors from your diagonalization and compute $\langle x^2\rangle$ for the ground state and for various excited states. The exact answer is $b^2(N+1/2)$.

Keep in mind the above was just for even functions; you could also do odd functions using $\sqrt{2/L}\sin(2n\pi x/L), n = 1, 2, \ldots$

Chapter 2

Introduction to many-body systems

> A person who never made a mistake never tried anything new. – *Albert Einstein*

2.1 Product wavefunctions

The starting point for quantum many-body systems is easy: write down a Hamiltonian $\hat{H}$ for N particles,

$$\hat{H} = \sum_{i=1}^{N} -\frac{\hbar^2}{2m}\nabla_i^2 + U(\vec{r}) + \sum_{i<j} V(\vec{r}_i - \vec{r}_j), \tag{2.1}$$

where $U(\vec{r})$ is some external potential, for example the Coulomb field of an atomic nucleus interacting on electrons, and where $V(\vec{r}-\vec{r}')$ is some interparticle interaction. I've also made the assumption, easily generalized, that the particles all have the same mass.

But now we want to solve the time-independent Schrödinger equation

$$\hat{H}\Psi(\vec{r}_1, \vec{r}_2, \vec{r}_3, \ldots, \vec{r}_N) = E\Psi. \tag{2.2}$$

Can we solve this as a differential equation? Keep in mind that even when solving for one particle in three-dimensions, we almost always reduce it via separation of variables to three one-dimensional problems. If one has two particles and no external field, one can go to relative coordinates and rewrite the problem as an effective one-body problem. There even exist methods for dealing with differential equations for three particles, such as Faddeev or hyperspherical harmonics. But these are specialized, difficult methods, and beyond a very few particles become intractably cumbersome.

Therefore we turn to expansion in a basis:

$$\Psi(\vec{r}_1, \vec{r}_2, \vec{r}_3, \ldots, \vec{r}_N) = \sum_\alpha c_\alpha \Phi_\alpha(\vec{r}_1, \vec{r}_2, \vec{r}_3, \ldots, \vec{r}_N). \tag{2.3}$$

What should we choose for our basis functions Φ_α? When in doubt, we fall back on what we know best–and we know best one-particle systems. Therefore we choose a product wavefunction, a many-body wavefunction constructed from the product of one-body wavefunctions:

$$\Phi(\vec{r}_1, \vec{r}_2, \vec{r}_3, \ldots, \vec{r}_N) = \phi_1(\vec{r}_1)\phi_2(\vec{r}_2)\phi_3(\vec{r}_3)\ldots\phi_N(\vec{r}_N). \tag{2.4}$$

Such a choice has several pleasant consequences.

First consider normalization. The normalization integral trivially factorizes:

$$\begin{aligned} &\int |\Phi(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N)|^2 d\vec{r}_1 d\vec{r}_1 d\vec{r}_2 \ldots d\vec{r}_N \\ &= \int |\phi_1(\vec{r}_1)|^2 d\vec{r}_1 \int |\phi_2(\vec{r}_2)|^2 d\vec{r}_2 \ldots \int |\phi_N(\vec{r}_N)|^2 d\vec{r}_N \end{aligned} \tag{2.5}$$

so that, if the single-particle functions ϕ_i are normalized, then the many-body product is automatically normalized too.

Orthogonality is also straightforward. Let the single-particle wavefunctions be not only normalized but also orthonormal, so that

$$\int \phi_a^*(\vec{r})\phi_b(\vec{r})d\vec{r} = \delta_{ab}, \tag{2.6}$$

Now consider two product wavefunctions, Φ_α and Φ_β, each for N particles. We can build each of them from any N of the single-particle states (in principle we have available an infinite number of singe-particle states ϕ_a, although in practice we take only a finite set); in fact, for now, we can even repeat the same single-particle wavefunctions.

For a specific example, consider 3 particles in an infinite well of width L. The single-particle basis functions are

$$\langle x|n\rangle = \phi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right). \tag{2.7}$$

So some possible product wavefunctions are:

$$\begin{aligned} \phi_1(x_1)\phi_1(x_2)\phi_1(x_3) &= \left(\frac{2}{L}\right)^{3/2} \sin\left(\frac{\pi x_1}{L}\right) \sin\left(\frac{\pi x_2}{L}\right) \sin\left(\frac{\pi x_3}{L}\right), \\ \phi_1(x_1)\phi_1(x_2)\phi_2(x_3) &= \left(\frac{2}{L}\right)^{3/2} \sin\left(\frac{\pi x_1}{L}\right) \sin\left(\frac{\pi x_2}{L}\right) \sin\left(\frac{2\pi x_3}{L}\right), \\ \phi_1(x_1)\phi_2(x_2)\phi_3(x_3) &= \left(\frac{2}{L}\right)^{3/2} \sin\left(\frac{\pi x_1}{L}\right) \sin\left(\frac{2\pi x_2}{L}\right) \sin\left(\frac{3\pi x_3}{L}\right), \\ \phi_5(x_1)\phi_{11}(x_2)\phi_4(x_3) &= \left(\frac{2}{L}\right)^{3/2} \sin\left(\frac{5\pi x_1}{L}\right) \sin\left(\frac{11\pi x_2}{L}\right) \sin\left(\frac{4\pi x_3}{L}\right), \end{aligned}$$

and so on.

We can introduce a general notation that, while slightly clunky at first glance, will give us a foretaste of the occupation representation:

$$\Phi_{a_1a_2a_3}(x_1,x_2,x_3) = \phi_{a_1}(x_1)\phi_{a_2}(x_2)\phi_{a_3}(x_3) \tag{2.8}$$
$$= \left(\frac{2}{L}\right)^{3/2} \sin\left(\frac{n_1\pi x_1}{L}\right)\sin\left(\frac{n_2\pi x_2}{L}\right)\sin\left(\frac{n_3\pi x_3}{L}\right).$$

Now, each of these many-body states are normalized. Furthermore, given the state $\Phi_{a_1a_2a_3}$ and $\Phi_{b_1b_2b_3}$, we can calculate their inner product:

$$\langle\Phi_{a_1a_2a_3}|\Phi_{b_1b_2b_3}\rangle$$
$$= \int\int\int \Phi^*_{a_1a_2a_3}(x_1,x_2,x_3)\Phi_{b_1b_2b_3}(x_1,x_2,x_3)\,dx_1\,dx_2\,dx_3$$
$$= \int \phi^*_{a_1}(x_1)\phi^*_{b_1}(x_1)\,dx_1 \int \phi^*_{a_2}(x_2)\phi^*_{b_2}(x_2)\,dx_2 \int \phi^*_{a_3}(x_3)\phi^*_{b_3}(x_3)\,dx_3$$
$$= \delta_{a_1b_1}\delta_{a_2b_2}\delta_{a_3b_3}. \tag{2.9}$$

This clearly generalizes to any number of particles and to any orthonormal single-particle basis: given $\Phi_{a_1a_2a_3a_4\ldots}$ and $\Phi_{b_1b_2b_3b_4\ldots}$, these two many-body basis states are orthogonal unless $a_1 = b_1, a_2 = b_2$, etc..

So, to summarize, we have an extremely useful result. If we start with an orthonormal set of single-particle states, we can construct a many-body basis that is automatically and intuitively also orthonormal.

As I reminded you in Chapter 1, the matrix formulation is a deep and fundamental way to think about quantum mechanics. Hence the next step is calculation of matrix elements of operators.

Before we do that, we have to think about how we define operators for many-body systems. For example, suppose we consider the position operator. What position are we measuring? While for the moment we *could* measure just the position of particle 1, x_1, later on we will consider indistinguishable particles. Instead we choose to measure the position of any particle, which is $\hat{x} = x_1 + x_2 + x_3 \ldots$.

(You might reasonable ask: in that case, why not measure the average position of all the particles, that is, $(x_1 + x_2 + x_3 \ldots)/N$ for N particles. But this is actually something quite different. In the first case, we are measuring the position of a *single* particle, and we don't care which one it is. This is a *one-body operator*. But to compute the average, one actually needs to know the positions of *all* the particles *simultaneously*, which is an N-particle operator. And though we haven't yet discussed it, computation of an N-particle operator is much harder than computation of a one-body operator.)

So the matrix element is then, in somewhat tedious detail,

$$\langle\Phi_{a_1a_2a_3}|\hat{x}|\Phi_{b_1b_2b_3}\rangle$$
$$= \int\int\int \Phi^*_{a_1a_2a_3}(x_1,x_2,x_3)\,(x_1+x_2+x_3)\,\Phi_{b_1b_2b_3}(x_1,x_2,x_3)\,dx_1\,dx_2\,dx_3$$

$$= \int \phi^*_{a_1}(x_1) x_1 \phi^*_{b_1}(x_1)\, dx_1 \int \phi^*_{a_2}(x_2)\phi^*_{b_2}(x_2)\, dx_2 \int \phi^*_{a_3}(x_3)\phi^*_{b_3}(x_3)\, dx_3$$
$$+ \int \phi^*_{a_1}(x_1)\phi^*_{b_1}(x_1)\, dx_1 \int \phi^*_{a_2}(x_2) x_2 \phi^*_{b_2}(x_2)\, dx_2 \int \phi^*_{a_3}(x_3)\phi^*_{b_3}(x_3)\, dx_3$$
$$+ \int \phi^*_{a_1}(x_1)\phi^*_{b_1}(x_1)\, dx_1 \int \phi^*_{a_2}(x_2)\phi^*_{b_2}(x_2)\, dx_2 \int \phi^*_{a_3}(x_3) x_3 \phi^*_{b_3}(x_3)\, dx_3 \quad (2.10)$$

which simplifies to just

$$= \delta_{a_2 b_2}\delta_{a_3 b_3} \int \phi^*_{a_1}(x_1) x_1 \phi^*_{b_1}(x_1)\, dx_1$$
$$+ \delta_{a_1 b_1}\delta_{a_3 b_3} \int \phi^*_{a_2}(x_2) x_2 \phi^*_{b_2}(x_2)\, dx_2 \quad (2.11)$$
$$+ \delta_{a_1 b_1}\delta_{a_2 b_2} \int \phi^*_{a_3}(x_3) x_3 \phi^*_{b_3}(x_3)\, dx_3. \quad (2.12)$$

Any operator that depends on just the coordinates of a single particle is called a *one-body operator*. This includes not only $\hat{x}$ but also the momentum $\hat{p}$ which depends upon the derivative in coordinate space, and so on.

For some one-body operator $\hat{\mathcal{O}}(x)$ we can write down the *one-body matrix element*,

$$O_{ab} = \langle a|\hat{\mathcal{O}}|b\rangle = \quad (2.13)$$
$$\int \phi^*_a(x)\hat{\mathcal{O}}(x)\phi_b(x)\, dx.$$

In this notation the matrix element of the one-body operator between many-body states is

$$\langle \Phi_{a_1 a_2 a_3}|\hat{\mathcal{O}}|\Phi_{b_1 b_2 b_3}\rangle = \delta_{a_2 b_2}\delta_{a_3 b_3} O_{a_1 b_1}$$
$$+ \delta_{a_1 b_1}\delta_{a_3 b_3} O_{a_2 b_2} + \delta_{a_1 b_1}\delta_{a_2 b_2} O_{a_3 b_3} \quad (2.14)$$

Already we can see an interesting pattern: for a one-body operator, if the single-particle labels $a_1, a_2, \ldots$ and $b_1, b_2, \ldots$ differ by more than one label, the matrix element is zero. So one can have a non-zero matrix element of a one-body operator between Φ_{123} and Φ_{123}, between Φ_{457} and Φ_{457}, and between Φ_{123} and Φ_{183}, but must perforce have zero matrix element of a one-body operator between Φ_{123} and Φ_{145} and between Φ_{457} and Φ_{789}.

This kind of pattern will generally hold even when we consider identical particles later on. Furthermore, we will see how the occupation representation arrives at this result smoothly and quickly; indeed, much of our justification for the occupation representation will be *because* it reproduces exactly this result.

Indeed, adopting the idea of occupation, we introduce the notation

$$|a_1 a_2 a_3 \ldots\rangle = |\Phi_{a_1 a_2 a_3 \ldots}\rangle \quad (2.15)$$

as a simplification.

Continuing on, let's now consider *two-body operators*, an example of which is the potential between two particles, $\hat{(}x, x')$. For N particles it is explicitly

$$\hat{V} = \sum_{i<j} V(x_i, x_j), \tag{2.16}$$

with the inequality introduced to make sure the interaction between each pair i, j is counted only once. We introduce the *two-body matrix element*

$$\begin{aligned} V^N_{ab,cd} &= \langle ab|\hat{V}|cd\rangle \\ &= \int\int \phi^*_a(x)\phi^*_b(x')\hat{V}(x,x')\phi_c(x)\phi_d(x'). \end{aligned} \tag{2.17}$$

The superscript ^{N} stands for 'nonsymmetric' and will be used later when we talk about identical particles.

As an exercise, you should derive the matrix elements for three particles

$$\begin{aligned} \langle a_1a_2a_3|\hat{V}|b_1b_2b_3\rangle &= \delta_{a_3b_3}V^N_{a_1a_2,b_1b_2} \\ &+\delta_{a_2b_2}V^N_{a_1a_3,b_1b_3} + \delta_{a_1b_1}V^N_{a_2a_3,b_2b_3} \end{aligned} \tag{2.18}$$

and also for four particles

$$\begin{aligned} &\langle a_1a_2a_3a_4|\hat{V}|b_1b_2b_3b_4\rangle \\ &= \delta_{a_3a_3}\delta_{a_4b_4}V^N_{a_1a_2,b_1b_2} + \delta_{a_2b_2}\delta_{a_4b_4}V^N_{a_1a_3,b_1b_3} \\ &+\delta_{a_1b_1}\delta_{a_2b_2}V^N_{a_3a_4,b_3b_4} + \delta_{a_2b_2}\delta_{a_3b_3}V^N_{a_1a_4,b_1b_4} \\ &+\delta_{a_1b_1}\delta_{a_3b_3}V^N_{a_2a_4,b_2b_4} + \delta_{a_1b_1}\delta_{a_2b_2}V^N_{a_3b_4,a_3b_4} \end{aligned} \tag{2.19}$$

The pattern is similar to that for one-body matrix elements: the single-particle labels must all agree except for, at most, differing in two labels.

Before going on, try Exercises (2.1) and (2.2) at the end of this chapter.

2.2 Example: particles in a well

Now that we can compute matrix elements, let's do for a sample problem: particles in a one-dimensional infinite well of length L. I'm going to use again the basis state for particles in a box, (2.7). Now let's choose a δ-interaction. This is the force between particles, so the Hamiltonian is

$$\hat{H} = \sum_i -\frac{\hbar^2}{2m}\frac{d^2}{dx_i^2} - V_0\sum_{i<j}\delta(x_i - x_j). \tag{2.20}$$

The kinetic energy, a one-body matrix element, is easy:

$$\left\langle m\left|-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\right|n\right\rangle = \frac{\hbar^2n^2\pi^2}{2mL^2}\delta_{mn}. \tag{2.21}$$

The two-body interaction matrix element is somewhat more tricky:

$$\begin{aligned}
&\langle mm'\,|-V_0\delta(x-x')|\,nn'\rangle = \\
&-V_0\left(\frac{2}{L}\right)^2\int_0^L dx\int_0^L dx'\sin\left(\frac{m\pi x}{L}\right)\sin\left(\frac{m'\pi x'}{L}\right) \\
&\qquad\qquad \delta(x-x')\sin\left(\frac{n\pi x}{L}\right)\sin\left(\frac{n'\pi x'}{L}\right) \\
&= -\frac{V_0}{L^2}\left(\delta_{m+n,m'+n'}+\delta_{m+n',m'+n}+\delta_{m+m',n+n'}\right. \\
&\left.-\delta_{m,m'+n+n'}-\delta_{n,m+m'+n'}-\delta_{m',m+n+n'}-\delta_{n',m+m'+n}\right). \qquad (2.22)
\end{aligned}$$

To simplify things, let's define $V_0 = W\hbar^2\pi^2/2m$, so that W is a dimensionless constant.

With these one- and two-body matrix elements, we can now compute the matrix elements of the many-body system. In any many-body calculations, we must choose a finite set of many-body states; deciding which to choose is far from obvious!

Let's first consider the two-particle system. We can label the states $|n_1, n_2\rangle$. One choice of basis states might be:

$$|1,1\rangle,\ |1,2\rangle,\ |2,1\rangle,\ |2,2\rangle.$$

Remember we are not yet assuming identical particles, so $|1,2\rangle$ is distinct from $|2,1\rangle$.

Restricting ourselves to these states, the truncated Hamiltonian matrix is

$$\frac{\hbar^2\pi^2}{2mL^2}\begin{pmatrix} 2-3W & 0 & 0 & -2W \\ 0 & 5-2W & -2W & 0 \\ 0 & -2W & 5-2W & 0 \\ -2W & 0 & 0 & 8-3W \end{pmatrix}. \qquad (2.23)$$

Why all the zeroes? This has to do with a conserved quantum number, in this case parity. If you consider the single-particle wavefunction, they are even about $x = L/2$ for n odd, that is,

$$\phi_n(x) = +\phi_n(L-x),$$

and odd about $x = L/2$, or

$$\phi_n(x) = -\phi_n(L-x),$$

for n even. (See illustrative figure.) When we construct a many body wavefunction, and send *every* coordinate x_i to $L - x_i$, the overall wavefunction is odd if there are an odd number of odd single-particle wavefunctions, otherwise it is even. (Convince yourself this is true.) Therefore the states $|1,1\rangle$ and $|2,2\rangle$ are even while $|1,2\rangle$ and $|2,1\rangle$ are odd. The Hamiltonian is invariant under reflection across $L/2$ and so its eigenstates are either even or odd.

Therefore let's take a truncated basis of even 2-body states:

$$|1,1\rangle,\ |1,3\rangle,\ |2,2\rangle,\ |3,1\rangle,\ |3,3\rangle$$

which now has the Hamiltonian matrix

$$\frac{\hbar^2\pi^2}{2mL^2}\begin{pmatrix} 2-3W & W & -2W & W & -2W \\ W & 10-2W & -W & -2W & 0 \\ -2W & -W & 8-3W & -W & -2W \\ W & -2W & -W & 10-2W & 0 \\ -2W & 0 & -2W & 0 & 18-3W \end{pmatrix}. \qquad (2.24)$$

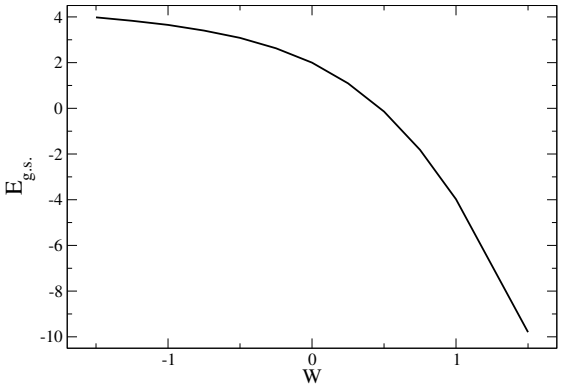

Figure 2.1: Ground state energy for particles in a box interacting via a δ-potential as a function of the dimensionless parameter W (see text), with $n_{\max} = 50$ (1250 two-particle basis states). Note that $W > 0$ is attractive and $W < 0$ repulsive.

If we restrict ourselves to $n_{\max}$ single-particle states, that is, $n = 1, 2, 3, \ldots, n_{\max}$, then the number of states is $n_{\max}^2$.

If you take $n_{\max} = 50$ there are 1250 even-parity two-particle basis states. Figure 2.1 shows the grounds state energy in this basis as a function of W.

It's natural to ask: is this a large enough basis? Actually, a δ-potential is problematic for many-body systems; because the δ is not actually a function, one must introduce a cutoff, a topic beyond the scope of this text. But in Figure 2.2 I illustrate the convergence for $W = 0.5$.

This starts to illustrate the difficulty of solving many-body problems. In general given N_p particles in N_s single particle states, the number of basis states is of the order of $N_s^{N_p}$. So, if we have four particles and five single-particle states, the number of basis states is $4^5 = 1024$, but if we have ten single-particle states, $4^10 = 1,048,576$. Thus the dimensions of the basis increase dramatically, both with the number of particles and the number of single-particle states. We will have more to say later about the dimension of basis states.

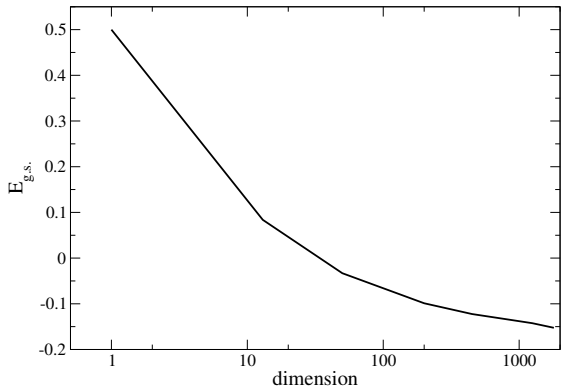

Figure 2.2: Convergence of the ground state energy of two particles in a box interacting via a δ-potential as a function of the dimension of the basis. Here the dimensionless parameter W (see text) is 0.5.

2.3 Identical particles

So far we have treated all the particles as distinguishable, as if we could paint 'one' on an electron, and 'two' on another, and so on. But we can't. So we assume that the electrons (and other kinds of particles) are indistinguishable, not just in practice due to our ignorance, but fundamentally. And let's take this assumption seriously and find the consequences, in the same way that Einstein took seriously his proposal that 'you cannot make an observation to determine absolute motion.' He wound up with $E = mc^2$; we're going to end up with chemistry.

Given a coordinate space wavefunction $\psi(\vec{r})$, the probability to find the particle at point $\vec{r}$ is $|\psi(\vec{r})|^2$. So clearly for a two-particle system, $|\Psi(\vec{r}_1, \vec{r}_2)|^2$ is the probability to find a particle at point $\vec{r}_1$ and a particle at point $\vec{r}_2$.

But we've assumed we cannot tell particle 1 from particle 2. So we must have

$$|\Psi(\vec{r}_1, \vec{r}_2)|^2 = |\Psi(\vec{r}_2, \vec{r}_1)|^2; \tag{2.25}$$

otherwise we could tell if particle 1 were at point $\vec{r}_1$ or $\vec{r}_2$.

Clearly, then, when we interchange $\vec{r}_1$ and $\vec{r}_2$, the wavefunction Ψ cannot change except for some phase, that is,

$$\Psi(\vec{r}_1, \vec{r}_2) = \pm\Psi(\vec{r}_2, \vec{r}_1). \tag{2.26}$$

(One could, and some researchers have, consider a more general complex phase. However this engenders difficulties because upon interchanging the same coordinates twice one expects to get back to the same wavefunction, hence the preference for a phase ± 1.)

More generally, under the interchange of any two coordinates of an N-particle system, we have wavefunctions that are either *symmetric*

$$\Psi(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_i, \ldots, \vec{r}_j, \ldots) = +\Psi(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_j, \ldots, \vec{r}_i, \ldots) \tag{2.27}$$

or *antisymmetric*:

$$\Psi(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_i, \ldots, \vec{r}_j, \ldots) = -\Psi(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_j, \ldots, \vec{r}_i, \ldots). \tag{2.28}$$

Particles whose wavefunction is symmetric under the intercharge of two coordinates are said to obey Bose-Einstein statistics and are called *bosons*, while particles with antisymmetric wavefunctions follow Fermi-Dirac statistics and are called *fermions*.

The *spin-statistics theorem* states that bosons must have intrinsic spin 0, 1, 2, ... (in units of $\hbar$) while fermions must have spin $\frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \ldots$. Examples of bosons are photons, gluons, and the W and Z weak vector bosons, as well as the composite particles pions, kaons, ^{4}He and ^{16}O nuclei, and so on. Examples of fermions are electrons, neutrinos, quarks, and composite particles protons, neutrons, ^{3}He, and so on. Even if a particle is composed of fundamental fermions, if the total angular momentum is an integer, it is a boson. (Rules for combining angular momentum can be found in the Appendix.)

We can already deduce some consequences. The most famous, is that for fermions, with the antisymmetric wavefunction (2.28), if $\vec{r}_i = \vec{r}_j$, the wavefunction is equal to its own negative and must vanish. In other words, two identical fermions cannot be at the same place, a statement also known as the Pauli exclusion principle. We will later develop this idea more fully, but the Pauli exclusion principle leads to chemistry as we know it.

Earlier we developed the idea of a product wavefunction as a simple basis for many-particle states. But in general a product of single-particle states will satisfy neither (2.27) nor (2.28). Therefore we enforce symmetry/antisymmetry by taking all possible permutations with the appropriate signs, as discussed in detail in the next two sections.

2.4 Boson permanents

I will start with systems of bosons. If you are primarily interested in fermion systems you can skip ahead to the next section. Be aware, however, that the antisymmetry of many-fermion wavefunctions lead to results that are even stranger and more unsettling than for bosons.

Let's jump right in. For two bosons the unnormalized *symmeterized* wavefunction is

$$\Phi(x_1, x_2) = \phi_1(x_1)\phi_2(x_2) + \phi_1(x_2)\phi_2(x_1). \tag{2.29}$$

and for three particles the unnormalized, symmeterized wavefunction is

$$\begin{aligned} &\Phi(x_1, x_2, x_3) = \\ &\phi_1(x_1)\phi_2(x_2)\phi_3(x_3) + \phi_1(x_2)\phi_2(x_3)\phi_3(x_1) + \phi_1(x_3)\phi_2(x_1)\phi_3(x_2) \\ &+\phi_1(x_1)\phi_2(x_3)\phi_3(x_2) + \phi_1(x_3)\phi_2(x_2)\phi_3(x_1) + \phi_1(x_2)\phi_2(x_1)\phi_3(x_3) \end{aligned} . \tag{2.30}$$

For N bosons one can write

$$\Phi(x_1, x_2, \ldots, x_N) = \phi_1(x_1)\phi_2(x_2)\ldots\phi_N(x_N) +$$

$$\phi_2(x_1)\phi_3(x_2)\dots\phi_1(x_N) + \phi_3(x_1)\phi_4(x_2)\dots\phi_2(x_N) + \dots$$
$$= \sum_{\mathrm{per}(a_1,a_2,a_3,\dots)} \phi_{a_1}(x_1)\phi_{a_2}(x_2)\dots\phi_{a_N}(x_N) \tag{2.31}$$

where the sum is over all permutations of $1, 2, 3, \dots, N$, the labels of the functions $\phi_{a_1}(x_1), \phi_{a_2}(x_2)$, etc.. Alternately one could permute the coordinates x_1, x_2, x_3, etc..

This might remind you of a mathematical construct you've seen before, a determinant, except without the minus signs. We'll actually use determinants in the next section, when we deal with fermions. The construct here is called a *permanent*. You are unlikely to have encountered permanents before, as they are not as ubiquitous as determinants nor do they have such interesting mathematical properties. Nonetheless we can symbolically write the general symmeterized boson wavefunction as

$$\Phi(x_1, x_2, \dots, x_N) = \mathrm{per} \begin{vmatrix} \phi_1(x_1) & \phi_1(x_2) & \dots & \phi_1(x_N) \\ \phi_2(x_1) & \phi_2(x_2) & \dots & \phi_2(x_N) \\ \vdots & & & \\ \phi_N(x_1) & \phi_N(x_2) & \dots & \phi_N(x_N) \end{vmatrix}. \tag{2.32}$$

Equation (2.32) is just a symbolic form of the expansion/definition (2.31). Because we take all possible permutations of the single-particle state labels a_i vis-a-vis the coordinates x_j, any boson permanent is known primarily by the list of labels $\{a_i\}$. Summing over the permutations means no one coordinate is associatedly exclusively with any one single-particle state label. This insight, we'll see, leads us to the occupation representation.

Let's return to normalization. (Eqn. (2.32) is *not* normalized, and we'll see that normalization is a bit tricky with bosons. I'll try to be clear when I am dealing with normalized states and when dealing with unnormalized states.) We continue to cling to the useful assumption that the single-particle states $\{\phi_a\}$ are orthonormalized. To illustrate, let's take two extremes.

First, suppose each of the bosons are in a unique single-particle state, so that no $\phi_a = \phi_b$. Note that while we'll later see this is obligatory for fermions, it is not for bosons. Expanding (2.32), we get $N!$ terms. Then we compute the normalization integral, relying upon the ideas we developed back in section 2.1, especially factorization of the integrals:

$$\int \Phi^*(x_1, x_2, \dots, x_N)\Phi(x_1, x_2, \dots, x_n)dx_1dx_2\dots dx_N \tag{2.33}$$

there will be $(N!)^2$ terms. Each of these will factorize, much as happened with the nonidentical case, and look like:

$$\int \phi^*_{a_1}(x_1)\phi_{a'_1}(x_1)dx_1 \times \int \phi^*_{a_2}(x_2)\phi_{a'_2}(x_2)dx_2\dots \tag{2.34}$$

which will equal $1 \times 1 \times 1 \dots = 1$ if and only if $a_i = a'_i$ for all i; otherwise orthogonality will force an integral to vanish. So, for each of the $N!$ permutations

of the a_i, there are also $N!$ permutations of the a'_i, but there is only one nonzero contribution. Thus the final value of (2.33) is $N!$. If this is not clear, I suggest you work out a few examples for yourself.

Now let's take the opposite extreme. Suppose all the bosons are in the same single-particle state (say ϕ_1 for convenience):

$$\Phi = \text{per} \begin{vmatrix} \phi_1(x_1) & \phi_1(x_2) & \dots & \phi_1(x_N) \\ \phi_1(x_1) & \phi_1(x_2) & \dots & \phi_1(x_N) \\ \vdots & & & \\ \phi_1(x_1) & \phi_1(x_2) & \dots & \phi_1(x_N) \end{vmatrix}. \tag{2.35}$$

This kind of state, called a *condensate*, is possible in boson systems, but impossible, we'll see, in fermion systems. There are still $N!$ terms, but they are all identical, and the expansion leaves:

$$\Phi = N! \prod_{i=1}^{N} \phi_1(x_i).$$

Unlike the previous case, no integral vanish, and the normalization integral for this permanent is $(N!)^2$ rather than $N!$.

In each of these cases we see we can label a permanent uniquely by the set of occupied states $\alpha = \{a_1, a_2, a_3, \dots, a_N\}$. Because we sum over all permutations, the ordering is irrelevant. And because it is possible to have a single-particle states occupied more than once, we introduce the *occupancy* n_a of the state a; this is the number of 'copies' of ϕ_a in a permanent. As a short hand one can write the many-particle label $\alpha = (a_1)^{n_1}(a_2)^{n_2}(a_2)^{n_3}\dots$. The sum of the occupancies must equal the total number of particles, $\sum_a n_a = N$. As an exercise you should work out the normalization and show the overlap integral for an unnormalized permanent (2.32) is

$$\langle (a_1)^{n_1}(a_2)^{n_2}(a_2)^{n_3}\dots | (a_1)^{n_1}(a_2)^{n_2}(a_2)^{n_3}\dots \rangle = N! n_1! n_2! n_3! \dots \tag{2.36}$$

so that a *normalized*, coordinate-space permanent is

$$\Phi(x_1, x_2, \dots, x_N) = \frac{1}{\sqrt{N! n_1! n_2! \dots}} \text{per} \begin{vmatrix} \phi_1(x_1) & \phi_1(x_2) & \dots & \phi_1(x_N) \\ \phi_2(x_1) & \phi_2(x_2) & \dots & \phi_2(x_N) \\ \vdots & & & \\ \phi_N(x_1) & \phi_N(x_2) & \dots & \phi_N(x_N) \end{vmatrix}. \tag{2.37}$$

This formula for the normalization agrees with our two extreme cases (the first has $n_1 = n_2 = n_3 \dots n_N = 1$ and the second has $n_1 = N$).

Now let's turn to matrix elements. From now on, assume we have *normalized* permanents, using (2.36), so that, given some set of occupied states $\alpha = \{a_1, a_2, a_3 \dots\}$ and $\beta = \{b_1, b_2, b_3, \dots\}$ (alternately we could use the occupancies $n_1, n_2, n_3, \dots$), we have $\langle \Phi_\alpha | \Phi_\beta \rangle = \delta_{\alpha,\beta}$.

We continue to use some of the insight developed for the case of nonidentical particles. For matrix elements of one-body operators, the integral factorizes as usual into sums of the form

$$\int \phi^*_{a_1}(x_1)\phi_{b_1}(x_1)dx_1 \times \int \phi^*_{a_2}(x_2)\phi_{b_2}(x_2)dx_2 \times \ldots \int \phi^*_{a_i}(x_i)\hat{\mathcal{O}}(x_i)\phi_{b_i}(x_i)dx_i$$

which becomes

$$\delta_{a_1 b_1} \times \delta_{a_2 b_2} \times \ldots O_{a_i b_i} \ldots$$

So, once again, such a term vanishes unless $a_1 = b_1, a_2 = b_2$, etc., with the only allowed (but not required) mismatch being a_i and b_i. This is very similar to the result for non-identical particles, the major difference being that there are $N!$ shuffling of the coordinates, which is accounted for in the normalization. Again like non-identical particles, there are two cases:

Case 1: Both permanents have identical occupations (keep in mind the ordering does not matter). Then

$$\langle\alpha|\hat{\mathcal{O}}|\alpha\rangle = \sum_{i=1}^{N} O_{a_i a_i} \tag{2.38}$$

which one can rewrite using occupancies

$$\sum_a n_a O_{aa}. \tag{2.39}$$

and

Case 2: The bra and ket permanents differ by exactly one occupancy. This case is actually a bit tricky because the occupancies can still be greater than 1. If we let the ket vector be

$$|\beta = (b_1)^{n_1}(b_2)^{n_2}(b_3)^{n_3}\ldots\rangle,$$

let $|\alpha\rangle$ have the same occupancies except it has one more in state b_m and one less in state b_i, so that

$$|\alpha = (b_1)^{n_1}(b_2)^{n_2}(b_3)^{n_3}\ldots(b_i)^{n_i-1}\ldots(b_m)^{n_m+1}\ldots\rangle,$$

the matrix element between *un*normalized states is

$$\langle\tilde{\alpha}|\hat{\mathcal{O}}|\tilde{\beta}\rangle = O_{mi}N!n_1!n_2!\ldots(n_m+1)!\ldots(n_i-1)!\ldots \tag{2.40}$$

(where I use $\tilde{\alpha}$ to denote an unnormalized state) and so the matrix element between *normalized* states is then

$$\langle\alpha|\hat{\mathcal{O}}|\beta\rangle = O_{mi}\sqrt{n_i(n_m+1)}. \tag{2.41}$$

Neither formula is obvious, so in the exercises you'll be asked to try to work out a couple of specific examples.

Actually, in general formulas such as (2.41) are not that useful. In Chapter 5 the operator formalism will reproduce all our hard-won results and give us a better way to derive them.

In light of that fact, I will only briefly touch upon matrix elements of two-body operators. First, consider the matrix element of $V(x, x')$ between *unnormalized* two-boson states $|a_1 a_2\rangle$ and $|b_1 b_2\rangle$. Expanding the permanents, the matrix element is the integral

$$\begin{aligned}\langle a_1 a_2|V|b_1 b_2\rangle = \\ \int \phi^*_{a_1}(x_1)\phi^*_{a_2}(x_2)V(x_1,x_2)\phi_{b_1}(x_1)\phi_{b_2}(x_2)dx_1dx_2 \\ + \int \phi^*_{a_1}(x_1)\phi^*_{a_2}(x_2)V(x_1,x_2)\phi_{b_2}(x_1)\phi_{b_1}(x_2)dx_1dx_2 \\ \int \phi^*_{a_2}(x_1)\phi^*_{a_1}(x_2)V(x_1,x_2)\phi_{b_1}(x_1)\phi_{b_2}(x_2)dx_1dx_2 \\ + \int \phi^*_{a_2}(x_1)\phi^*_{a_1}(x_2)V(x_1,x_2)\phi_{b_2}(x_1)\phi_{b_1}(x_2)dx_1dx_2.\end{aligned} \tag{2.42}$$

But any physical interaction potential must be symmetric $V(x, x') = V(x', x)$. This means we can swap the integration variables in the last two terms and arrive at

$$2\int \phi^*_{a_1}(x_1)\phi^*_{a_2}(x_2)V(x_1,x_2)\left(\phi_{b_1}(x_1)\phi_{b_2}(x_2) + \phi_{b_2}(x_1)\phi_{b_1}(x_2)\right)dx_1dx_2. \tag{2.43}$$

Building upon this and the definition (2.17), let's define the *symmetric* two-body matrix elements, which are the matrix elements of a two-body operator between two *normalized* two-boson states:

$$V^S(ab,cd) = \frac{1}{\sqrt{2(1+\delta_{ab})(1+\delta_{bc})}}\left(V^N(ab,cd) - V^N(ab,dc)\right) \tag{2.44}$$

which have the property

$$V^S(ab,cd) = +V^S(ab,dc) = +V^S(ba,cd) = +V^S(ba,dc). \tag{2.45}$$

We'll return to two-body matrix elements in Chapter 5.

Before going on, derive (2.36), and show that (2.38), (2.39) are true (exercises 2.3 and 2.4 at the end of the chapter).

2.5 Fermion determinants

I'll start with the fermion case because in some important respects it is simpler. Consider a product wavefunction for two particles:

$$\Phi(x_1, x_2) = \phi_1(x_1)\phi_2(x_2). \tag{2.46}$$

We make this antisymmetric by hand, by simply adding (with a minus sign in front) a term with the coordinates switched:

$$\Phi(x_1, x_2) = \phi_1(x_1)\phi_2(x_2) - \phi_1(x_2)\phi_2(x_1). \tag{2.47}$$

I'll discuss normalization shortly. We can do also write down by hand an antisymmeterized product wavefunction for three particles as well:

$$\begin{aligned} &\psi(x_1, x_2, x_3) = \\ &\phi_1(x_1)\phi_2(x_2)\phi_3(x_3) + \phi_1(x_2)\phi_2(x_3)\phi_3(x_1) + \phi_1(x_3)\phi_2(x_1)\phi_3(x_2) \\ &-\phi_1(x_1)\phi_2(x_3)\phi_3(x_2) - \phi_1(x_3)\phi_2(x_2)\phi_3(x_1) - \phi_1(x_2)\phi_2(x_1)\phi_3(x_3) \end{aligned}. \tag{2.48}$$

This is straightforward but slightly tedious. We can write this in a somewhat more compact form if we remember how we form determinants:

$$\det \begin{vmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{vmatrix} = a_{11}a_{22} - a_{12}a_{21}; \tag{2.49}$$

$$\det \begin{vmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{vmatrix} = \begin{array}{c} a_{11}a_{22}a_{33} + a_{12}a_{23}a_{31} + a_{13}a_{21}a_{32} \\ -a_{11}a_{23}a_{32} - a_{12}a_{21}a_{33} - a_{13}a_{22}a_{31} \end{array} \tag{2.50}$$

Thus inspired, we can rewrite the many-body wavefunctions as

$$\Phi(x_1, x_2,) = \frac{1}{\sqrt{2}} \det \begin{vmatrix} \phi_1(x_1) & \phi_1(x_2) \\ \phi_2(x_1) & \phi_2(x_2) \end{vmatrix}; \tag{2.51}$$

$$\Phi(x_1, x_2, x_3) = \frac{1}{\sqrt{6}} \det \begin{vmatrix} \phi_1(x_1) & \phi_1(x_2) & \phi_1(x_3) \\ \phi_2(x_1) & \phi_2(x_2) & \phi_2(x_3) \\ \phi_3(x_1) & \phi_3(x_2) & \phi_3(x_3) \end{vmatrix}. \tag{2.52}$$

I'll justify the normalization below. This is easily generalized to N particles:

$$\Phi(x_1, x_2, \ldots, x_N) = \frac{1}{\sqrt{N!}} \det \begin{vmatrix} \phi_1(x_1) & \phi_1(x_2) & \ldots & \phi_1(x_N) \\ \phi_2(x_1) & \phi_2(x_2) & \ldots & \phi_2(x_N) \\ \vdots & & & \\ \phi_N(x_1) & \phi_N(x_2) & \ldots & \phi_N(x_N) \end{vmatrix}. \tag{2.53}$$

We call these *Slater determinants*. They are actually an intermediate step in our development, as while they encompass antisymmetry determinants of coordinate functions must be expanded and are still clumsy to work with. In later chapters we'll develop the full-fledged formalism of the occupation representation using creation and annihilation operators, we will shed this clumsiness. But we will still call antisymmeterized product wavefunctions Slater determinants.

We can use the well-known properties of determinants to gain insight into the wavefunctions. In the Slater determinant wavefunction (2.53), interchange of any two coordinates x_i and x_j is equivalent to interchange of any two columns, which leads to a minus sign and the desired antisymmetry.

Furthermore, if any two coordinates are the same, that is, if any two fermions are at the same place, $x_i = x_j$, then two columns are identical and the determinant is zero. This is the first understanding of the Pauli exclusion principal. But we can generalize it in an important way: for also if any two *rows* are identical, that is, if any $\phi_a = \phi_b$, then the determinant also vanishes. In other words, any two fermions occupying the same *same single-particle state* is forbidden.

We see this in chemistry. Each orbital in an atom can be labeled by principal quantum number N, by orbital angular momentum l, and magnetic quantum number m (which is the z-projection of the orbital angular momentum). Hund's rule tells us we can place two electrons in each of these orbits. Where this comes from is an additional labeling of the states, the spin. Each electron, with total spin $s = 1/2$, can have third component of spin up or down, that is $m_s = \pm\frac{1}{2}$. So in an atom, each electron is assigned a unique combination of N, l, m, m_s. We'll talk more about this at great length later.

Now let's return to the issue of normalization. We can recycle some of the understanding we already used for systems of non-identical particles. Let's consider the normalization of the two-particle system starting from (2.47):

$$\begin{aligned}
\int |\Phi(x_1,x_2)|^2 dx_1 dx_2 = \qquad (2.54)\\
\int (\phi_1^*(x_1)\phi_1(x_1)\phi_2^*(x_2)\phi_2(x_2) + \phi_2^*(x_1)\phi_2(x_1)\phi_1^*(x_2)\phi_1(x_2)\\
-\phi_1^*(x_1)\phi_2(x_1)\phi_2^*(x_2)\phi_1(x_2) - \phi_2^*(x_1)\phi_1(x_1)\phi_1^*(x_2)\phi_2(x_2))\, dx_1 dx_2\\
= \int \phi_1^*(x_1)\phi_1(x_1)dx_1 \times \int \phi_2^*(x_2)\phi_2(x_2)dx_2\\
+ \int \phi_2^*(x_1)\phi_2(x_1)dx_1 \times \int \phi_1^*(x_2)\phi_1(x_2)dx_2\\
- \int \phi_1^*(x_1)\phi_2(x_1)dx_1 \times \int \phi_2^*(x_2)\phi_1(x_2)dx_2\\
- \int \phi_2^*(x_1)\phi_1(x_1)dx_1 \times \int \phi_1^*(x_2)\phi_2(x_2)dx_2\\
= 1\times 1 + 1\times 1 - 0\times 0 - 0\times 0 = 2
\end{aligned}$$

where I used the orthonormality of the single-particle wavefunctions.

We can easily generalize. Expanding any N-particle determinant Φ, you will get $N!$ terms of the form

$$\pm\phi_1(x_a)\phi_2(x_b)\phi_3(x_c)\ldots\phi_N(x_z) \qquad (2.55)$$

where $x_a, x_b, x_c, \ldots$ are even or odd permutations of $x_1, x_2, x_3, \ldots$. Expanding Φ^* yields similar terms. But when performing the integral, any term

$$\int \phi_a^*(x)\phi_b(x)dx = 0$$

unless $a = b$. This means the only nonzero contributions arise when you match $\phi_1(x_i)$ with $\phi_1^*(x_i)$, $\phi_2(x_j)$ with $\phi_2^*(x_j)$, etc.. So although there are a total of

$(N!)^2$ terms, only $N!$ are nonzero, and if the single-particle states are normalized, each term is $= 1$. It's also easy to see the sign of every nonzero term is $+$. Hence the total normalization is $N!$, which is why there is a coefficient $(N!)^{-1/2}$ in front of (2.53).

If this is not yet clear, I recommend you try the three-particle case, which has a total of 36 terms with 6 nonzero.

Now consider the overlap between two Slater determinants composed from different single-particle states, for example, one with ϕ_1, ϕ_2, ϕ_3 and the other with ϕ_1, ϕ_2, ϕ_4. (In a much later chapter I'll deal with *oblique* Slater determinants, where the single-particle states are not taken from the same set or are not orthonormal.) The overlap integral is

$$\int |\Phi^* \Phi'|^2 dx_1 dx_2 dx_3.$$

But when expanding this integral, one always will have factors of the form $\int \phi_4^*(x)\phi_b(x)dx$ with $b = 1, 2, 3$ and hence $= 0$. Thus the overlap integral must vanish, and the two Slater determinants are orthogonal. Again, I encourage you to do a few examples to convince yourself of this.

What we have learned: if we construct Slater determinants from orthonormal single-particle states, then we get easily normalized many-body wavefunctions and trivial orthogonality. Furthermore the properties are clearly dependent only upon the list of single-particle states ϕ_1, ϕ_2, ϕ_4 in a given Slater determinant, that is, the single-particle states that are *occupied*. So we can write $|\Phi_{a_1,a_2,a_3,\ldots}\rangle$. The idea of describing the states primarily through occupation will reach full flower when we introduce creation and annihilation operators and we will all but completely drop the coordinates $x_1, x_2, \ldots$; in anticipation we use the occupation notation

$$|a_1 a_2 a_3 \ldots\rangle = |\Phi_{a_1 a_2 a_3 \ldots}\rangle.$$

A significant difference from boson permanents is that a state a_i can be occupied at most *once*, that is, $n_a = 0$ or 1, only.

We need more than just orthonormality relation among Slater determinants; we also require matrix elements. Fortunately we can again apply much of what we have learned from the non-identical case and from bosons.

First consider matrix elements of a one-particle operator $\hat{\mathcal{O}}^{(1)}$. Between two-particle Slater determinants,

$$\begin{aligned}\langle a_1 a_2 | \hat{\mathcal{O}}^{(1)} | b_1 b_2 \rangle = \delta_{a_2 b_2} O_{a_1 b_1} + \delta_{a_1 b_1} O_{a_2 b_2} \\ -\delta_{a_1 b_2} O_{a_2 b_1} - \delta_{a_2 b_1} O_{a_1 b_2}.\end{aligned} \tag{2.56}$$

Here we see a phase that can arise due to the ordering, and this phase is one of the most important, and problematic, issues for many-fermion systems. Often one insists upon a strict ordering, for example $a_1 < a_2 < a_3 < \ldots$. The actual ordering is not important, only the consistency. Even with a strict ordering, however, phases ineluctably arise.

For example, consider the matrix element of a one-body operator between three-particle Slater determinants (assuming strict ordering $a_1 < a_2 < a_3$ and $b_1 < b_2 < b_3$)

$$\begin{aligned}\langle a_1 a_2 a_3|\hat{\mathcal{O}}^{(1)}|b_1 b_2 b_3\rangle = \delta_{a_2 b_2}\delta_{a_3 b_3} O_{a_1 b_1} \\ +\delta_{a_1 b_1}\delta_{a_3 b_3} O_{a_2 b_2} + \delta_{a_1 b_1}\delta_{a_2 b_2} O_{a_3 b_3} \\ -\delta_{a_2 b_1}\delta_{a_3 b_3} O_{a_1 b_2} - \delta_{a_2 b_1}\delta_{a_3 b_2} O_{a_1 b_3} - \delta_{a_1 b_1}\delta_{a_3 b_2} O_{a_2 b_3}\end{aligned} \tag{2.57}$$

(I leave detailed derivation as an exercise to the reader.)

As for non-identical particles and for bosons, there are two general cases for matrix elements of one-body operators between two fermion Slater determinants:

Case 1 for one-body matrix elements: the N-particle Slater determinants are identical, leaving

$$\langle a_1 a_2 \ldots|\hat{\mathcal{O}}^{(1)}|a_1 a_2 \ldots\rangle = \sum_{i=1}^{N} O_{a_i a_i}; \tag{2.58}$$

or

Case 2 for one-body matrix elements: the N-particle Slater determinants differ by exactly one occupation, so that $a_1 = b_1, a_2 = b_2$, and so on, except for exactly one mismatched pair $a_x \neq b_x$,. The matrix element is then

$$\langle a_1 a_2 \ldots|\hat{\mathcal{O}}^{(1)}|b_1 b_2 \ldots\rangle = (\text{phase}) O_{a_x b_x}. \tag{2.59}$$

Determining the phase is straightforward but tedious. I encourage you to try the examples in the exercises.

Matrix elements of two-body operators are more interesting. To deal with them we must take care with notation, or else it is easy to get confused. Begin with two normalized 2-particle Slater determinants,

$$\Phi_{a_1,a_2}(x_1, x_2) = \frac{1}{\sqrt{2}}\left[\phi_{a_1}(x_1)\phi_{a_2}(x_2) - \phi_{a_2}(x_1)\phi_{a_1}(x_2)\right]$$

and

$$\Phi_{b_1,b_2}(x_1, x_2) = \frac{1}{\sqrt{2}}\left[\phi_{b_1}(x_1)\phi_{b_2}(x_2) - \phi_{b_2}(x_1)\phi_{b_1}(x_2)\right].$$

The matrix element of a two-body operator $\hat{V}$ between them is

$$\begin{aligned}\langle\Phi_{a_1,a_2}|\hat{V}|\Phi_{b_1,b_2}\rangle = \frac{1}{2}\int \phi^*_{a_1}(x)\phi^*_{a_2}(x')V(x,x')\phi_{b_1}(x)\phi_{b_2}(x') \\ -\frac{1}{2}\int \phi^*_{a_1}(x)\phi^*_{a_2}(x')V(x,x')\phi_{b_2}(x)\phi_{b_1}(x') \\ +\frac{1}{2}\int \phi^*_{a_2}(x)\phi^*_{a_1}(x')V(x,x')\phi_{b_2}(x)\phi_{b_1}(x') \\ -\frac{1}{2}\int \phi^*_{a_2}(x)\phi^*_{a_1}(x')V(x,x')\phi_{b_1}(x)\phi_{b_2}(x').\end{aligned}$$

This can be simplified further by using the fact that the interaction must be symmetric, $V(x,x') = V(x',x)$; then the first and third terms are identical except for the dummy variables of integration, and the same for the second and fourth terms. Then the final result is

$$\langle \Phi_{a_1,a_2} | \hat{V} | \Phi_{b_1,b_2} \rangle = \int \phi^*_{a_1}(x)\phi^*_{a_2}(x')V(x,x')\phi_{b_1}(x)\phi_{b_2}(x') - \int \phi^*_{a_1}(x)\phi^*_{a_2}(x')V(x,x')\phi_{b_2}(x)\phi_{b_1}(x'). \tag{2.60}$$

The first term is called the *direct* term, while the second is the *exchange* term, which arises from the indistinguishability of the particles.

Earlier I introduced the nonsymmetric matrix elements in Eqn. (2.17). Now I can introduce the *antisymmeteric two-body matrix elements*

$$V^A(ab,cd) = V^N(ab,cd) - V^N(ab,dc). \tag{2.61}$$

We have the following relations:

$$V^A(ab,cd) = -V^A(ab,dc) = -V^A(ba,cd) = +V^A(ba,dc). \tag{2.62}$$

From these antisymmetric two-body matrix elements (TBMEs) we can build matrix elements of two-body operators between any two Slater determinants.

Similar to the one-body operator, given any two N-particle Slater determinants, there will be a nonzero matrix element only if the Slater determinants differ by at most two different occupied states, and those can be categorized into three cases:

Case 1 for two-body matrix elements: the N-particle Slater determinants are identical, leaving

$$\langle a_1 a_2 \ldots | \hat{V} | a_1 a_2 \ldots \rangle = \sum_{a<b} V^A(ab,ab) \tag{2.63}$$

or

Case 2 for two-body matrix elements: the N-particle Slater determinants are identical, except for exactly one occupancy each, $a_x \neq b_x$:

$$\langle a_1 a_2 \ldots | \hat{V} | b_1 b_2 \ldots \rangle = \sum_{i \neq x} (\text{phase}) V^A(a_i a_x, a_i b_x) \tag{2.64}$$

or

Case 3 for two-body matrix elements: the N-particle Slater determinants are identical, except for exactly two occupancy each, $a_x \neq b_x$ and $a_y \neq b_y$:

$$\langle a_1 a_2 \ldots | \hat{V} | \Phi_{b_1 b_2 \ldots} \rangle = (\text{phase}) V^A(a_x a_y, b_x b_y). \tag{2.65}$$

In both cases 2 and 3 above, the phase that appears is straightforward but tedious to determine. Rather than try to give a rule, I will postpone detailed discussion of the phase. Practice can be found in the exercises, as well as in

Chapter 6 and Chapter 9.6. You will note, however, that I only give problems up to three particles; for four particles, each Slater determinant has 4!=24 terms, which becomes difficult to handle. When we develop the full operator formalism in Chapter 6, handling cases with four, five, six, or more fermions will become much easier.

2.6 Summary

What you should get from this chapter:

• To tackle the quantum mechanics of many-particle systems, we turn to the matrix formulation of quantum mechanics.

• Products of orthonormalized single-particle wavefunctions make for a convenient basis for many-body systems.

• The many-body wavefunctions for systems of identical particles must be either symmetric (bosons) or antisymmetric (fermions) under interchange of coordinates. When married to product wavefunctions, this leads to permanents (for bosons) and determinants (for fermions).

• Despite the apparent complexity of symmeterizing/antisymmeterizing wavefunctions, the normalization and orthogonality of permanent and determinant basis wavefunctions is straightforward. Furthermore the matrix elements between such wavefunctions are also surprisingly simple. It is clear, despite the origin in a coordinate-space form, that the orthonormality relations and matrix elements depend primarily upon the list of single-particle states used to construct the permanents/determinants, that is, upon the *occupied* single-particle states.

2.7 Exercises

(2.1) For *non-identical* particles, show that there are the following two nontrivial cases for matrix elements of one-body operators $\hat{\mathcal{O}}$:

Case 1: The initial and final single-particle labels all agree, that is, if we have $|\alpha = a_1 a_2 a_3 \ldots\rangle$ and $|\beta = b_1 b_2 b_3 \ldots\rangle$ then $a_i = b_i$ for all i. The matrix element is

$$\langle\alpha|\hat{\mathcal{O}}|\alpha\rangle = \sum_i O_{a_i a_i}. \tag{2.66}$$

and

Case 2: The single-particle labels all agree, $a_i = b_i$, except for exactly one pair, $a_j \neq b_j$. Then

$$\langle\alpha|\hat{\mathcal{O}}|\beta\rangle = O_{a_j b_j}. \tag{2.67}$$

(2.2) Derive the three nontrivial cases for matrix elements of two-body operators, taken between product wavefunctions of non-identical particles.

(2.3) Derive (2.36), or at least convince yourself it is correct.

(2.4) Show that (2.38), (2.39) are true.

(2.5) For the following boson permanents (assume normalized), show in detail the following matrix elements of a one-body operator $\hat{\mathcal{O}}$ are correct (that is, confirm for these cases that (2.41) :

$$\langle 13|\hat{\mathcal{O}}|12\rangle = O_{32};$$

$$\langle 1^2|\hat{\mathcal{O}}|12\rangle = \sqrt{2}O_{12};$$

$$\langle 124|\hat{\mathcal{O}}|123\rangle = O_{43};$$

$$\langle 1^2 3|\hat{\mathcal{O}}|123\rangle = \sqrt{2}O_{12};$$

$$\langle 1^2 2|\hat{\mathcal{O}}|1^3\rangle = \sqrt{3}O_{21}.$$

(2.6) For the following Slater determinants (normalized), show in detail the following matrix elements of a one-body operator $\hat{\mathcal{O}}$ are correct:

$$\langle 123|\hat{\mathcal{O}}|123\rangle = O_{11} + O_{22} + O_{33};$$

$$\langle 124|\hat{\mathcal{O}}|123\rangle = O_{34};$$

$$\langle 123|\hat{\mathcal{O}}|134\rangle = -O_{34};$$

$$\langle 123|\hat{\mathcal{O}}|234\rangle = O_{14}.$$

(2.7) For the following Slater determinants (normalized), show in detail the following matrix elements of a two-body operator $\hat{V}$ are correct:

$$\langle 123|\hat{\mathcal{O}}|123\rangle = V^A(12,12) + V^A(13,13) + V^A(23,23);$$

$$\langle 123|\hat{\mathcal{O}}|124\rangle = V^A(13,14) + V^A(23,24);$$

$$\langle 123|\hat{\mathcal{O}}|145\rangle = V^A(23,45);$$

$$\langle 123|\hat{\mathcal{O}}|235\rangle = V^A(13,35) + V^A(12,25);$$

$$\langle 123|\hat{\mathcal{O}}|245\rangle = -V^A(13,45).$$

Chapter 3

Operator methods for the harmonic oscillator

Steter Tropfen höhlt den Stein. – *German saying.*

Before delving further into many-body systems, let's review carefully the simple one-dimensional simple harmonic oscillator, that is a particle of mass m attached to a spring of spring constant k and thus with classical oscillator frequency $\omega = \sqrt{k/m}$. Even though this is a single-particle system, we can learn a lot from it. The Hamiltonian is

$$\hat{H}_{\rm SHO} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2. \tag{3.1}$$

There are two ways to find the eigenenergies and eigenfunctions of this fundamental system. The first is to solve the differential equation through a series of straightforward, if occasionally tedious steps that can be found in any textbook on basic quantum mechanics. The ultimate result is the eigenenergies are $E_n = \hbar\omega(n + 1/2), n = 0, 1, 2, 3, \ldots$, and the eigenfunctions are, up to some normalization, of the form,

$$\Psi_n(x) = H_n\left(x\sqrt{\frac{m\omega}{\hbar}}\right)\exp\left(-\frac{m\omega x^2}{2\hbar}\right), \tag{3.2}$$

where H_n is a Hermite polynomial of order n. The quantity $b = \sqrt{\hbar/m\omega}$ is known as the 'oscillator length.'

Somewhat curiously, in most textbooks this straightforward method of solution via solving the differential equation directly is often presented second. The other method, often presented first, is in a very real sense simpler, and ultimately very powerful. Indeed, we will use it as a starting paradigm to motivate much of the rest of this book. But it is far from being intuitive. This is the method of creation and annhilation operators, also known as ladder operators.

3.1 Ladder operators

First let's take a step in abstraction. You know that the coordinate-space representation of the momentum operator is

$$\hat{p} = \frac{\hbar}{i}\frac{d}{dx}. \tag{3.3}$$

Then the harmonic oscillator Hamiltonian can be written in a form more congruent to classical mechanics:

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2. \tag{3.4}$$

I put the hat on both the momentum p and coordinate x to emphasize that both are operators, and that neither truly is more fundamental than the other.

From algebra we know that $a^2 + b^2 = (a + ib)(a - ib)$. Inspired by this, we introduce new operators,

$$\hat{B} = \frac{1}{\sqrt{2}}\left(\frac{\hat{x}}{b} + i\frac{b}{\hbar}\hat{p}\right), \hat{B}^\dagger = \frac{1}{\sqrt{2}}\left(\frac{\hat{x}}{b} - i\frac{b}{\hbar}\hat{p}\right). \tag{3.5}$$

These operators, helpfully, are dimensionless (the oscillator length b has, naturally, units of length, and the units of $\hbar$ are length $\times$ momentum). And as both position $\hat{x}$ and momentum $\hat{p}$ are Hermitian operators, we can see that these two operators are indeed Hermitian adjoints of each other.

(The notation $\hat{B}, \hat{B}^\dagger$ is nonstandard, but I want to reserve later $\hat{a}$ for fermions and $\hat{b}$ for bosons.)

Does this help? If you have been paying attention, you may have a concern: $\hat{x}, \hat{p}$ are operators, not scalars, so we do not expect them to commute. Indeed, the basic commutation relation is

$$[\hat{x}, \hat{p}] = i\hbar. \tag{3.6}$$

(As I mentioned earlier, physicists tend to be obsessed with commutators. After a while, when presented with a set of operators, your first instinct is to take their mutual commutators. Part of the reason is that if the commutation relation looks like something familiar, say the commutation relations of angular momentum operators, then often we can apply our intuition. We'll see examples of this later.)

With these simple operators, we can rewrite (3.4)

$$\hat{H} = \hbar\omega\left(\hat{B}^\dagger\hat{B} + \frac{1}{2}\right). \tag{3.7}$$

But don't think we are done with commutators. First, the commutators among the the new operators are (you should prove as an exercise)

$$\left[\hat{B}, \hat{B}^\dagger\right] = 1, \tag{3.8}$$

a nicely simple result. Note that both $\hat{B}$ and $\hat{B}^\dagger$ trivially commute with itself.

But let's not stop there. Let's compute the commutator of $\hat{B}^\dagger$ with the Hamiltonian; this boils down to the commutator

$$\begin{aligned}\left[\hat{B}^\dagger\hat{B},\hat{B}^\dagger\right] &= \hat{B}^\dagger\hat{B}\hat{B}^\dagger - \hat{B}^\dagger\hat{B}^\dagger\hat{B} \\ &= \hat{B}^\dagger\left(1+\hat{B}^\dagger\hat{B}\right) - \hat{B}^\dagger\hat{B}^\dagger\hat{B} = \hat{B}^\dagger\end{aligned} \tag{3.9}$$

using just (3.8). But now we can use this to get the commutator of $\hat{B}^\dagger$ with the simple harmonic oscillator Hamiltonian (3.4):

$$\left[\hat{H}_{\rm SHO},\hat{B}^\dagger\right] = \hbar\omega\hat{B}^\dagger. \tag{3.10}$$

It's important to emphasize here that for a more general Hamiltonian this simple commutator will not result. But for the harmonic oscillator we can exploit this.

As for any Hamiltonian there must exist the eigensolutions, which for convenience we label simply as $|n\rangle$,

$$\hat{H}_{\rm SHO}|n\rangle = E_n|n\rangle. \tag{3.11}$$

We don't have to yet know the value of E_n. But now we are in a position to prove the state $\hat{B}^\dagger|n\rangle$ is also an eigensolution:

$$\begin{aligned}\hat{H}_{\rm SHO}\left(\hat{B}^\dagger|n\rangle\right) = \hat{H}_{\rm SHO}\hat{B}^\dagger|n\rangle &= \left(\hat{B}^\dagger\hat{H}_{\rm SHO}+\hbar\omega\hat{B}^\dagger\right)|n\rangle \\ = \hat{B}^\dagger\hat{H}_{\rm SHO}|n\rangle + \hbar\omega\hat{B}^\dagger|n\rangle &= \hat{B}^\dagger E_n|n\rangle + \hbar\omega\hat{B}^\dagger|n\rangle \\ &= (E_n+\hbar\omega)\,\hat{B}^\dagger|n\rangle,\end{aligned} \tag{3.12}$$

that is, $\hat{B}^\dagger|n\rangle$ is also an eigenstate, with energy $E_n+\hbar\omega$.

Because of this, we call $\hat{B}$ a *raising* operator, because it raises the energy by $\hbar\omega$. We also call it a *creation* operation because it creates $\hbar\omega$ energy.

Similarly, one can prove (and you should do it) that $\hat{B}|n\rangle$ is also an eigenstate of $\hat{H}_{\rm SHO}$, with eigenenergy $E_n-\hbar\omega$. Thus $\hat{B}$ is a *lowering* or *annihilation* (or *destruction*) operator. Together they are *ladder* operators, because they take us up and down on the ladder of the spectrum.

But there must be some ground state energy, that is, some $|n\rangle$ with the lowest energy. In that case

$$\hat{B}|n\rangle = 0 \tag{3.13}$$

We set $n=0$, and while this is the ground state, we also call $|0\rangle$ the *vacuum*. Notice, peculiarly, that the vacuum is not zero. This is like the difference between the empty set, and no set at all.

We have to find the ground state energy: This is easy:

$$E_0 = \langle 0|\hat{H}_{\rm SHO}|0\rangle = \hbar\omega\langle 0|\left(\hat{B}^\dagger\hat{B}+\frac{1}{2}\right)|0\rangle = \frac{1}{2}\hbar\omega \tag{3.14}$$

where I used (3.13).

From this we conclude the spectrum is $E_n = (\hbar\omega + 1/2)$. (One has to worry if there are states we cannot reach this way starting from the ground state, but I will simply assert there are no such states.) Not only that, but also we inexorably conclude that

$$|n\rangle \propto \left(\hat{B}^\dagger\right)^n |0\rangle. \tag{3.15}$$

This is a rather astounding result. We wrote the simple harmonic oscillator Hamiltonian in terms of the ladder operators. We deduced the spectrum. We can construct any and all harmonic oscillator states using the raising operator.

When I first learned the method of ladder operators, and how powerful they were, I was disappointed to realized one couldn't apply them to an arbitrary one-body potential. It was only much later that I understand one could apply ladder operators to other systems, but it turns out that one must have an exact symmetry or symmetries represented by a group structure underneath. We'll see this when we come to angular momentum in the next chapter.

3.2 Normalization and matrix elements

Even more powerful results await us. First thing is the normalization of $\hat{B}^\dagger|n\rangle$, assuming $|n\rangle$ is already normalized. For this we need the adjoint:

$$\left(\hat{B}^\dagger|n\rangle\right)^\dagger = \langle n|\hat{B}. \tag{3.16}$$

Then we need $\langle n|\hat{B}\hat{B}^\dagger|n\rangle$. Using the fundamental commutation relation (3.8):

$$\langle n|\hat{B}\hat{B}^\dagger|n\rangle = \langle n|\left(1 + \hat{B}^\dagger\hat{B}\right)|n\rangle. \tag{3.17}$$

Now for this we can use already-proven results that $\hat{B}^\dagger\hat{B} = \hat{H}_{\rm SHO}/\hbar\omega - 1/2$ and $\hat{H}_{\rm SHO}|n\rangle = \hbar\omega(n+1/2)|n\rangle$, we conclude that $\hat{B}\,\dagger\,\hat{B}|n\rangle = n|n\rangle$. Putting this all together, we get

$$\langle n|\hat{B}\hat{B}^\dagger|n\rangle = (n+1)\langle n|n\rangle = n+1. \tag{3.18}$$

From this, we deduce

$$\hat{B}^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle. \tag{3.19}$$

Alternately, we can write this as a matrix element:

$$\langle n'|\hat{B}^\dagger|n\rangle = \sqrt{n+1}\delta_{n',n+1}. \tag{3.20}$$

By taking the adjoint, we get

$$\langle n|\hat{B}|n'\rangle = \sqrt{n+1}\delta_{n',n+1} = \sqrt{n'}\delta_{n,n'-1}. \tag{3.21}$$

or

$$\hat{B}|n\rangle = \sqrt{n}|n-1\rangle. \tag{3.22}$$

Notice that, consistent with our expectation, we get $\hat{B}|0\rangle = 0$.

Now we can construct normalized eigenstates:

$$|n+1\rangle = \frac{1}{\sqrt{n+1}}\hat{B}^\dagger|n\rangle, \tag{3.23}$$

or

$$|n\rangle = \frac{1}{\sqrt{n!}}\left(\hat{B}^\dagger\right)^n|0\rangle. \tag{3.24}$$

Not only that, but we can go further. We can write

$$\hat{x} = b\frac{1}{\sqrt{2}}\left(\hat{B}^\dagger + \hat{B}\right), \tag{3.25}$$

$$\hat{p} = i\frac{\hbar}{b}\frac{1}{\sqrt{2}}\left(\hat{B}^\dagger - \hat{B}\right). \tag{3.26}$$

This allows us to compute matrix elements of functions of x and p in the harmonic oscillator basis *without resorting to integrals*.

So, for example, if we want to compute the matrix elements of $\hat{x}$,

$$\langle n'|\hat{x}|n\rangle = \frac{b}{\sqrt{2}}\left(\langle n'|\hat{B}^\dagger|n\rangle + \langle n'|\hat{B}|n\rangle\right), \tag{3.27}$$

we can use the fact that $\hat{B}^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle$ and get

$$\langle n'|\hat{x}|n\rangle = \frac{b}{\sqrt{2}}\left(\delta_{n',n+1}\sqrt{n+1} + \delta_{n,n'+1}\sqrt{n'+1}\right). \tag{3.28}$$

When we take powers of $\hat{x}$ it gets more complicated, because we have to pay attention to ordering. For example,

$$\hat{x}^2 = \frac{b}{2}\left(\hat{B}^\dagger + \hat{B}\right)^2 = \frac{b^2}{2}\left(\hat{B}^\dagger\hat{B}^\dagger + \hat{B}\hat{B} + \hat{B}^\dagger\hat{B} + \hat{B}\hat{B}^\dagger\right). \tag{3.29}$$

Now there are various tricks to simplifying such expressions, and they take some practice. For example, we often want to put operators into *normal order*, with all the creation operators to the left and all the annihilation operators to the right, that is, of the form $\hat{B}^\dagger\hat{B}^\dagger\hat{B}^\dagger\ldots\hat{B}\hat{B}\hat{B}$. Sometimes it is more convenient to put into *antinormal order*, which is exactly what it sounds like. At other times, however, it may be convenient to group operators into the number operator $\hat{N} = \hat{B}^\dagger\hat{B}$ even if one doesn't have normal or antinormal order, because the basis states are eigenstates of the number operator and so its action is easy to evaluate. To determine which strategy is best, you must rely upon experience, as well as a little or a lot of experimentation. When in doubt, put into normal order.

Therefore we use the basic commutation relation to rewrite $\hat{B}\hat{B}^\dagger = 1 + \hat{B}^\dagger\hat{B}$, and we get

$$\hat{x}^2 = \frac{b^2}{2}\left(1 + 2\hat{N} + \hat{B}^\dagger\hat{B}^\dagger + \hat{B}\hat{B}\right). \tag{3.30}$$

To evaluate the matrix element, use

$$\hat{B}^\dagger \hat{B}^\dagger |n\rangle = \hat{B}^\dagger \sqrt{n+1}|n+1\rangle = \sqrt{(n+1)(n+2)}|n+2\rangle,$$

etc. The final matrix element is $\langle n'|\hat{x}^2|n\rangle$

$$= \frac{b^2}{2}\left(\delta_{n',n}(2n+1) + \delta_{n',n+2}\sqrt{(n+1)(n+2)} + \delta_{n,n'+2}\sqrt{(n'+1)(n'+2)}\right). \tag{3.31}$$

In a similar fashion one can (and you should) derive $\langle n'|\hat{p}^2|n\rangle$

$$= \frac{\hbar^2}{2b^2}\left(\delta_{n',n}(2n+1) - \delta_{n',n+2}\sqrt{(n+1)(n+2)} - \delta_{n,n'+2}\sqrt{(n'+1)(n'+2)}\right). \tag{3.32}$$

When computing the matrix elements of $\hat{p}^2/2m + m\omega^2\hat{x}^2$, one finds the off-diagonal matrix elements cancel, leaving only the diagonal terms with the correct energy.

3.3 Example: Diagonalizing the quartic oscillator

With these tools in hand, we can revisit the quartic oscillator (1.75), which we looked at variationally in section 1.7. But now we can compute all the matrix elements using creation and annihilation operators.

By manipulating the ladder operators, one can derive

$$\begin{aligned}\hat{x}^4 = \frac{b^4}{4}\Big(&3 + 6\hat{N} + 6\hat{N}^2 + (1+2\hat{N})(\hat{B}^\dagger\hat{B}^\dagger + \hat{B}\hat{B}) \\ &+ (\hat{B}^\dagger\hat{B}^\dagger + \hat{B}\hat{B})(1+2\hat{N}) + (\hat{B}^\dagger)^4 + (\hat{B})^4\Big)\end{aligned} \tag{3.33}$$

From this we can compute the matrix elements of x^4 in the oscillator basis, remembering that $\hat{N}|n\rangle = n|n\rangle$ and $\langle n|\hat{N} = \langle n|n$:

$$\langle n|x^4|n\rangle = \frac{b^4}{4}(3 + 6n(n+1)), \tag{3.34}$$

$$\langle n+2|x^4|n\rangle = \frac{b^4}{4}(6+4n)\sqrt{(n+1)(n+2)}, \tag{3.35}$$

$$\langle n+4|x^4|n\rangle = \frac{b^4}{4}\sqrt{(n+1)(n+2)(n+3)(n+4)}, \tag{3.36}$$

plus of course the trivial Hermitian conjugates. Then, using from variational theory

$$b_{\min} = \left(\frac{\hbar^2}{m\lambda}\right)^{1/6}, \tag{3.37}$$

we can compute the Hamiltonian matrix elements.

$$\langle n|\hat{H}|n\rangle = \frac{\hbar^{4/3}\lambda^{1/3}}{8m^{2/3}}(3+6n+2n^2), \tag{3.38}$$

$$\langle n+2|\hat{H}|n\rangle = \frac{\hbar^{4/3}\lambda^{1/3}}{6m^{2/3}}(n\sqrt{(n+1)(n+2)}, \tag{3.39}$$

$$\langle n+4|\hat{H}|n\rangle = \frac{\hbar^{4/3}\lambda^{1/3}}{24m^{2/3}}\sqrt{(n+1)(n+2)(n+3)(n+4)}. \tag{3.40}$$

As a check, note that the diagonal term reproduces the variational result for $n=0$; in the exercises you will check it for $n=1$.

Again parity plays a role: the matrix elements do not connect even n with odd n. Taking $n=0,2,4,6$, the matrix is

$$\mathbf{H} = \frac{\hbar^{4/3}\lambda^{1/3}}{24m^{2/3}}\begin{pmatrix} 9 & 0 & 2\sqrt{6} & 0 \\ 0 & 69 & 2/\sqrt{3} & 6\sqrt{10} \\ 2\sqrt{6} & 2/\sqrt{3} & 177 & \sqrt{40/3} \\ 0 & 6\sqrt{10} & \sqrt{40/3} & 333 \end{pmatrix}. \tag{3.41}$$

(Note: although I write everthing out in terms of integers and radicals, ultimately one must solve numerically. Also, be aware that some platforms, such as Mathematica, will attempt to solve integer matrices exactly.)

Already at this point the ground state of this truncated matrix, 0.367639, is very close to the numerically exactly answer of 0.367607. (The convergence is much faster than for the δ-potential we saw in Figure 1.1, because the latter requires many more basis states, of increasingly small wavelength, to resolve the zero-range interaction.)

With the numerical solution in hand, one can also compute observables, such as $\langle x^2\rangle$. Solving $\mathbf{H}\vec{v} = E\vec{v}$ is equivalent to expanding

$$|\Psi\rangle = \sum_n v_n|n\rangle$$

and then

$$\langle x^2\rangle = \langle\Psi|x^2|\Psi\rangle = \sum_{n',n} v^*_{n'}v_n\langle n'|x^2|n\rangle \tag{3.42}$$

where we can use the matrix elements computed in (3.31). If we truncate at $n=0$, then we get $\langle x^2\rangle = 0.5(\hbar^2/m\lambda)^{1/6}$, but adding more states we quickly converge to the correct answer of $0.522127(\hbar^2/m\lambda)^{1/6}$.

3.4 Example: Return of the δ-potential

We can also revisit the δ-potential (1.48); this time in a harmonic oscillator basis rather a basis of cosines. We already have in hand the matrix elements for the kinetic energy. Now we need

$$\langle n'|\delta(x)|n\rangle = \int \psi^*_{n'}(x)\delta(x)\psi_n(x)dx = \psi_{n'}(0)\psi_n(0), \tag{3.43}$$

where use the fact the harmonic oscillator wavefunctions can be made real. Although it is beyond the immediate scope of this chapter, from most quantum textbooks one can find for the one-dimensional harmonic oscillator for even n,

$$\psi_n(0) = (-1)^{n/2}\sqrt{\frac{n!}{b2^n\sqrt{\pi}\left(\frac{n}{2}!\right)^2}}, \tag{3.44}$$

for n even (and vanishes for n odd). Again choosing the variational solution

$$b = \frac{\hbar^2\sqrt{\pi}}{2m\lambda}, \tag{3.45}$$

we can work out the matrix elements for the Hamiltonian,

Again note for $n = 0$ we regain the variational limit. Only even n contribute, so taking $n = 0, 2, 4, 6$ we have

$$\mathbf{H} = \frac{m\lambda^2}{\hbar^2\pi}\begin{pmatrix} -1 & 0 & \sqrt{3/2} & \sqrt{5}/2 \\ 0 & 4 & -3\sqrt{3}/2 & -\sqrt{5/8} \\ -\sqrt{3/2} & -3\sqrt{3}/2 & 33/4 & -7\sqrt{30}/8 \\ \sqrt{5}/2 & -\sqrt{5/8} & -7\sqrt{30}/8 & 99/8 \end{pmatrix}. \tag{3.46}$$

The numerical convergence is much slower than for the quartic oscillator, as shown in Figure 3.1. Again, to dissect the convergence I put the difference between the numerical energy and the exact value on a log-log plot (Figure 3.2).

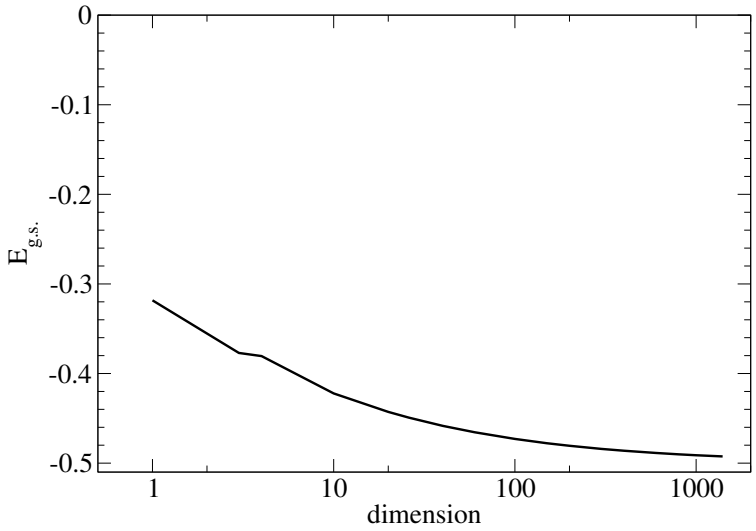

Figure 3.1: Convergence of the ground state energy for the δ-potential in a harmonic oscillator basis. Energy is in units of $\hbar^2/m\lambda$.

In the same way as in the previous section we can compute the variance $\langle x^2\rangle$ in the ground state wavefunction, in Figure 3.3.

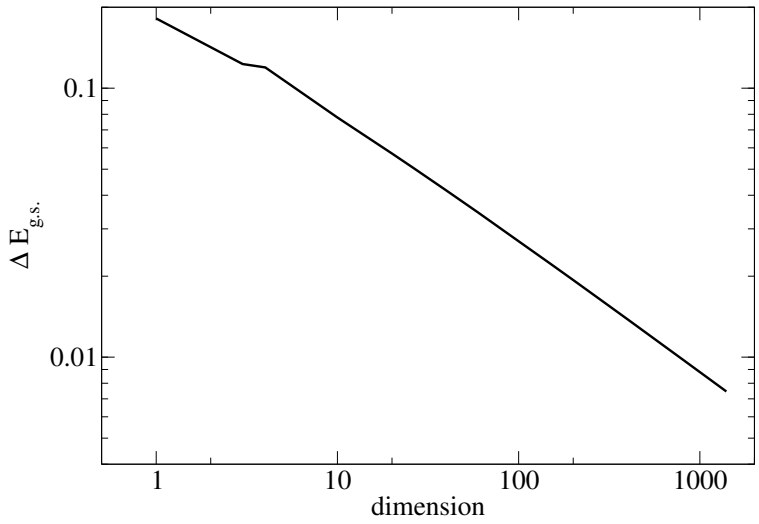

Figure 3.2: Error of the numerical ground state energy for the δ-potential in a harmonic oscillator basis. $\Delta E_{g.s.} = E_{\text{numerical}} - E_{\text{exact}}$.

3.5 Coherent states

The *coherent state* is defined by

$$|z\rangle = \exp(z\hat{B}^\dagger)|0\rangle = \sum_{n=0} \frac{z^n \left(\hat{B}^\dagger\right)^n}{n!}|0\rangle = \sum_{n=0} \frac{z^n}{\sqrt{n!}}|n\rangle \tag{3.47}$$

where z is a complex number. One can show the normalization is

$$\langle z|z\rangle = \exp(|z|^2) \tag{3.48}$$

and also that the coherent (ket) state is an eigenstate of the annihilation operator,

$$\hat{B}|z\rangle = z|z\rangle \tag{3.49}$$

so that consequently we also have the adjoint equation $\langle z|\hat{B}^\dagger = z^*\langle z|$.

Among the many uses of coherent states is the explicit demonstration of the *correspondence principle*, that is, an exact quantum state which goes over to the exact classical solution. This is left to the exercises.

3.6 Summary

What you should get from this chapter:

• One can rewrite the Schrödinger equation for the simple harmonic oscillator using ladder or creation/annihilation operators. While the operators are

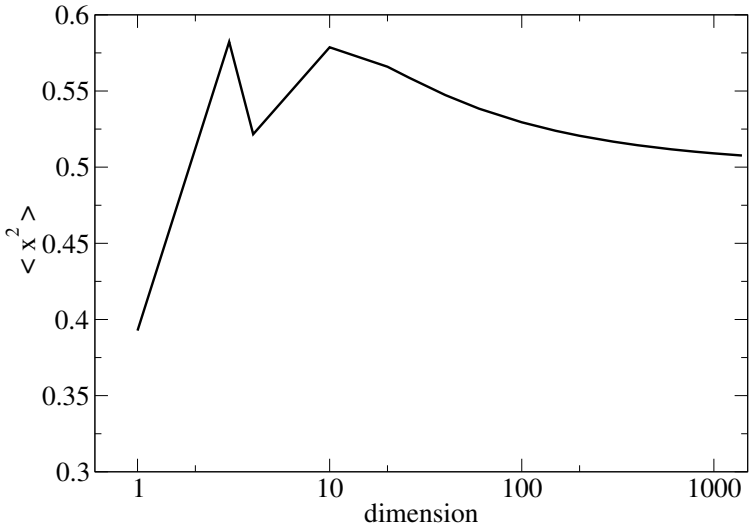

Figure 3.3: Convergence of the ground state variance $\langle x^2 \rangle$ for the δ-potential in a harmonic oscillator basis. Units are $m\lambda/\hbar^2$.

abstract, by simple manipulation one can derive the eigenenergies as well as many interesting observables (expectation value of x^2, etc.).

• The creation/annihilation operators facilitate the matrix formulation of quantum mechanics, by making many matrix elements straightforward to calculate.

3.7 Exercises

(3.1) Prove (3.7) using (3.6).

(3.2) The coordinate-space ground state wavefunction is a Gaussian,

$$\psi_0(x) = \langle x|0\rangle = c \exp\left(-m\omega x^2/2\hbar\right),$$

where c is just an uninteresting normalization constant. Using the coordinate-space form of $\hat{B}$, show explicitly that $\hat{B}|0\rangle = 0$.

(3.3) For each harmonic oscillator state $|n\rangle$, compute $\Delta x \Delta p$, where

$$\Delta x = \sqrt{\langle n|x^2|n\rangle - \langle n|x|n\rangle^2}$$

and similarly for Δp. Show that every oscillator eigenstate satisfies the Heisenberg bound , $\Delta x \Delta p \geq \hbar/2$, with equality only for $n = 0$.

(3.4) Compute the matrix elements of $\hat{p}^4$ in the harmonic oscillator basis.

(3.5) Show that $\hat{B}^\dagger \hat{B}^\dagger \hat{B}\hat{B} = \hat{N}^2 - \hat{N}$, while $\hat{B}\hat{B}\hat{B}^\dagger \hat{B}^\dagger = 2 + 3\hat{N} + \hat{N}^2$.

(3.6) It's useful to be good at Gaussian integrals. For the ground state, the wavefunction is

$$\psi_0(x) = \langle x|0\rangle = \frac{1}{b^{1/2}\pi^{1/4}}\exp(-x^2/2b^2);$$

show this is normalized. The first excited state is

$$\psi_1(x) = \langle x|1\rangle = \frac{\sqrt{2}}{b^{3/2}\pi^{1/4}}x\exp(-x^2/2b^2);$$

show *this* is normalized. Furthermore, compute $\langle x^2\rangle$ and $\langle x^4\rangle$ for both $n = 0, 1$. Finally, show that, for the harmonic oscillator Hamiltonian, $\langle\hat{H}\rangle$ agrees with the diagonal matrix elements in (3.31) and (3.32).

(3.7) Find numerically the energy of the first excited state of the quartic oscillator, and the value of $\langle x^2\rangle$. To get the eigenpairs, diagonalize the matrix in the harmonic oscillator basis given by (3.38)-(3.40), and for the expectation value use (3.31). You should get 1.317272 and 1.300342, respectively.

(3.8) Show that (3.45) gives the minimum for a Gaussian *ansatz* for the δ-potential.

(3.9) Derive (3.48) and (3.49).

(3.10) For a coherent state, derive $\langle x\rangle, \langle x^2\rangle, \langle p\rangle$, and $\langle p^2\rangle$. From this demonstrate that a coherent state, like a Gaussian, minimally satisfies the Heisenberg uncertainty relation.

(3.11) For the harmonic oscillator Hamiltonian, $\hat{H} = \hbar\omega(\hat{B}^\dagger\hat{B} + \frac{1}{2})$, show that an exact solution to the time-dependent Schrödinger equation is given by

$$|\psi(t)\rangle = e^{-i\omega t/2}|z_0 e^{-i\omega t}\rangle,$$

(that is, a coherent state with $z(t) = z_0\exp(-i\omega t)$ plus an additional time-dependent phase), specifically by showing that this satisfies

$$\langle\psi(t)|\hat{H} - i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = 0.$$

From this and from problem (3.10), derive $\langle x(t)\rangle$ and $\langle p(t)\rangle$ and show they are the classical trajectories for a harmonic oscillator; furthermore they satisfy the Ehrenfest theorem,

$$\langle p(t)\rangle = m\frac{d}{dt}\langle x(t)\rangle.$$

These results are true for any value of z_0, so that you can express any classical harmonic oscillator motion via a coherent state which, I repeat, is an exact solution to the quantum time-dependent Schrödinger equation. This shows that quantum mechanics goes smoothly to macroscopic classical physics, at least in this case.

(3.12) **Advanced**. Compute the matrix elements of the quartic oscillator for a coherent state. From

$$\langle\psi(t)|\hat{H} - i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = 0.$$

find an equation of motion for $z(t)$ for the quartic oscillator. Solve this numerically for random starting values of z and let evolve for a long time. Now take the Fourier transform. Generalize your matrix solutions from problem (3.7), and compare the eigenenergies to the peaks in the power spectrum of your time-dependent solution.

Chapter 4

Operator methods for angular momentum

> I have had my results for a long time: but I do not yet know how I am to arrive at them. – *Carl Friederich Gauss*

In the last chapter we reviewed the use of creation and annihilation operators, also known as ladder operators, for the simple harmonic oscillator. In this chapter I'll discuss another application of using abstract operators to a well-known system, specifically angular momentum. While this chapter can be safely skipped, it will help to get the reader used to using abstract operator formalism. In addition, several of our later detailed examples of applying the occupation representation will rely heavily upon appealing to our intuition about angular momentum in quantum mechanics.

Some of the basics–and some of the more advanced topics–of angular momentum in quantum systems can be found in the Appendices.

We begin with the classical definition of angular momentum, $\vec{L} = \vec{r} \times \vec{p}$. The quantum operator in coordinate space is then

$$\hat{\vec{L}} = \vec{r} \times \frac{\hbar}{i} \vec{\nabla}. \tag{4.1}$$

We call this the *orbital* angular momentum because it is relative between particles. In classical mechanics orbital angular momentum is the only option, but in quantum mechanics it is possible for particles to have *intrinsic* angular momentum, also called *spin*. (In practice, however, physicists are sometimes careless and use the word 'spin' to refer to any kind of angular momentum, mostly because the former is far fewer syllables than the latter.) More of this in a moment.

In Cartesian coordinates, the three components of $\hat{\vec{L}}$ are:

$$\hat{L}_x = \frac{\hbar}{i} \left(y \frac{\partial}{\partial z} - z \frac{\partial}{\partial y} \right);$$

$$\hat{L}_y = \frac{\hbar}{i}\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right); \tag{4.2}$$
$$\hat{L}_z = \frac{\hbar}{i}\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right).$$

As an exercise, show that the following commutation relations hold:

$$\left[\hat{L}_x, \hat{L}_y\right] = i\hbar\hat{L}_z,$$
$$\left[\hat{L}_y, \hat{L}_z\right] = i\hbar\hat{L}_x,$$
$$\left[\hat{L}_z, \hat{L}_x\right] = i\hbar\hat{L}_y.$$

You may at this point think we've gone commutator-crazy, but everything else we'll do in this chapter will be strictly based upon (4.3). Using commutation relations we can prove very powerful results that go far beyond the orbital angular momentum operators in (4.2). To emphasize this, I introduce the generic operators $\hat{J}_x, \hat{J}_y, \hat{J}_z$, with the same commutation relations

$$\left[\hat{J}_x, \hat{J}_y\right] = i\hbar\hat{J}_z,$$
$$\left[\hat{J}_y, \hat{J}_z\right] = i\hbar\hat{J}_x, \tag{4.3}$$
$$\left[\hat{J}_z, \hat{J}_x\right] = i\hbar\hat{J}_y.$$

These commutation relations, widely known as the SU(2) commutation relations, apply to operators far beyond just (4.2). For example, in section 15.2 I will introduce the spin matrices for spin-1/2 systems–where, despite the name, nothing is actually "spinning"–and in section 7.1 I will use apply the SU(2) commutation relations to solve a toy model of superconductivity! A third application is the toy model of Lipkin, Meshkov, and Glick, section 7.3, which is a boiled-down version of the shell model.

In the exercises you'll show that each of $\hat{J}_x, \hat{J}_y, \hat{J}_z$ commute with $\hat{J}^2 = \hat{J}_x^2 + \hat{J}_y^2 + \hat{J}_z^2$. Thus, choosing one (and only one) of them, traditionally $\hat{J}_z$, and as discussed in a previous chapter it must be possible to find a simultaneous eigenstate $|\alpha, \beta\rangle$, that is,

$$\hat{J}^2|\alpha,\beta\rangle = \alpha|\alpha,\beta\rangle; \quad \hat{J}_z|\alpha,\beta\rangle = \beta|\alpha,\beta\rangle. \tag{4.4}$$

We can actually determine quite a lot about the allowed values of α and β. To do this, introduce the raising and lowering operators:

$$\hat{J}_\pm = \hat{j}_x \pm i\hat{J}_y. \tag{4.5}$$

These are called *raising* and *lowering* operators because they do raise or lower β, the eigenvalue of $\hat{J}_z$, by one unit (of $\hbar$, but I'm going to set $\hbar = 1$ hereafter):

$$\hat{J}_\pm|\alpha,\beta\rangle = C_\pm(\alpha,\beta)|\alpha,\beta\pm 1\rangle. \tag{4.6}$$

To prove (4.6), we first need more commutators! You can work these out direct from (4.3)

$$\left[\hat{J}_z, \hat{J}_\pm\right] = \pm\hat{J}_\pm, \tag{4.7}$$

$$\left[\hat{J}_+, \hat{J}_-\right] = 2\hat{J}_z. \tag{4.8}$$

Now to prove (4.6) we need to show that $\hat{J}_\pm|\alpha,\beta\rangle$ is an eigenstate of both $\hat{J}^2$ with eigenvalue α and of $\hat{J}_z$ with eigenvalue $\beta \pm 1$. The first is easy, because $\hat{J}^2$ commutes with $\hat{J}_\pm$. This second requires a little more manipulation. Starting from

$$\hat{J}_z\left(\hat{J}_\pm|\alpha,\beta\rangle\right) \tag{4.9}$$

we apply (4.7)

$$= \left(\hat{J}_\pm\hat{J}_z \pm \hat{L}_\pm\right)|\alpha,\beta\rangle = \hat{J}_\pm\left(\hat{J}_z \pm 1\right)|\alpha,\beta\rangle = (\beta\pm 1)\left(\hat{J}_\pm|\alpha,\beta\rangle\right), \tag{4.10}$$

and so $\hat{J}_\pm|\alpha,\beta\rangle$ must be proportional to $|\alpha,\beta\pm 1\rangle$, that is, we've proven (4.6).

To find the actual value of the coefficient $C_\pm(\alpha,\beta)$ we simply must find the magnitude of $\hat{J}_\pm|\alpha,\beta\rangle$.

Before doing that, I would like to remind the reader about adjoints: if we have $\hat{A}\hat{B}|v\rangle$ the adjoint is

$$\left(\hat{A}\hat{B}|v\rangle\right)^\dagger = \langle v|\hat{B}^\dagger\hat{A}^\dagger. \tag{4.11}$$

(We'll have many occasions later on to use this so remember it!) Thus the adjoint of $\hat{J}_\pm|\alpha,\beta\rangle$ is $\langle\alpha,\beta|\hat{J}_\pm^\dagger = \langle\alpha,\beta|\hat{J}_\mp$.

Hence , if we assume $|\alpha,\beta\rangle$ already normalized, we compute the magnitude, which is the square root of

$$\begin{aligned}\langle\alpha,\beta|\hat{J}_\mp\hat{J}_\pm|\alpha,\beta\rangle &= \langle\alpha,\beta|\left(\hat{J}_x \mp i\hat{J}_y\right)\left(\hat{J}_x \pm i\hat{J}_y\right)|\alpha,\beta\rangle \\ = \langle\alpha,\beta|\hat{J}_x^2 + \hat{J}_y^2 \pm i\left[\hat{J}_x,\hat{J}_y\right]|\alpha,\beta\rangle &= \langle\alpha,\beta|\hat{J}_x^2 + \hat{J}_y^2 \mp \hat{J}_z|\alpha,\beta\rangle \\ &= \langle\alpha,\beta|\hat{J}^2 - \hat{J}_z^2 \mp \hat{J}_z|\alpha,\beta\rangle = \alpha - \beta^2 \mp \beta.\end{aligned} \tag{4.12}$$

From this we get $C_\pm(\alpha,\beta) = \sqrt{\alpha - \beta^2 \mp \beta}$. But we also get a more powerful and more important result. We *must* have $\alpha - \beta^2 \mp \beta \geq 0$, which means that $\alpha \geq \beta^2 \pm \beta$. This in turn means for a given α there are maximal and minimal values of β. Furthermore, at those extremal values, we must have $C_\pm(\alpha,\beta_{\max/\min}) = 0$, that is, $\hat{J}_\pm|\alpha,\beta_{\max/\min}\rangle = 0$, or else we could continue.

Now because $\alpha = \beta_{\max}^2 \pm \beta_{\max}$ we realize that $\beta_{\max} = -\beta_{\min}$. And because we increase β in unit steps from $\beta_{\min}$ to $\beta_{\max}$, we must have $2\beta_{\max} = N$ an integer. Then, $\beta_{\max} = j = N/2$, and $\beta_{\min} = -j$, and finally $\alpha = j(j+1)$.

We can now rewrite (4.6) as

$$\hat{J}_\pm|j,m\rangle = \sqrt{j(j+1) - m^2 \mp m}|j,m\pm 1\rangle. \tag{4.13}$$

I used $\hat{J}_\pm$ etc. rather than $\hat{L}_\pm$ to emphasize the generic nature: this is not restricted to orbital angular momentum, and in fact works for any operators that satisfy the SU(2) commutation relations (4.3).

Thus we see that we the quantum number j can take on either integer or half-integer values. For orbital angular momentum $\hat{\vec{L}}$ in (4.2) only integer values are possible. Half-integer values come from intrinsic angular momentum or spin; in particular it arises in Dirac's relativistic wave equation. It is important to note that despite the name 'spin' one does not have a little tiny ball of matter spinning around; in that case, one would still get integer values. Even without the Dirac equation, however, half-integer values of j are mathematically possible, although not obligatory (as are integer values, as one cannot escape orbital angular momentum). It is interesting that nature nonetheless provides us particles with half-integer values of j. This is perhaps fortunate, as chemistry would have been much less interesting (see exercise on the bosonic atom).

Although the above argument may seem overly abstract, that abstraction is actually its power, a power I hope you'll come to appreciate. In all of the above we *never* referenced the coordinate-space representation of $\hat{\vec{L}}$ but only commutation relations. This has tremendous impact: it means whenever we have operators, however abstract, that satisfy the SU(2) commutation relations (4.3), we can apply the intuition we have built up for angular momentum. Indeed, later on we'll do just that for two toy examples, the Lipkin model and the seniority model for pairing.

The most important point of this chapter, however, is to emphasize the power of abstract operators, using only commutation relations. Believing in the power of that abstraction is important. Up to now when we have used operators, such as $\hat{b}, \hat{b}^\dagger$ for the harmonic oscillator and $\hat{L}_z$ etc for angular momentum, you knew that behind them were coordinate space operators such as derivatives and so on, and so one might feel the use of commutation relations, while definitely useful, are simply a short hand for the 'real' coordinate-space work.

In the next two chapters, however, you will have to abandon any such notion. We will have operators that we manipulate using commutation relations and the like. But there will not be any explicit coordinate-space representation. This can be a difficult fact to swallow, but let's plunge in.

4.1 Summary

What you should get from this chapter:

• Similar to the harmonic oscillator, one can recast angular momentum in terms of ladder operators. These operators allow one to deduce facts about angular momentum, for example that one can have either integer or half-integer quantum numbers, and to calculate some matrix elements, without recourse to coordinate-space representations.

4.2 Exercises

(4.1): Using Eq. (4.3), show that $\left[\hat{J}_x, \hat{J}^2\right] = \left[\hat{J}_y, \hat{J}^2\right] = \left[\hat{J}_z, \hat{J}^2\right] = 0$, where $\hat{J}^2 = \hat{J}_x^2 + \hat{J}_y^2 + \hat{J}_z^2$.

(4.2) Show that the spin matrices

$$\mathbf{S}_x = \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \ \mathbf{S}_y = \frac{1}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \ \mathbf{S}_z = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{4.14}$$

satisfy the SU(2) commutation relations.

(4.3) Show the matrices

$$\mathbf{L}_x = \frac{1}{2}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \ \mathbf{L}_y = \frac{i}{2}\begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix},$$
$$\mathbf{L}_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \tag{4.15}$$

satisfy the SU(2) commutation relations.

(4.4) Find the raising and lowering operators $\mathbf{L}_\pm$ from the matrices in problem (4.3). Confirm they satisfy (4.7), (4.8)

(4.5) Problems 4.2 and 4.3 provide matrix representations for angular momentum 1/2 and 1. What about 3/2? We can guess the form for

$$\mathrm{J}_z = \frac{1}{2}\begin{pmatrix} 3 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -3 \end{pmatrix} \tag{4.16}$$

as well as the raising

$$\mathrm{J}_+ = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{pmatrix} \tag{4.17}$$

and lowering

$$\mathrm{J}_- = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix} \tag{4.18}$$

operators. Confirm these satisfy (4.7), (4.8), then construct $\mathbf{J}_x, \mathbf{J}_y$, and the finally confirm (4.3) for these matrices.

(4.6) **Advanced**. The above matrix representations for angular momentum 1/2, 1, and 3/2 are the minimal nontrivial representations. One can have non-minimal representations as well. One way to do this is to add angular momenta,

using Clebsch-Gordan (a.k.a. vector coupling coefficients) described in Chapter 15. Try

- adding together as an outer product two 2×2 spin-1/2 matrices to get a 4×4 representation of angular momentum 1;
- adding together as an outer product 2×2 spin-1/2 matrices with 3×3 spin-1 matrices to get a 5×5 representation of angular momentum 3/2;
- adding together as an outer product 2×2 spin-1/2 matrices with the derivative operators (4.2).

Chapter 5

Boson creation and annihilation operators

> Research is what I'm doing when I don't know what I'm doing. – *Werner von Braun*

Our story so far:

We've reviewed the basic of quantum mechanics, at least for one-particle systems. We started by thinking about many-body systems, and set upon using products of single-particle wavefunctions to construct our many-body wavefunctions. We then introduced symmetric (for bosons) and antisymmetric (for fermions) wavefunctions, in the form of permanents and determinants.

These, we found, could be conveniently, indeed nearly automatically orthonormalized if we started with an orthonormal single-particle basis. We also investigated some typical matrix elements and, despite the faintly clunky form of the permanents and determinants, found the final matrix elements were considerably simplified. So simplified, in fact, that you would be justified in thinking there must be some cleaner, simpler formalism.

And there is: the occupation representation, using the formalism of second quantization with creation and annihilation operators.

The downside of the occupation representation, and second quantization in particular, is its high level of abstraction. To get us warmed up a bit, I provided two chapters with analogous material, reminding you of the use of abstract operators for the simple harmonic oscillator in 1-D, and for the quantum theory of angular momentum.

Thus prepared, you are, I hope, ready to face the full formalism of the occupation representation, for bosons in this chapter, and for fermions in the next chapter. If you wish to skip directly to fermions, I'll repeat most of this argumentation there.

I start with boson systems because they are more closely related to the simple harmonic oscillator; furthermore, as we'll see in the next chapter, the

antisymmetry of fermion wavefunctions can make them quite counterintuitive.

On the other hand, there are generally far more detailed calculations of many-fermion systems than of many-boson systems. While the recent laboratory development of atomic Bose-Einstein condensates have lead to a surge of theoretical interest, most microscopic calculations involve mean-field approximations such as the Gross-Pitaevskii equation. While there are a host of well-worn approximations for fermion systems, as will be discussed later on, the main calculations of many-boson systems beyond the mean-field are in algebraic frameworks such as the interacting boson model (IBM) for nuclei. I won't be covering algebraic models; see instead the books by Arima and Iachello and by Talmi.

Already we have been slouching towards the occupation representation and the operator formalism, as we developed the boson permanent in section 2.4, which takes a product of single-particle wavefunctions and symmeterizes. Because of the symmeterization, we no longer associate a particular coordinate x_i to a particular boson or a particular single-particle wavefunction ϕ_i. Indeed, the best way to interpret a permanent is: choose a finite set of single particle wavefunctions, some of which may occur multiple times, and then take all possible symmetric permutation of the coordinates among them.

In slow motion: we start with an orthonormal set of single-particle wavefunctions $\phi_1, \phi_2, \phi_3 \ldots$. (In principle there are an infinite number of these, but in practice one chooses a finite set.) For an N-boson systems, we take n_1 copies of ϕ_1, n_2 copies of ϕ_2, and so on, with $n_1 + n_2 + n_3 \ldots = N$. We call n_i the *occupancy* of ϕ_i. (One of the differences with the fermion case is for the latter $n_i = 0, 1$ only.)

To construct the permanent we then distribute the coordinates $x_1, x_2, x_3, \ldots, x_N$ with all possible permutations (and with the same + sign in front) among the occupied ϕ_i. But this step seems a bit superfluous. All we *really* need to know are the occupancies, that is, how many times each state ϕ_i is occupied. So when we write a permanent wavefunction

And so: we introduce the notation $\hat{b}_i^\dagger$ to indicate a particle occupies the ith single-particle state. This is inspired by the ladder operators for the simpler harmonic oscillator and for angular momentum, but with a difference. For those latter two cases, they have explicit interpretations in terms of coordinates and derivatives. But this is no longer the case for boson creation operators: unlike the operator $\hat{B}^\dagger, \hat{B}$ from Chapter 3 which we think of as being a convenient combination of $\hat{x}$ and $\hat{p}$, we *cannot* do that for $\hat{b}_i^\dagger$. It is merely a placeholder for the single-particle state in the wavefunction. But it is so powerful a notation that soon we will forget all about permanents.

So: let us consider a system of N bosons, with single particle states $\phi_i(x)$. In the same way that the harmonic oscillator creation operator 'creates' one unit of excitation energy, we use the *boson creation operator,* $\hat{b}_i^\dagger$, to create a boson in state ϕ_i.

(The use of creation and annihilation operators is sometimes referred to as *second quantization.* The reason is historical and developmental: in the early days of quantum mechanics, as in standard introductory courses on quantum

mechanics, one treats a particle quantum mechanically, but the potential is purely classical. But of course one should treat the potential quantum mechanically as well. In order to treat replace a static, classical potential with a dynamic quantum field, one needs creation and annihilation operators. Hence these operators are used in the second quantization–the quantization of fields–following the first quantization of particles.)

We represent a permanent, that is a symmeterized product of single-particle wavefunctions, by

$$|\Phi\rangle = \hat{b}_1^\dagger \hat{b}_2^\dagger \dots \hat{b}_N^\dagger |0\rangle. \tag{5.1}$$

Now comes the key idea. Because we now have operators $\hat{b}_i^\dagger$, we have to worry about the ordering. We want the states to be symmetric under interchange, that is, we want $\hat{b}_i^\dagger \hat{b}_j^\dagger = \hat{b}_j^\dagger \hat{b}_i^\dagger$, or, writing as a commutator

$$\left[\hat{b}_i^\dagger, \hat{b}_j^\dagger\right] = 0 \tag{5.2}$$

(also its adjoint).

But we also need a rule for creation and annihilation operators. We borrow the commutation relation from the harmonic oscillator, but only for the same state:

$$\left[\hat{b}_i, \hat{b}_j^\dagger\right] = \delta_{ij}. \tag{5.3}$$

Finally, we need a definition of the vacuum:

$$\hat{b}_i |0\rangle = 0 \tag{5.4}$$

and the adjoint equation, $\langle 0|\hat{b}_i^\dagger = 0$.

Mostly we will justify these rules by showing in detail that they ultimately yield exactly the same results as using permanents in Chapter 2, only more efficiently.

Let's take a couple of examples. First, consider the operator representation of one-particle, in this case one-boson, states:

$$|i\rangle = \hat{b}_i^\dagger |0\rangle. \tag{5.5}$$

Now let's show that $|i\rangle$ is normalized and is orthogonal to $|j\rangle$ for $i \neq j$. Start by computing the overlap

$$\langle j|i\rangle = \langle 0|\hat{b}_j \hat{b}_i^\dagger |0\rangle, \tag{5.6}$$

where I've used the rule for taking the adjoint,

$$\langle j| = (|j\rangle)^\dagger = \left(\hat{b}_j^\dagger |0\rangle\right)^\dagger = \langle 0|\hat{b}_j.$$

Next, I use the commutation relation (13.28)

$$\langle 0|\hat{b}_j \hat{b}_i^\dagger |0\rangle = \langle 0|\delta_{ij} + \hat{b}_i^\dagger \hat{b}_j |0\rangle. \tag{5.7}$$

But $\hat{b}_j |0\rangle = 0$ so all that remains is $\delta_{ij}\langle 0|0\rangle = \delta_{ij}$, completing our proof.

What about a two-boson state? For normalization and orthogonality we need to compute

$$\langle ij|kl\rangle = \langle 0|\hat{b}_j\hat{b}_i\hat{b}_k^\dagger\hat{b}_l^\dagger|0\rangle. \tag{5.8}$$

The basic strategy is to systematically apply commutation relations to bring the boson operators into normal ordering. Along the way one of two things happens: either an annihilation operator $\hat{b}_x$ meets up with its creation counterpart $\hat{b}_x^\dagger$ and in the process of commutation leaves behind a 1, or the annihilation operator proceeds merrily on its way towards the vacuum ket $|0\rangle$ and annihilates it. In detail:

$$\begin{aligned}
&= \langle 0|\hat{b}_j\left(\delta_{ik} + \hat{b}_k^\dagger\hat{b}_i\right)\hat{b}_l^\dagger|0\rangle = \delta_{ik}\langle 0|\hat{b}_j\hat{b}_l^\dagger|0\rangle + \langle 0|\hat{b}_j\hat{b}_k^\dagger\hat{b}_i\hat{b}_l^\dagger|0\rangle \\
&= \delta_{ik}\langle 0|\delta_{jl} + \hat{b}_l^\dagger\hat{b}_j|0\rangle + \langle 0|\left(\delta_{jk} + \hat{b}_k^\dagger\hat{b}_j\right)\left(\delta_{il} + \hat{b}_l^\dagger\hat{b}_i\right)|0\rangle \\
&= \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}.
\end{aligned} \tag{5.9}$$

In the exercises I ask you to generalize these results. The result is straightforward, which I summarize now. Any normalized boson permanent can be represented as

$$\prod_i \frac{1}{\sqrt{n_!}}(\hat{b}_i^\dagger)^{n_i}|0\rangle \equiv |n_1, n_2, n_3, \ldots\rangle \tag{5.10}$$

where n_i is the *occupancy* of the ith state, with $n_i = 0, 1, 2, 3, \ldots$. This is very similar to the normalized coordinate-space form of a permanent, (2.37), except for the overall factor of $1/\sqrt{N!}$, which arose from taking the $N!$ permutations of the coordinates.

Here we see the full expression of the occupancy representation. Because the bosons are indistinguishable, we cannot say that the ith boson is in state j. We can only say that state j is occupied by a boson (or two bosons, three bosons, and so on). Creation and annihilation operators are the most efficient way to express this idea.

Let me pause here and emphasize: the occupation representation of a boson wavefunction is not just shorthand for a 'true' wavefunction in the form of a permanent such as (2.37); the occupation representation is just as true and real, in the same way that a momentum-space representation of a wavefunction is just as true and real as coordinate-space wavefunction.

5.1 The number operator

Now that we have boson permanents and their occupation representation using boson and creation annihilation operators, we can compute matrix elements.

Let's begin with one of the simplest of operators, the number operator. This is just a generalization of the number operator for the harmonic oscillator:

$$\hat{N} = \sum_i \hat{b}_i^\dagger\hat{b}_i. \tag{5.11}$$

As with the harmonic oscillator, it is easy to show that

$$\left[\hat{b}_i^\dagger \hat{b}_i, \hat{b}_j^\dagger\right] = \delta_{ij}\hat{b}_j^\dagger. \tag{5.12}$$

Then it is clear that

$$\left[\hat{N}, \hat{b}_j^\dagger\right] = \hat{b}_j^\dagger, \tag{5.13}$$

which is a compact form of writing

$$\hat{N}\hat{b}_j^\dagger = \hat{b}_j^\dagger \hat{N} + \hat{b}_j^\dagger. \tag{5.14}$$

Then, in the same was as we did for the harmonic oscillator, it is straightforward to show that

$$\hat{N}|n_1, n_2, n_3 \ldots\rangle = (n_1 + n_2 + n_3 + \ldots)|n_1, n_2, n_3 \ldots\rangle. \tag{5.15}$$

The key to deriving this result is to commute the operator $\hat{N}$ rightwards until we get $\hat{N}|0\rangle$. But we have the rule that $\hat{b}_i|0\rangle = 0$ so that term vanishes, and we are left with the result. This is a common strategy, though by no means the only one: try to move annihilation operators rightward, where they can vanish against the vacuum state $|0\rangle$, and/or move creation operators leftward to vanish against the adjoint vacuum states $\langle 0|$.

Now the way we derived this is to use commutation relations. But there is another way to think about more general matrix elements as we'll see in the next section.

5.2 General one-body operators

Let's think about how we represent one- and two-body operators in the occupation representation. Rather than an axiomatic derivation, I am simply going to state how we represent such operators, and then show that they reproduce the laborious results from Chapter 2.

First, consider a one-body operator, $\hat{\mathcal{O}}$. In second quantization we write this as

$$\hat{\mathcal{O}} = \sum_{ij} O_{ij}\hat{b}_i^\dagger \hat{b}_j \tag{5.16}$$

where

$$O_{ij} = \langle i|\hat{\mathcal{O}}|j\rangle = \int \phi_i^*(x)\hat{\mathcal{O}}\phi_j(x)dx \tag{5.17}$$

is the one-body matrix element. How do we understand this representation? The operator moves a single particle from the jth state to the ith state, with strength O_{ij}.

Let's compute some matrix elements. To warm up, start by computing matrix elements of a one-body operator between two one-body states; this is almost trivial, but it helps to illustrate. Let the initial state be $|a\rangle = \hat{b}_a^\dagger|0\rangle$ and

the final state $|b\rangle = \hat{b}_b^\dagger|0\rangle$. The matrix element of a one body operator between them is

$$\langle a|\hat{\mathcal{O}}|b\rangle = \langle 0|\hat{b}_a\hat{\mathcal{O}}\hat{b}_b^\dagger|0\rangle.$$

Now let's expand this term by term using the definition (5.16):

$$= \sum_{ij} O_{ij}\langle 0|\hat{b}_a\hat{b}_i^\dagger\hat{b}_j\hat{b}_b^\dagger|0\rangle. \tag{5.18}$$

So the key is to reduce $\langle 0|\hat{b}_a\hat{b}_i^\dagger\hat{b}_j\hat{b}_b^\dagger|0\rangle$ to a scalar (that is, a number rather than a vector or a function), through a combination of commutators and annihilating the vacuum.

Let me do this in slow motion.

$$\begin{aligned}\langle 0|\hat{b}_a\hat{b}_i^\dagger\hat{b}_j\hat{b}_b^\dagger|0\rangle &= \langle 0|\hat{b}_a\hat{b}_i^\dagger\left(\delta_{jb} - \hat{b}_b^\dagger\hat{b}_j\right)|0\rangle \\ = \delta_{jb}\langle 0|\hat{b}_a\hat{b}_i^\dagger|0\rangle &= \delta_{jb}\langle 0|\left(\delta_{ai} + \hat{b}_i^\dagger\hat{b}_a\right)|0\rangle \\ &= \delta_{ai}\delta_{jb},\end{aligned} \tag{5.19}$$

and plugging into the sum, we get the final result:

$$\langle a|\hat{\mathcal{O}}|b\rangle = O_{ab}.$$

While this may seem tautological, it is an important test of consistency.

Next, move up to matrix elements of a one-body operator between two-boson states. Let the initial state be $\hat{b}_a^\dagger\hat{b}_b^\dagger|0\rangle$ and the final state $\hat{b}_c^\dagger\hat{b}_d^\dagger|0\rangle$; for the moment don't worry about normalization. The matrix element of $\hat{\mathcal{O}}$ between these states is

$$\langle 0|\hat{b}_d\hat{b}_c\hat{\mathcal{O}}\hat{b}_a^\dagger\hat{b}_b^\dagger|0\rangle = \sum_{ij} O_{ij}\langle 0|\hat{b}_d\hat{b}_c\hat{b}_i^\dagger\hat{b}_j\hat{b}_a^\dagger\hat{b}_b^\dagger|0\rangle. \tag{5.20}$$

To evaluate the bracketed term, I choose to start by moving the annihilation operator $\hat{b}_j$ rightward until it crashes against the vacuum:

$$\begin{aligned}\langle 0|\hat{b}_d\hat{b}_c\hat{b}_i^\dagger\hat{b}_j\hat{b}_a^\dagger\hat{b}_b^\dagger|0\rangle &= \langle 0|\hat{b}_d\hat{b}_c\hat{b}_i^\dagger\left(\delta_{ja} + \hat{b}_a^\dagger\hat{b}_j\right)\hat{b}_b^\dagger|0\rangle \\ &= \delta_{ja}\langle 0|\hat{b}_d\hat{b}_c\hat{b}_i^\dagger\hat{b}_b^\dagger|0\rangle + \langle 0|\hat{b}_d\hat{b}_c\hat{b}_i^\dagger\hat{b}_a^\dagger\hat{b}_j\hat{b}_b^\dagger|0\rangle \\ = \delta_{ja}\langle 0|\hat{b}_d\hat{b}_c\hat{b}_i^\dagger\hat{b}_b^\dagger|0\rangle &+ \langle 0|\hat{b}_d\hat{b}_c\hat{b}_i^\dagger\hat{b}_a^\dagger\left(\delta_{jb} + \hat{b}_b^\dagger\hat{b}_j\right)|0\rangle \\ &= \delta_{ja}\langle 0|\hat{b}_d\hat{b}_c\hat{b}_i^\dagger\hat{b}_b^\dagger|0\rangle + \delta_{jb}\langle 0|\hat{b}_d\hat{b}_c\hat{b}_i^\dagger\hat{b}_a^\dagger|0\rangle.\end{aligned} \tag{5.21}$$

Now at this point we stop and notice we have two terms that look like the overlap between two boson permanents. What has happened is the operator $\hat{b}_j$ has annihilated either of the occupied states $\hat{b}_a^\dagger$ or $\hat{b}_b^\dagger$. They are then replaced by the creation operator $\hat{b}_i^\dagger$.

The final result is

$$\delta_{ja}\delta_{ci}\delta_{db} + \delta_{ja}\delta_{di}\delta_{cb} + \delta_{jb}\delta_{ci}\delta_{da} + \delta_{jb}\delta_{di}\delta_{ca}. \tag{5.22}$$

Formally the annihilation of operators is called a contraction, but a useful way to think about the action of operators is one of replacement or movement. So, for example (you should work these out in detail to convince yourself they are correct),

$$\hat{b}_3^\dagger \hat{b}_1 \times \left(\hat{b}_2^\dagger \hat{b}_1^\dagger\right)|0\rangle = \hat{b}_3^\dagger \hat{b}_2^\dagger |0\rangle,$$

that is, moving a boson from state 1 to state 3,

$$\hat{b}_4^\dagger \hat{b}_2 \left(\hat{b}_3^\dagger \hat{b}_2^\dagger \hat{b}_1^\dagger\right)|0\rangle = \hat{b}_4^\dagger \hat{b}_3^\dagger \hat{b}_1^\dagger |0\rangle$$

moving a boson from state 2 to state 4, and

$$\hat{b}_3^\dagger \hat{b}_7 \left(\hat{b}_{10}^\dagger \left[\hat{b}_7^\dagger\right]^4\right)|0\rangle = 4\left(\hat{b}_{10}^\dagger \left[\hat{b}_7^\dagger\right]^3 \hat{b}_3^\dagger\right)|0\rangle,$$

moving any one of 4 bosons in state 7 into state 3. We'll see a similar pattern when we come to fermions; the main differences will be that we can pick up a minus sign, and no more than one particle can occupy any given state. This is why $\hat{b}_i^\dagger \hat{b}_j$ is a *one-body* operator: it moves only one particle at a time.

5.3 Two-body operators

Two-body operators, as you might expect, move two bosons at a time. To see this, consider the action

$$\hat{b}_i^\dagger \hat{b}_j^\dagger \hat{b}_l \hat{b}_k \times \hat{b}_a^\dagger \hat{b}_b^\dagger |0\rangle = (\delta_{ka}\delta_{lb} + \delta_{kb}\delta_{la})\hat{b}_i^\dagger \hat{b}_j^\dagger |0\rangle, \tag{5.23}$$

which can be derived with the usual rules. Then the elementary matrix element

$$\langle 0|\hat{b}_d \hat{b}_c \cdot \hat{b}_i^\dagger \hat{b}_j^\dagger \hat{b}_l \hat{b}_k \cdot \hat{b}_a^\dagger \hat{b}_b^\dagger |0\rangle = (\delta_{ka}\delta_{lb} + \delta_{kb}\delta_{la})(\delta_{ic}\delta_{jd} + \delta_{id}\delta_{jc}). \tag{5.24}$$

5.4 Example problem: bosonic pairing

As practice in working with bosons, let's consider the *boson pairing model*. This is made in analogy with fermionic pairing as discussed below in Section 6.5, which is widely referred to in the literature. Bosonic pairing is much less commonly discussed, but is a useful exercise nonetheless. If you have difficult with this section, you can return to it after you have successfully tackled 6.5.

Suppose you have 2Ω bosonic states, labeled by $\alpha = 1, 2, 3, 4, \ldots, \Omega$ and $-\alpha = -1, -2, \ldots, -\Omega$. The use of Ω is taken from the convention in fermionic pairing. Now consider the boson pair creation operator

$$\hat{P}^\dagger = \hat{b}_1^\dagger \hat{b}_{-1}^\dagger + \hat{b}_2^\dagger \hat{b}_{-2}^\dagger + \hat{b}_3^\dagger \hat{b}_{-3}^\dagger + \ldots = \sum_{\alpha=1}^{\Omega} \hat{b}_\alpha^\dagger \hat{b}_{-\alpha}^\dagger. \tag{5.25}$$

The Hermitian conjugate of this operator is

$$\hat{P} = \left(\hat{P}^\dagger\right)^\dagger = \sum_{\alpha=1}^{\Omega} \hat{b}_{-\alpha}\hat{b}_\alpha. \tag{5.26}$$

Note that $\hat{P}|0\rangle = 0$ and $\langle 0|\hat{P}^\dagger = 0$; we will use these results.

As an exercise, you should show that

$$\left[\hat{P}^\dagger, \hat{P}\right] = -\left(\hat{N} + \Omega\right) \tag{5.27}$$

where $\hat{N} = \sum_{\alpha=1}^{\Omega} \hat{b}_\alpha^\dagger \hat{b}_\alpha + \hat{b}_{-\alpha}^\dagger \hat{b}_{-\alpha}$ is the boson number operator.

Now let's consider unnormalized states with $2m$ bosons of the form

$$|m\rangle = \left(\hat{P}^\dagger\right)^m |0\rangle. \tag{5.28}$$

The first step is to convince yourself that

$$\langle m = 1|m = 1\rangle = \langle 0|\hat{P}\hat{P}^\dagger|0\rangle = \Omega. \tag{5.29}$$

This is actually pretty easy to see: $\hat{P}^\dagger|0\rangle = \hat{b}_1^\dagger\hat{b}_{-1}^\dagger|0\rangle + \hat{b}_2^\dagger\hat{b}_{-2}^\dagger|0\rangle + \hat{b}_3^\dagger\hat{b}_{-3}^\dagger|0\rangle + \ldots$, that is, there are Ω 2-boson permanents, which are trivially orthogonal (and, here, orthonormal) to each other. I encourage the reader to work it out in detail until it becomes obvious to her or him.

There's another way to arrive at this solution: use the commutation relation (5.27) so that

$$\langle 0|\hat{P}\hat{P}^\dagger|0\rangle = \langle 0|\hat{P}^\dagger\hat{P} + \hat{N} + \Omega|0\rangle. \tag{5.30}$$

But, as noted above, $\hat{P}|0\rangle = 0$ and similarly, $\hat{N}|0\rangle = 0$ because the vacuum is a zero-boson state. Then it reduces to a value of Ω as above.

Next, let's find the normalization for $m > 1$. We can do this by further exploiting the commutation relation (5.27) and using induction. Suppose we know the normalization $\langle m|m\rangle$. Let's find the normalization for $\langle m+1|m+1\rangle = \langle m|\hat{P}\hat{P}^\dagger|m\rangle$. One way to do this is to commute the $\hat{P}$ continually rightward. We remember our previous result:

$$\hat{P}\hat{P}^\dagger|0\rangle = \hat{P}^\dagger\hat{P}|0\rangle + \left(\hat{N} + \Omega\right)|0\rangle = 0 + \Omega|0\rangle; \tag{5.31}$$

and from this we can then consider

$$\hat{P}\hat{P}^\dagger\hat{P}^\dagger|0\rangle = \hat{P}^\dagger\hat{P}\hat{P}^\dagger|0\rangle + \left(\hat{N} + \Omega\right)\hat{P}^\dagger|0\rangle \tag{5.32}$$

but we can use our prior results to get

$$\hat{P}^\dagger\left(\hat{N} + \Omega\right)|0\rangle + (2 + \Omega)\,\hat{P}^\dagger|0\rangle = (2 + 2\Omega)\,\hat{P}^\dagger|0\rangle \tag{5.33}$$

using the fact that $\hat{N}|0\rangle = 0$ (because it is a zero-boson state) and $\hat{N}\hat{P}^\dagger|0\rangle = 2\hat{P}^\dagger|0\rangle$ (because it is a 2-boson state). From this we can conclude that $\langle 2|2\langle = (2\Omega + 2)\langle 1|1\rangle$ as well as

$$\hat{P}\hat{P}^\dagger\hat{P}^\dagger|0\rangle = (2\Omega + 2)\hat{P}^\dagger|0\rangle \tag{5.34}$$

Adding another pair,

$$\hat{P}\hat{P}^\dagger\hat{P}^\dagger\hat{P}^\dagger|0\rangle = \hat{P}^\dagger\hat{P}\hat{P}^\dagger\hat{P}^\dagger|0\rangle + \left(\hat{N}+\Omega\right)\hat{P}^\dagger\hat{P}^\dagger|0\rangle \tag{5.35}$$

$$= \hat{P}^\dagger(2\Omega+2)\hat{P}^\dagger|0\rangle + (4+\Omega)\,\hat{P}^\dagger\hat{P}^\dagger|0\rangle = (6+3\Omega)\hat{P}^\dagger\hat{P}^\dagger|0\rangle \tag{5.36}$$

so that $\langle 3|3\rangle = (6+3\Omega)\langle 2|2\rangle$. With a few more example you can prove that

$$\langle m|m\rangle = m(\Omega+m-1)\langle m-1|m-1\rangle, \tag{5.37}$$

from which it is easy to deduce that

$$\langle m|m\rangle = m!\frac{(\Omega+m-1)!}{(\Omega-1)!}. \tag{5.38}$$

Finally, suppose we have a boson Hamiltonian of the form $\hat{H} = -G\hat{P}^\dagger\hat{P}$. Although it is not at first obvious, the states $|m\rangle = \left(\hat{P}^\dagger\right)^m|0\rangle$ are eigenstates of this Hamiltonian. To see this, consider

$$\hat{H}|m\rangle = -G\hat{P}^\dagger\hat{P}|m\rangle. \tag{5.39}$$

But we have shown above that $\hat{P}|m\rangle = m(\Omega+m-1)|m-1\rangle$ so that

$$\hat{H}|m\rangle = -Gm(\Omega+m-1)|m\rangle. \tag{5.40}$$

Considering there are $N = 2m$ bosons in the wavefunction, we can instead write

$$\hat{H}\left|\frac{N}{2}\right\rangle = -\frac{G}{4}N(N+2\Omega-2)\left|\frac{N}{2}\right\rangle, \tag{5.41}$$

which gives us the ground state energy of the boson pairing Hamiltonian, something we will have occasion to use later on.

5.5 Summary

What you should get from this chapter:

• While boson permanents give us the desired symmetry for a many-boson wavefunction, they are clunky to expand and use. Instead, boson *creation* and *annihilation* operators yield exactly the same results with considerable efficiency.

• While boson creation and annihilation operators are inspired by the operators for the simple harmonic oscillator and for angular momentum, they differ in that they do not have a specific coordinate space representation that leads to the boson commutation relations.

• Formally one manipulates boson operators through commutation and contraction (annihilation of two operators); but a useful way to visualize the process is one of moving bosons from one state to another. A one-body operator moves one boson, while a two-body operator moves two bosons.

5.6 Exercises

(5.1) Show explicitly that a two-boson state is always orthogonal to a one-boson state, that is,

$$\langle 0|\hat{b}_i\hat{b}_j^\dagger\hat{b}_k^\dagger|0\rangle = 0.$$

(5.2) For 3-body states derive the overlap:

$$\langle ijk|lmn\rangle = \delta_{il}\delta_{jm}\delta_{kn}+\delta_{im}\delta_{jn}\delta_{kl}+\delta_{in}\delta_{jl}\delta_{km}+\delta_{il}\delta_{jn}\delta_{km}+\delta_{im}\delta_{jl}\delta_{kn}+\delta_{in}\delta_{jl}\delta_{km}.$$

(5.3) Derive the normalization of a condensate of bosons: show that the norm of

$$(\hat{b}_i^\dagger)^n|0\rangle$$

is $n!$, that is,

$$\langle 0|(\hat{b}_i)^n(\hat{b}_i^\dagger)^n|0\rangle = n!.$$

Hint: we already did this for the harmonic oscillator. This immediately leads us to (5.10).

(5.4) Find the normalization of the following states: $\hat{b}_1^\dagger\hat{b}_2^\dagger|0\rangle$; $\hat{b}_1^\dagger\hat{b}_3^\dagger|0\rangle$; $(\hat{b}_1^\dagger)^2|0\rangle$; $\hat{b}_1^\dagger\hat{b}_2^\dagger\hat{b}_3^\dagger|0\rangle$; $\hat{b}_1^\dagger\hat{b}_2^\dagger\hat{b}_4^\dagger|0\rangle$; $(\hat{b}_1^\dagger)^2\hat{b}_2^\dagger|0\rangle$; $(\hat{b}_1^\dagger)^2\hat{b}_3^\dagger|0\rangle$; $(\hat{b}_1^\dagger)^3|0\rangle$.

(5.5) Using the normalizations from (5.4), compute the following matrix elements:

$$\langle 13|\hat{\mathcal{O}}|12\rangle;\ \ \langle 1^2|\hat{\mathcal{O}}|12\rangle;\ \ \langle 124|\hat{\mathcal{O}}|123\rangle;$$

$$\langle 1^2 3|\hat{\mathcal{O}}|123\rangle;\ \ \langle 1^2 2|\hat{\mathcal{O}}|1^3\rangle.$$

Do you get the same results as in Exercise (2.5)?

(5.6) For the operators in Section 5.4, show that

$$\left[\hat{N},\hat{P}^\dagger\right] = 2\hat{P}^\dagger,$$

$$\left[\hat{N},\hat{P}\right] = -2\hat{P}.$$

Chapter 6

Fermion creation and annihilation operators

> Everything should be as simple as can be, but not simpler. – *attributed to Albert Einstein*

When we introduced the idea of indistinguishable particles and using symmetric or antisymmetric wavefunctions, we found that even for product wavefunctions we could not assign a specific coordinate, e.g. x_4, to a particular single-particle state. Instead, the best we could do was to write down a list of *occupied* single-particle states we used to construct the wavefunction. In the case of bosons we were able to introduce creation and annihilation operators which efficiently reproduce all the matrix elements between permanents.

In this chapter we will do the same for fermions: we will introduce fermion creation and annihilation operators that allow us to efficiently calculate matrix elements between Slater determinants. By now you ought to be getting used to using operators as a calculational tool. Nonetheless, there are some strange twists for fermions.

6.1 Anticommutators and Slater determinants

In analogy with using boson creation operators $\hat{b}_i^\dagger$ to construct a permanent, we introduce fermion creation operators $\hat{a}_i^\dagger$ which we'll use to construct a Slater determinant. This represents the occupation of a single-particle state, $\phi_i(x)$, and at the single-particle level there is no difference between fermion states and boson states.

So for a Slater determinant we write:

$$\hat{a}_1^\dagger \hat{a}_2^\dagger \hat{a}_3^\dagger \dots \hat{a}_N^\dagger |0\rangle. \tag{6.1}$$

There are important differences from the boson case. The most fundamental is that the wavefunction is antisymmetric under interchange of any two quantum numbers, so that

$$\hat{a}_i^\dagger \hat{a}_j^\dagger = -\hat{a}_j^\dagger \hat{a}_i^\dagger$$

which we write compactly with an *anticommutator*

$$\left\{\hat{a}_i^\dagger, \hat{a}_j^\dagger\right\} = \hat{a}_i^\dagger \hat{a}_j^\dagger + \hat{a}_j^\dagger \hat{a}_i^\dagger = 0. \tag{6.2}$$

Sometimes one encounters the notation $[A, B]_+$ for the anticommutator. Anticommutation guarantees the occupation of any unique fermion state is only 0 or 1, as $(\hat{a}^\dagger)^2 = -(\hat{a}^\dagger)^2 = 0$.

As with bosons, the annihilation operator annihilates the vacuum:

$$\hat{a}_i|0\rangle = 0 \tag{6.3}$$

for any i, as well as the adjoint expression,

$$\langle 0|\hat{a}_i^\dagger = 0.$$

But now we need a relation between the creation and annihilation operators. We again go with an anticommutator:

$$\left\{\hat{a}_i, \hat{a}_j^\dagger\right\} = \delta_{ij}. \tag{6.4}$$

We these rules we can regain all the results we clumsily derived using the functional form of Slater determinants back in Chapter 2.

Let's start with orthonormality. For one-fermion systems, the overlap between $\hat{a}_i^\dagger|0\rangle$ and $\hat{a}_j^\dagger|0\rangle$ is

$$\langle 0|\hat{a}_i\, \hat{a}_j^\dagger|0\rangle = \langle 0|\left(\delta_{ij} - \hat{a}_j^\dagger \hat{a}_i\right)|0\rangle = \delta_{ij}\langle 0|0\rangle - \langle 0|\hat{a}_j^\dagger \hat{a}_i|0\rangle = \delta_{ij} - 0 \tag{6.5}$$

as one might expect.

The two-fermion cases is also straightforward. The overlap between state $|ij\rangle = \hat{a}_i^\dagger \hat{a}_j^\dagger|0\rangle$ and state $|kl\rangle$ is

$$\begin{aligned}
\langle ij|kl\rangle &= \langle 0|\hat{a}_j \hat{a}_i\, \hat{a}_k^\dagger \hat{a}_l^\dagger|0\rangle \\
&= \langle 0|\hat{a}_j\left(\delta_{ik} - \hat{a}_k^\dagger \hat{a}_i\right)\hat{a}_l^\dagger|0\rangle = \delta_{ik}\langle 0|\hat{a}_j \hat{a}_l^\dagger|0\rangle - \langle 0|\hat{a}_j \hat{a}_k^\dagger \hat{a}_i \hat{a}_l^\dagger|0\rangle \\
&= \delta_{ik}\langle 0|\left(\delta_{jl} - \hat{a}_l^\dagger \hat{a}_j\right)|0\rangle - \langle 0|\hat{a}_j \hat{a}_k^\dagger\left(\delta_{il} - \hat{a}_l^\dagger \hat{a}_i\right)|0\rangle \\
&= \delta_{ik}\delta_{jl} - \delta_{il}\langle 0|\hat{a}_j \hat{a}_k^\dagger|0\rangle \\
&= \delta_{ik}\delta_{jl} - \delta_{il}\langle 0|\left(\delta_{jk} - \hat{a}_k^\dagger \hat{a}_j\right)|0\rangle = \delta_{ik}\delta_{jl} - \delta_{il}\delta_{jk}
\end{aligned} \tag{6.6}$$

In the exercises you'll try some three-fermion cases. But the end result is that all Slater determinants of the form (6.1) are already normalized. This is in fact exactly like the normalization for boson permanents found in (2.36), as all occupations n_i are either 0 or 1.

6.2 Again, the number operator

The number operator for fermions is, as you might expect,

$$\hat{N} = \sum_i \hat{a}_i^\dagger \hat{a}_i. \tag{6.7}$$

Similar to the boson number operator, one can using fermion anticommutation relations derive the *commutator* (not anti-commutator; a crude way to intuit this is we have *two* fermion operators moving past another fermion, and so we pick up two minus signs which cancel)

$$\left[\hat{N}, \hat{a}_j^\dagger\right] = \hat{a}_j^\dagger. \tag{6.8}$$

To derive this, consider just one term:

$$\left[\hat{a}_i^\dagger \hat{a}_i, \hat{a}_j^\dagger\right] = \hat{a}_i^\dagger \hat{a}_i \hat{a}_j^\dagger - \hat{a}_j^\dagger \hat{a}_i^\dagger \hat{a}_i \tag{6.9}$$

$$= \hat{a}_i^\dagger(\delta_{ij} - \hat{a}_j^\dagger \hat{a}_i) - \hat{a}_j^\dagger \hat{a}_i^\dagger \hat{a}_i$$

$$= \delta_{ij}\hat{a}_i^\dagger + \hat{a}_j^\dagger \hat{a}_i^\dagger \hat{a}_i - \hat{a}_j^\dagger \hat{a}_i^\dagger \hat{a}_i = \delta_{ij}\hat{a}_i^\dagger; \tag{6.10}$$

taking the sum over j yields the final result.

Now any n-particle Slater determinant is an eigenstate of the number operator with eigenvalue n:

$$\hat{N}\hat{a}_1^\dagger \hat{a}_2^\dagger \hat{a}_3^\dagger \dots \hat{a}_n^\dagger |0\rangle = n\hat{a}_1^\dagger \hat{a}_2^\dagger \hat{a}_3^\dagger \dots \hat{a}_n^\dagger |0\rangle. \tag{6.11}$$

You can show this by commuting $\hat{N}$ past each creation operator; in the end one has $\hat{a}_1^\dagger \dots \hat{a}_n^\dagger \hat{N}|0\rangle = 0$ because the annihilation operator in $\hat{N}$ destroys the vacuum when it touches it.

6.3 One-body operators

From the number operator we go on to general one-body operators. The form is identical to the boson cases, which should be unsurprising as the difference between bosons and fermions only shows up in many-particle systems: given a one-body operator $\hat{\mathcal{O}}$, the operator expansion is

$$\hat{\mathcal{O}} = \sum_{ij} O_{ij} \hat{a}_i^\dagger \hat{a}_j, \tag{6.12}$$

where the matrix element is the usual one:

$$O_{ij} = \langle i|\hat{\mathcal{O}}|j\rangle = \int \phi_i^*(x)\hat{\mathcal{O}}\phi_j(x)dx. \tag{6.13}$$

As always, the actual value of the matrix elements O_{ij} depend on the choice of basis.

To convince yourself this expression is correct, let's work out some many-body matrix elements and see they give the same results as from section 2.5.

First, and somewhat tediously, in exercise (6.2) you're asked to confirm that the definition (6.12) is consistent, that is, using the creation/annihilation operator expansion of $\hat{\mathcal{O}}$ the matrix element between two one-fermion states $|a\rangle = \hat{a}_a^\dagger|0\rangle$ and $|b\rangle$ is, as you would expect , O_{ab}.

Next, let's tackle matrix elements of a *one-body operator* between *two-fermion* states, $|ab\rangle = \hat{a}_a^\dagger\hat{a}_b^\dagger|0\rangle$ and $|cd\rangle = \hat{a}_c^\dagger\hat{a}_d^\dagger|0\rangle$. Expanding

$$\langle ab|\hat{\mathcal{O}}|cd\rangle = \sum_{ij} O_{ij}\langle 0|\hat{a}_b\hat{a}_a\hat{a}_i^\dagger\hat{a}_j\hat{a}_c^\dagger\hat{a}_d^\dagger|0\rangle. \tag{6.14}$$

Again, we want to turn $\langle 0|\hat{a}_b\hat{a}_a\hat{a}_i^\dagger\hat{a}_j\hat{a}_c^\dagger\hat{a}_d^\dagger|0\rangle$ into a number. While there are different strategies, a useful one is to have $\hat{a}_j$ annihilate either $\hat{a}_c^\dagger$ or $\hat{a}_d^\dagger$ and replace it with $\hat{a}_i^\dagger$. In slow motion

$$\begin{aligned}\hat{a}_j\hat{a}_c^\dagger\hat{a}_d^\dagger|0\rangle &= \left(\delta_{jc} - \hat{a}_c^\dagger\hat{a}_j\right)\hat{a}_d^\dagger|0\rangle \\ = \delta_{jc}\hat{a}_d^\dagger|0\rangle - \hat{a}_c^\dagger\left(\delta_{jd} - \hat{a}_d^\dagger\hat{a}_j\right)|0\rangle &= \delta_{jc}\hat{a}_d^\dagger|0\rangle - \delta_{jd}\hat{a}_c^\dagger|0\rangle\end{aligned} \tag{6.15}$$

and so

$$\hat{a}_i^\dagger\hat{a}_j\hat{a}_c^\dagger\hat{a}_d^\dagger|0\rangle = \delta_{jc}\hat{a}_i^\dagger\hat{a}_d^\dagger|0\rangle - \delta_{jd}\hat{a}_i^\dagger\hat{a}_c^\dagger|0\rangle = \delta_{jc}\hat{a}_i^\dagger\hat{a}_d^\dagger|0\rangle + \delta_{jd}\hat{a}_c^\dagger\hat{a}_i^\dagger|0\rangle \tag{6.16}$$

where I've moved either a fermion in state c or in state d into state i.

So now we need to finish up and compute

$$\begin{aligned}\langle 0|\hat{a}_b\hat{a}_a\hat{a}_i^\dagger\hat{a}_j\hat{a}_c^\dagger\hat{a}_d^\dagger|0\rangle &= \delta_{jc}\langle 0|\hat{a}_b\hat{a}_a\hat{a}_i^\dagger\hat{a}_d^\dagger|0\rangle + \delta_{jd}\langle 0|\hat{a}_b\hat{a}_a\hat{a}_c^\dagger\hat{a}_i^\dagger|0\rangle \\ &= \delta_{jc}(\delta_{ai}\delta_{bd} - \delta_{ad}\delta_{bi}) + \delta_{jd}(\delta_{ac}\delta_{bi} - \delta_{ai}\delta_{bc}).\end{aligned} \tag{6.17}$$

Finally, plugging back into (6.14) and taking the sum over i, j we get

$$O_{ac}\delta_{bd} - O_{bc}\delta_{ad} + O_{bd}\delta_{ac} - O_{ad}\delta_{bc}. \tag{6.18}$$

But this is exactly what we got in (2.56). While more abstract, the use of creation and annihilation operators is ultimately easier.

6.4 Two-body operators

For two-body operators, the occupation representation is

$$\hat{V} = \sum_{a<b,c<d} V^A(ab,cd)\hat{a}_a^\dagger\hat{a}_b^\dagger\hat{a}_d\hat{a}_c \tag{6.19}$$

where the antisymmetric two-body matrix element is taken between *normalized* two-body states as described above. The restriction $a < b, c < d$ is to prevent

double-counting; alternately, one can have an unrestricted sum with a factor of 1/4 in front. This is somewhat simpler than for bosons, if only because normalization is a simpler issue: using operators, the Slater determinant $\hat{a}_a^\dagger \hat{a}_b|0\rangle$ is already and always normalized.

The reason one has the reversed order $\hat{a}_d\hat{a}_c$ in the annihilation operators is to get the sign right. To see this, let's confirm consistency by computing

$$\langle ij|\hat{V}|mn\rangle = \frac{1}{4}\sum_{abcd} V^A(ab,cd)\langle 0|\hat{a}_j\hat{a}_i\hat{a}_a^\dagger\hat{a}_b^\dagger\hat{a}_d\hat{a}_c\hat{a}_m^\dagger\hat{a}_n^\dagger|0\rangle. \tag{6.20}$$

I'll sketch out the process, and you should fill in the missing steps. First, the annihilation operators $\hat{a}_d\hat{a}_c$ will of course annihilate $\hat{a}_m^\dagger\hat{a}_n^\dagger$:

$$\hat{a}_d\hat{a}_c\hat{a}_m^\dagger\hat{a}_n^\dagger|0\rangle = (\delta_{cm}\delta_{dn} - \delta_{cn}\delta_{dm})|0\rangle. \tag{6.21}$$

If c annihilates m and d annihilates n then we pick up a + sign, else in the reverse order we pick up a − sign.

The next step is to replace the now-missing operators $\hat{a}_m^\dagger\hat{a}_n^\dagger$ with $\hat{a}_a^\dagger\hat{a}_b^\dagger$; that is, we've moved particles from states m and n to states a and b:

$$\hat{a}_a^\dagger\hat{a}_b^\dagger\hat{a}_d\hat{a}_c\hat{a}_m^\dagger\hat{a}_n^\dagger|0\rangle = \hat{a}_a^\dagger\hat{a}_b^\dagger|0\rangle(\delta_{cm}\delta_{dn} - \delta_{cn}\delta_{dm}). \tag{6.22}$$

This we have to take the dot product with the adjoint $\langle 0|\hat{a}_j\hat{a}_i$, and from this we have (setting aside for the moment the Kronecker δs we've generated)

$$\langle 0|\hat{a}_j\hat{a}_i\hat{a}_a^\dagger\hat{a}_b^\dagger|0\rangle = \delta_{ai}\delta_{bj} - \delta_{aj}\delta_{bi}. \tag{6.23}$$

Putting this all together

$$\begin{aligned}\langle ij|\hat{V}|mn\rangle &= \frac{1}{4}\sum_{abcd} V^A(ab,cd)(\delta_{ai}\delta_{bj} - \delta_{aj}\delta_{bi})(\delta_{cm}\delta_{dn} - \delta_{cn}\delta_{dm}) \\ &= \frac{1}{4}(V^A(ij,mn) - V^A(ji,mn) - V^A(ij,nm) + V^A(ji,nm)).\end{aligned} \tag{6.24}$$

But now we remember the antisymmetry relations $V^A(ab,cd) = -V^A(ba,cd) = -V^A(ab,dc) = +V^A(ba,dc)$ and collapse to the simple result $\langle ij|\hat{V}|mn\rangle = V^A(ij,mn)$, as we would like.

While this looks terribly complicated, with practice you can learn to do this much more swiftly. The basic rules are, as one moves an annihilation operator rightward, it must at some point annihilate against a creation operator, yielding a 1; if it instead it reaches the vacuum $|0\rangle$ we'll get zero. Each time the operator moves past another operator we pick up a − sign.

6.5 Example problem: pairing

For our first detailed example working with fermion operators, we take a simplified model for pairing. Coordinated pairs of fermions explain many important

phenomena in many-body physics, from superconductivity in solid state materials to the spectra of atomic nuclei. In following chapters we will revisit pairing several times, with tools of increasing sophistication. For now we will just use this to practice manipulating fermion operators.

We start with 2Ω single-particle states. The states come in pairs, labeled by k and $-k$, with $k > 0$ taking on Ω distinct values. If you are a condensed matter physicist, you might think of these as states of linear momentum, with k labeling a momentum state $\vec{p}$ and $-k$ labeling $-\vec{p}$. If you are a nuclear physicist (or atomic physicist, although despite its origin seniority is a less useful concept for atomic electrons), you might think a shell of single-particle states with angular momentum $j = \Omega - 1/2$ and k labeling the third component $m > 0$ and $-k$ labeling $-m < 0$. The important point is that the single-particle states come in pairs of equal but opposite 'momentum;' in a later chapter we'll write out how to generalize this.

We now consider a specific pair of time-reversed partners, $\hat{a}_k^\dagger \hat{a}_{-k}^\dagger$, and then taking a sum of all of them:

$$\hat{P}_+ = \sum_{k>0} \hat{a}_k^\dagger \hat{a}_{-k}^\dagger. \tag{6.25}$$

The Hamiltonian for this system is very simple:

$$\hat{H} = -G\hat{P}_+\hat{P}_-, \tag{6.26}$$

where

$$\hat{P}_- = (\hat{P}_+)^\dagger = \sum_{k>0} \hat{a}_{-k}\hat{a}_k. \tag{6.27}$$

Now we want to show that

$$\left[\hat{P}_+, \hat{P}_-\right] = \sum_{k>0} \left(\hat{a}_k^\dagger \hat{a}_k + \hat{a}_{-k}^\dagger \hat{a}_{-k} - 1\right) = \hat{N} - \Omega. \tag{6.28}$$

Let's go through this in slow motion. First,

$$\left[\hat{P}_+, \hat{P}_-\right] = \sum_{k>0} \sum k' > 0 \left[\hat{a}_k^\dagger \hat{a}_{-k}^\dagger, \hat{a}_{-k'}\hat{a}_{k'}\right], \tag{6.29}$$

but unless $k = k'$ the two pairs trivially commute. Now taking the nontrivial term,

$$\left[\hat{a}_k^\dagger \hat{a}_{-k}^\dagger, \hat{a}_{-k}\hat{a}_k\right] = \hat{a}_k^\dagger \hat{a}_{-k}^\dagger \hat{a}_{-k}\hat{a}_k - \hat{a}_{-k}\hat{a}_k\hat{a}_k^\dagger \hat{a}_{-k}^\dagger.$$

Now consider the first term. Applying the standard anticommutation relation,

$$\hat{a}_k^\dagger \hat{a}_{-k}^\dagger \hat{a}_{-k}\hat{a}_k = \hat{a}_k^\dagger \left(1 - \hat{a}_{-k}\hat{a}_{-k}^\dagger\right)\hat{a}_k = \hat{a}_k^\dagger \hat{a}_k - \hat{a}_k^\dagger \hat{a}_{-k}\hat{a}_{-k}^\dagger \hat{a}_k$$

but because $k \neq -k$ we can trivially anticommute twice, leaving an overall $+$ sign:

$$= \hat{a}_k^\dagger \hat{a}_k - \hat{a}_{-k}\hat{a}_k^\dagger \hat{a}_k \hat{a}_{-k}^\dagger = \hat{a}_k^\dagger \hat{a}_k - \hat{a}_{-k}\left(1 - \hat{a}_k\hat{a}_k^\dagger\right)\hat{a}_{-k}^\dagger$$

$$= \hat{a}_k^\dagger \hat{a}_k - \hat{a}_{-k}\hat{a}_{-k}^\dagger - \hat{a}_{-k}\hat{a}_k\hat{a}_k^\dagger\hat{a}_{-k}^\dagger = \hat{a}_k^\dagger\hat{a}_k + \hat{a}_{-k}^\dagger\hat{a}_{-k} - 1 - \hat{a}_{-k}\hat{a}_k\hat{a}_k^\dagger\hat{a}_{-k}^\dagger.$$

Thus the overall commutator is

$$\left[\hat{a}_k^\dagger\hat{a}_{-k}^\dagger, \hat{a}_{-k}\hat{a}_k\right] = \hat{a}_k^\dagger\hat{a}_k + \hat{a}_{-k}^\dagger\hat{a}_{-k} - 1. \tag{6.30}$$

Then k sums from 1 to Ω, and we arrive at (6.28).

Next consider states of the form, for n even,

$$|n\rangle = (\hat{P}_+)^{n/2}|0\rangle. \tag{6.31}$$

We will first normalize them; then demonstate they are eigenstates of the Hamiltonian (6.26); and finally find the energy of these states.

First the normalization, which is far from obvious. Define

$$\mathcal{N}(n) = \left\langle 0 \left| \left(\hat{P}_-\right)^{n/2} \left(\hat{P}_+\right)^{n/2} \right| 0 \right\rangle. \tag{6.32}$$

We can compute this easily for $n = 2$ using the basic commutator (6.28):

$$\mathcal{N}(2) = \left\langle 0 \left| \hat{P}_-\hat{P}_+ \right| 0 \right\rangle = \left\langle 0 \left| \hat{P}_+\hat{P}_- - \hat{N} + \Omega \right| 0 \right\rangle.$$

But: $\hat{P}_-|0\rangle = 0$ (because any $\hat{a}_k|0\rangle = 0$) and $\hat{N}|0\rangle = 0$ as well. And because we assume the vacuum is always normalized, $\langle 0|0\rangle = 1$, we get

$$N(2) = \Omega. \tag{6.33}$$

Now let's generalize this via induction. We want

$$\mathcal{N}(n+2) = \left\langle 0 \left| \left(\hat{P}_-\right)^{n/2+1} \left(\hat{P}_+\right)^{n/2+1} \right| 0 \right\rangle. \tag{6.34}$$

To start, we peel off one of the $\hat{P}_-$ operators

$$= \left\langle 0 \left| \left(\hat{P}_-\right)^{n/2} \hat{P}_- \left(\hat{P}_+\right)^{n/2+1} \right| 0 \right\rangle$$

and commute it rightwards until it reaches the vacuum and destroys it. Every time we commute it past a $\hat{P}_+$ we pick up a $\Omega - \hat{N}$, so that

$$\hat{P}_- \left(\hat{P}_+\right)^{n/2+1}|0\rangle = \hat{P}_-\hat{P}_+\hat{P}_+\hat{P}_+\ldots\hat{P}_+|0\rangle$$

$$= (\Omega - \hat{N})\left(\hat{P}_+\right)^{n/2}|0\rangle + \hat{P}_+\hat{P}_-\hat{P}_+\hat{P}_+\ldots\hat{P}_+|0\rangle$$

$$= (\Omega - \hat{N})\left(\hat{P}_+\right)^{n/2}|0\rangle + \hat{P}_+(\Omega - \hat{N})\hat{P}_+\hat{P}_+\ldots\hat{P}_+|0\rangle + \hat{P}_+\hat{P}_+\hat{P}_-\hat{P}_+\ldots\hat{P}_+|0\rangle =$$

$$(\Omega - \hat{N})\left(\hat{P}_+\right)^{n/2}|0\rangle$$

$$+\hat{P}_+(\Omega - \hat{N})\hat{P}_+\hat{P}_+\ldots\hat{P}_+|0\rangle + \hat{P}_+\hat{P}_+(\Omega - \hat{N})\hat{P}_+\ldots\hat{P}_+|0\rangle\ldots$$

$$+\hat{P}_+\hat{P}_+\hat{P}_+\ldots(\Omega - \hat{N})\hat{P}_+|0\rangle + \hat{P}_+\hat{P}_+\hat{P}_+\ldots\hat{P}_+(\Omega - \hat{N})|0\rangle \tag{6.35}$$

While Ω is just a number, or scalar in our parlance, the operator $\hat{N}$ takes on the value of the number of particles to the right of it (but only because in this case there are a fixed number of particles to the right), that is,

$$((\Omega - n) + (\Omega - n + 2) + (\Omega - n + 4) \ldots + (\Omega - 2) + \Omega)) \left(\hat{P}_+\right)^{n/2} |0\rangle$$
$$= \frac{1}{4}(2\Omega - n)(n + 2) \left(\hat{P}_+\right)^{n/2} |0\rangle, \quad (6.36)$$

which then leads to

$$\mathcal{N}(n + 2) = \frac{1}{4}(2\Omega - n)(n + 2)\mathcal{N}(n). \quad (6.37)$$

Note this returns the correct answer when $n = 0$.

From this one can work out the full normalization

$$\mathcal{N}(n) = \frac{\Omega! \left(\frac{n}{2}\right)!}{\left(\Omega - \frac{n}{2}\right)!} \quad (6.38)$$

and the energy of a normalizes state with n particles,

$$E_n = -\frac{Gn}{4}(2\Omega + 2 - n) \quad (6.39)$$

(see exercises).

6.6 Summary

What you should learn from this chapter:

• As in the case of bosons, we can introduce fermion *creation* and *annihilation* operators to efficiently reproduce our results using antisymmeterized fermion Slater determinants. Also like the boson case, and unlike for the harmonic oscillator and for angular momentum, these operators do not have any coordinate-space representation.

• Unlike boson operators, however, the fermion operators *anti*commute. One major result is that the maximum occupation of any single fermion state is one, which is rigorous way to arrive at the Pauli exclusion principle.

• Because of the antisymmetry, matrix elements can have non-intuitive phases (minus signs) arise. Furthermore, when dealing with interactions between particles, the most natural starting point are antisymmeterized two-body matrix elements.

• One can think of a one-body operator $\hat{a}_i^\dagger \hat{a}_j$ as *moving* a particle from state j to state i, with possibly an additional phase. Similarly one can think of a two-body operator $\hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_l \hat{a}_k$ as moving two particles from states k and l to states i and j – again possibly with an induced phase.

6.7 Exercises

(6.1) Show that the state $|123\rangle$ and $|124\rangle$ are normalized and orthogonal to each other, where $|123\rangle = \hat{a}_1^\dagger \hat{a}_2^\dagger \hat{a}_3^\dagger |0\rangle$.

(6.2) Confirm Eq. (6.11).
(6.3) Show that the definition (6.12) is consistent, that is, show that using the occupation-representation form

$$\langle a|\hat{\mathcal{O}}|b\rangle = \langle a| \sum_{ij} O_{ij} \hat{a}_i^\dagger \hat{a}_j |b\rangle = O_{ab}.$$

(6.4) Compute for a one-body operator $\langle 123|\hat{\mathcal{O}}|124\rangle$

(6.5) Confirm Equation (6.38)

(6.6) Confirm the expectation value of the Hamiltonian (6.26) is given by (6.39). *Hint*: Use the commutation relation (6.28) and the normalization relation (6.37)
.

The following two exercises will be useful warmup for Chapter 9

(6.7). Confirm the following matrix elements:

$$\langle 124|\hat{a}_1^\dagger \hat{a}_4^\dagger \hat{a}_3 \hat{a}_1|123\rangle = 1;$$

$$\langle 256|\hat{a}_5^\dagger \hat{a}_6^\dagger \hat{a}_3 \hat{a}_1|123\rangle = -1;$$

$$\langle 456|\hat{a}_1^\dagger \hat{a}_4^\dagger \hat{a}_3 \hat{a}_1|123\rangle = 0;$$

$$\langle 123|\hat{a}_1^\dagger \hat{a}_4^\dagger \hat{a}_3 \hat{a}_1|123\rangle = 0;$$

$$\langle 256|\hat{V}|123\rangle = -V_{56,13};$$

$$\langle 124|\hat{V}|123\rangle = V_{14,13} + V_{24,23}$$

$$\langle 789|\hat{V}|123\rangle = 0.$$

(6.8) Compute the following:

$$\langle 1245|\hat{a}_1^\dagger \hat{a}_5^\dagger \hat{a}_3 \hat{a}_1|1234\rangle;$$

$$\langle 2456|\hat{a}_5^\dagger \hat{a}_6^\dagger \hat{a}_3 \hat{a}_1|1234\rangle;$$

$$\langle 1234|\hat{a}_1^\dagger \hat{a}_5^\dagger \hat{a}_3 \hat{a}_1|1234\rangle;$$

$$\langle 2567|\hat{a}_5^\dagger \hat{a}_6^\dagger \hat{a}_3 \hat{a}_1|1234\rangle;$$

$$\langle 1256|\hat{V}|1234\rangle;$$

$$\langle 1456|\hat{V}|1234\rangle;$$

$$\langle 1567|\hat{V}|1234\rangle;$$

(6.9) What is $\hat{a}_1^\dagger \hat{a}_2|123\rangle = ?$

Part II

A first portfolio of applications

Chapter 7

Classic toy models

Errors are not in the art but in the artificers. – *Isaac Newton*

While we've done some simple calculations with creation and annihilation operators, it is useful to tackle some toy models: systems of sufficient complexity to allow us to flex our muscles in working with creation and annihilation operators, but simple enough that most everything can be done by hand. Later on we will draw upon some of these toy models to illustrate in some detail various approximations.

The examples I'll give are for fermion systems. For bosons, there exist analytic models, such as special cases of for the *s-d* interacting boson model, but they require group theory far before the scope of this text. For those cases I recommend Arima and Iachello's book, or Talmi's book.

The methods of exact solution presented here are *tricks*, special to these cases, drawing upon our experience with and intuition about angular momentum algebra–hence we use the name *quasi-spin* to denote the trick. They do not apply to more general cases. We will return to these toy models and tackle them using less clever, but more general, methods in Chapter 9. The trick method of quasi-spin is nonetheless useful because, first, it gives us easy solutions to systems against which we can compare various approximations, and second because quasi-spin gives us additional, if simplified, practice in using operator formalism.

7.1 Pairing, quasi-spin, and seniority

We return to the interaction between pairs of fermions from section 6.5, but with more sophisticated tools that will allow us to compute the full spectrum and not just the ground state energy: quasi-spin and seniority.

The concept of seniority was introduced by Giulio Racah, originally for atomic systems, although soon it was taken up for nuclear structure. The simplest seniority model is exactly solvable using *quasi-spin*, that is, rewriting the

problem in terms of operators that have SU(2) commutation relations. Even though the dynamics of the system have nothing to do with angular momentum, we can apply the same mathematics to derive our solution.

Seniority, it turns out, is related to pairing of fermions and thus is a starting point to understanding superconductivity and the structure and spectra of atomic nuclei. We'll use seniority to help illuminate quasiparticles, the Bogoliubov transformation, and the BCS approach to superconductivity.

Let me remind you: we take 2Ω single-particle states. The states come in pairs, labeled by k and $-k$, with $k > 0$. Then we define

$$\hat{P}_+ = \sum_{k>0} \hat{a}_k^\dagger \hat{a}_{-k}^\dagger. \tag{7.1}$$

The reason for this unusual notation will become clear in a moment. The Hamiltonian for this system is very simple:

$$\hat{H} = -G\hat{P}_+\hat{P}_-, \tag{7.2}$$

where $\hat{P}_- = (\hat{P}_+)^\dagger$.

Now previously we proved:

$$\left[\hat{P}_+, \hat{P}_-\right] = \sum_{k>0} \left(\hat{a}_k^\dagger \hat{a}_k + \hat{a}_{-k}^\dagger \hat{a}_{-k} - 1\right) = \hat{N} - \Omega. \tag{7.3}$$

Now let's define

$$\hat{P}_z = \frac{1}{2}(\hat{N} - \Omega). \tag{7.4}$$

As an exercise, show

$$\left[\hat{P}_z, \hat{P}_\pm\right] = \pm\hat{P}_\pm. \tag{7.5}$$

But these are just the SU(2) commutation relations, and although this system has nothing to do with angular momentum, we can apply ideas and intuition from angular momentum to the system. We call this "quasi-spin."

So, for example: we can define operators

$$\hat{P}_x = \frac{1}{2}\left(\hat{P}_+ + \hat{P}_-\right), \;\; \hat{P}_i = \frac{i}{2}\left(-\hat{P}_+ + \hat{P}_-\right), \tag{7.6}$$

and then, in the same way as we did back in (4.12),

$$\hat{H} = -G\hat{P}_+\hat{P}_- = -G\left(\hat{P}_x^2 + \hat{P}_y^2 + i\left[\hat{P}_y, \hat{P}_x\right]\right) = -G\left(\hat{P}^2 - P_z^2 + \hat{P}_z\right),$$

where we define $\hat{P}^2 = \hat{P}_x^2 + \hat{P}_y^2 + \hat{P}_z^2$. Because of the SU(2) algebra, we *know* that the eigenvalues of $\hat{P}^2$ must be of the form $p(p+1)$, with p either integer or half-integer, and the eigenvalues of $\hat{P}_z$ are m_p with $p \geq |m_p|$, with m_p also integer or half-integer.

But because $\hat{P}_z = (1/2)(\hat{N} - \Omega)$, we know that for n particles the value $m_p = (n - \Omega)/2$. Furthermore, the values of m_p range from $-\Omega/2$ (for $n = 0$) to

$+\Omega/2$ (for $n = 2\Omega$, with all states filled). Because of this we deduce the maximal $p = \Omega/2$ and for a given n the values range of p range from $|n - \Omega|/2$ to $\Omega/2$ in steps of 1. (Here we are only dealing with an even number of particles.)

Racah introduced the notation

$$p = (\Omega - v)/2, \tag{7.7}$$

where $v = 0, 2, 4, ..., \Omega - |n - \Omega|$ (the upper bound being the lesser of either n or $2\Omega - n$). The symbol v comes from the Hebrew word *vetek* or 'seniority.' From this one can show the eigenvalues of the pairing Hamiltonian are

$$-G(n - v)(2\Omega + 2 - n - v)/4. \tag{7.8}$$

You can see that we obtain not only the ground state energy, not only more easily than previously, but also the excitation spectrum with $v > 0$, which is interpreted as the number of unpaired particles. Not only that, but this also works for n odd, with $v = 1, 3, 5, \ldots$.

On the other hand, quasi-spin is a trick. We'll use it again for several other systems, but for a general system it is not applicable. The main use is to help us gain experience in manipulating fermion operators, as well as providing a few toy systems on which we can test various approximations.

7.2 Bosonic pairing model

You may well be wondering if we can use a similar trick for the boson pairing model back in Section 5.4. We can, mostly, although with some key differences.

Recall: we have 2Ω bosonic states, labeled by $\alpha = 1, 2, 3, 4, \ldots, \Omega$ and $-\alpha = -1, -2, \ldots, -\Omega$, and the boson pairing creation operator, which we now label by $\hat{P}_+$:

$$\hat{P}_+ = \sum_{\alpha=1}^{\Omega} \hat{b}^\dagger_\alpha \hat{b}^\dagger_{-\alpha}. \tag{7.9}$$

The Hermitian conjugate of this operator is $\hat{P}_- = \left(\hat{P}_+\right)^\dagger$. If we introduce the operator

$$\hat{P}_0 = \frac{1}{2}\left(\hat{N} + \Omega\right), \tag{7.10}$$

then we can use our prior work to establish the following commutation relations:

$$\left[\hat{P}_+, \hat{P}_-\right] = -2\hat{P}_0, \quad \left[\hat{P}_0, \hat{P}_\pm\right] = \pm\hat{P}_\pm. \tag{7.11}$$

These are *almost* the SU(2) commutation relations we used in the previous section, except the first one has a minus sign! Instead these are called SU(1,1) commutation relations, which are less familiar to many physics students. It is beyond the scope of this book to go into much detail about SU(1,1); you may find your own references, e.g. http://sbfisica.org.br/rbef/pdf/040704.pdf. With SU(1,1) one may quickly establish our previous results.

Briefly: one can show that the second-order SU(1,1) Casimir operator (which commutes with all generators of the group, for example $\hat{J}^2$ in SU(2)) is

$$\hat{C}_2 = \hat{P}_0^2 - \frac{1}{2}\left(\hat{P}_+\hat{P}_- + \hat{P}_-\hat{P}_+\right) = \hat{P}_0^2 - \hat{P}_0 - \hat{P}_+\hat{P}_-. \tag{7.12}$$

Furthermore one can then show that there exist simultaneous eigenstates of both $\hat{C}_2$ and $\hat{P}_0$ labeled by p and m:

$$\hat{C}_2|p,m\rangle = p(p-1)|p,m\rangle; \tag{7.13}$$

$$\hat{P}_0|p,m\rangle = (p+m)|p,m\rangle. \tag{7.14}$$

As with SU(2), the irreps are labeled by p, where p is any nonzero real number, while m is any nonnegative integer. One can start from the state $|p,0\rangle$ and then raise the value of m using the $\hat{P}_+$ operator:

$$|p,m\rangle = A\left(\hat{P}_+\right)^m |p,0\rangle \tag{7.15}$$

where A is a normalization.

In our case, we have $m = N/2$, but we also have eigenvalues of $\hat{P}_0$ $\frac{1}{2}(N+\Omega)$, so for the ground state irrep we must have $k = \Omega/2$. Then the eigenvalue of the second-order Casimir is $\frac{1}{4}\Omega(\Omega-2)$ and the eigenvalue of $\hat{P}_+\hat{P}_-$ is exactly what we established previously,

Note that unlike the case for fermionic pairing, where there is a maximal value of N, we can add bosons indefinitely. In group-theoretic language, this is because SU(1,1) is a *non-compact* group. The details are best left to more thorough treatments.

7.3 The Lipkin model

Another simple but illuminating toy many-fermion system is the model of Lipkin, Meshkov, and Glick, or simply the Lipkin model. Like seniority, the Lipkin model also uses operators with an SU(2) structure. The Hamiltonian has a more complex structure, however, and to obtain the final solution one must diagonalize small matrices. We will use the Lipkin model to illustrate the use of several approximations, including Hartree-Fock and the random phase approximation.

In the seniority model considered in the previous section, all the single-particle states were degenerate, that is, there was no one-body term, no single-particle energies arising from a central potential (i.e., the Coulomb field of the nucleus of an atom) or a mean-field potential. But this is highly unrealistic. The Lipkin model addresses this by inserting single-particle energies. Thus the Lipkin model offers a kind of simplified shell model, like that found in atoms and nuclei. I emphasize, however, that there is no direct correspondence to a physical system.

The Hamiltonian is

$$\hat{H} = \frac{1}{2}\epsilon\sum_{i=1}^{N}\left(\hat{a}_{i\uparrow}^\dagger\hat{a}_{i\uparrow} - \hat{a}_{i\downarrow}^\dagger\hat{a}_{i\downarrow}\right) - \frac{1}{2}V\sum_{i,j}\left(\hat{a}_{i\uparrow}^\dagger\hat{a}_{j\uparrow}^\dagger\hat{a}_{j\downarrow}\hat{a}_{i\downarrow} + \hat{a}_{i\downarrow}^\dagger\hat{a}_{j\downarrow}^\dagger\hat{a}_{j\uparrow}\hat{a}_{i\uparrow}\right). \tag{7.16}$$

This is a cartoon version of a many-body system, illustrated by Figure 7.1. It has N particles, each of which can be in one of two states separated by an energy ϵ; the splitting in energy echoes single-particle energies that arise from, for example, the Coulomb potential from a nucleus in an atom, or from the self-consistent mean-field potential inside a nucleus itself. The lower states are labeled as 'down' or $\downarrow$, while the upper states are labeled as 'up' or $\uparrow$. The first term in (7.16), which you should recognize by now as a one-body operator, accounts for the single-particle energy.

The second term in (7.16) is the interaction term. The action of the operator $\hat{a}^\dagger_{i\uparrow}\hat{a}^\dagger_{j\uparrow}\hat{a}_{j\downarrow}\hat{a}_{i\downarrow}$ is to take two particles, one in the down ($\downarrow$) i state and in the down j state, and promote them up ($\uparrow$). In popular culture terms, this is much like the transporter in *Star Trek*: the particles are destroyed in one place and recreated in another. To ensure Hermiticity, the conjugate term $\hat{a}^\dagger_{i\downarrow}\hat{a}^\dagger_{j\downarrow}\hat{a}_{j\uparrow}\hat{a}_{i\uparrow}$ demotes two particles from up to down. For simplicity, the strength of the interaction, V, does not depend on the labels of the particles.

Thus the model has just three parameters, N, ϵ, and V, and because we can always rescale the energy, there are just two relevant parameters, N and V/ϵ. In more realistic systems the potential usually does depend on i and j and there can be more than two single-particle levels. Additionally, more realistic systems generally do not have just the "up or down" restriction; for example, in atoms one can have both a spin-up and a spin-down electron in what is otherwise the same orbit. Nonetheless, the Lipkin model is useful for practicing our skills and to illustrate basic concepts and approximations.

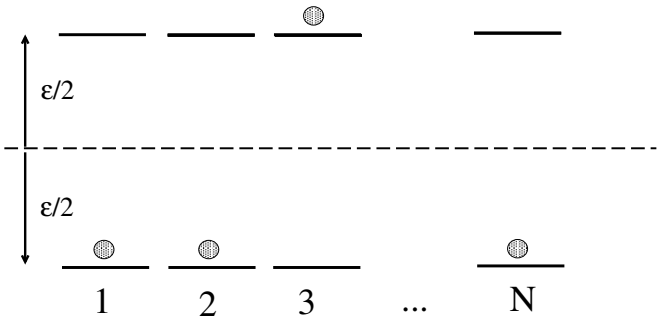

Figure 7.1: The Lipkin model: N particles, each of which can be in one of two levels, separated in energy by ϵ.

7.3.1 Exact solution of the Lipkin model

One advantage of the Lipkin model is that it is of intermediate difficulty. The seniority model is purely algebraic; once we recast the Hamiltonian using quasi-spin, the spectrum falls out immediately. While this simplicity is appealing, it leaves little to teach us about messier, decidedly un-algebraic problems. The Lipkin model, on the other hand, can be simplified using similar quasi-spin

techniques, albeit with a different formulation, but there still remains a modest diagonalization, enough to get our feet wet.

Later on, in section 9.5, we will discuss how to "naively" solve this Hamiltonian, by computing the Hamiltonian matrix in a basis of Slater determinants. For this chapter, however, we instead tackle exact solutions using tricks. Much as we used quasi-spin to solve seniority Hamiltonian, despite the lack of physical angular momentum, we rewrite the Lipkin Hamiltonian by introducing operators that also *act* like SU(2) generators even through they too have *nothing* to do with angular momentum:

$$\begin{aligned} \hat{J}_z &= \frac{1}{2}\sum_{i=1}^{N}\left(\hat{a}^\dagger_{i\uparrow}\hat{a}_{i\uparrow} - \hat{a}^\dagger_{i\downarrow}\hat{a}_{i\downarrow}\right), \\ \hat{J}_+ &= \sum_{i=1}^{i}\hat{a}^\dagger_{i\uparrow}\hat{a}_{i\downarrow}, \\ \hat{J}_- &= \left(\hat{J}_+\right)^\dagger = \sum_{i=1}^{i}\hat{a}^\dagger_{i\downarrow}\hat{a}_{i\uparrow}. \end{aligned} \tag{7.17}$$

We also call these quasi-spin operators, although they look nothing like the quasi-spin operators for seniority. With these operators and commutation relations in hand we rewrite the Lipkin Hamiltonian into the form

$$\hat{H} = \epsilon J_z - \frac{1}{2}V\left(\hat{J}_+^2 + \hat{J}_-^2\right) \tag{7.18}$$

Let me emphasize that this trick of rewriting using SU(2)-like operators is *not* generic. It's only in a few cases, specially designed to be analytically tractable, that one can do this. But these special cases help to illustrate the methods, both approximate and exact, that we will apply to messier, more general cases.

For example, the Lipkin Hamiltonian, being built from the operators $\hat{J}_\pm, \hat{J}_z$, must commute with $\hat{J}^2$. That is, the eigenstates of the Lipkin Hamiltonian must have j as a good quantum number, even though we have no easy physical interpretation of this number.

On the other hand, $\hat{J}_z$ does not commute with the Lipkin Hamiltonian. Therefore any eigenstate must have fixed j but be a mixture of different ms. That is, in order to find the exact solutions, we can fix j, and then take as a truncated basis all the states $m = -j, -j+1, \ldots, j-1, j$. Our basis states we then label by $|j, m\rangle$. Later, in section (9.5) we'll explore these in more detail as a way of illustrating more general, more numerical approaches.

In the basis $|j, m\rangle$, we can compute the matrix elements of the Hamiltonian. We do that by using

$$\hat{J}_z|j, m\rangle = m|j, m\rangle, \tag{7.19}$$

$$\hat{J}_\pm|j, m\rangle = \sqrt{j(j+1) - m^2 \mp m}|j, m \pm 1\rangle, \tag{7.20}$$

the latter which comes from (4.13). The only nonzero matrix elements are

$$\langle j, m|\hat{H}|j, m\rangle = \epsilon m, \tag{7.21}$$

$$\langle j, m+2|\hat{H}|j,m\rangle = -\frac{V}{2}\sqrt{[j(j+1)-m(m+1)]} \times\sqrt{[j(j+1)-(m+1)(m+2)]}. \tag{7.22}$$

Before going further, we can deduce some properties of the quantum numbers. We do this much in the same way as we did for the seniority Hamiltonian. For example, the extremal possible values of m are either $N/2$ (all states $\uparrow$) or $-N/2$ (all $\downarrow$). Thus, for a given N, the maximal value of j must be $N/2$.

Second, because the interaction is of the form $\hat{J}_+^2+\hat{J}_-^2$, which either promotes two particles from $\downarrow$ to $\uparrow$ or demotes two from $\downarrow$ to $\uparrow$, we can define a conserved 'parity', which is $(-1)^{N_\uparrow}$. That is, the Hamiltonian will connect two many-body states, both of which have either an even number of up particles or an odd number of up particles, but will never connect an even number of up particles with an odd number of up particles. This is reflected in the matrix element (7.22), which connects states that differ in m by 2 but not by 1.

So, for a given j, there are two separate sets of solutions: those constructed from states with $m = j, j-2, j-4, \ldots$ and those with $m = j-1, j-3, \ldots$.

Furthermore, for a given N, the possible js are $N/2, N/2-1, N/2-2, \ldots$. This can be confusing, because it means systems with N particles have a spectrum that includes the energies for $N-2$ particles, $N-4$ particles, etc.. This arises because of the simple, semi-algebraic nature of the Hamiltonian, but is not unknown in more realistic systems: in nuclei we have *isospin analogs* found in neighboring isobars (nuclei with the same $A = Z + N$ but different Z, N).

Let's consider a specific case: $N = 3$, so that the maximal $j = 3/2$ and the possible js are $3/2, 1/2$. For simplicity we set $\epsilon = 1$. For $j = 1/2$, the Hamiltonian is trivial:

$$\mathbf{H}_{j=1/2} = \begin{pmatrix} 1/2 & 0 \\ 0 & -1/2 \end{pmatrix}. \tag{7.23}$$

For $j = 3/2$ the Hamiltonian matrix is slightly more interesting:

$$\mathbf{H}_{j=3/2} = \begin{pmatrix} 3/2 & 0 & -\sqrt{3}V & 0 \\ 0 & 1/2 & 0 & -\sqrt{3}V \\ -\sqrt{3}V & 0 & -1/2 & 0 \\ 0 & -\sqrt{3}V & 0 & -3/2 \end{pmatrix}. \tag{7.24}$$

and we see that we get either $m = 3/2, -1/2$ (which we label as "odd parity" although it has no physical meaning aside from having an odd number of particles "up") or $m = 1/2, -3/2$ (even parity). We can solve for the eigenvalues exactly, and get $E = 1/2 \pm \sqrt{1+3V^2}$ for odd parity solutions and $E = -1/2 \pm \sqrt{1+3V^2}$ for even solutions.

For larger N, of course, one must diagonalize numerically. An example is given below.

7.3.2 Variational solution of the Lipkin model

The Lipkin model is easy to solve exactly, but it is still instructive to apply approximation techniques. First we tackle it using variational theory, akin to

mean-field theory (also known as Hartree-Fock, discussed later in Chapter 11), but simplified.

For a variational limit on the Lipkin model, we transform the $\uparrow$ and $\downarrow$ states into a different basis, labeled $+$ and $-$:,

$$\hat{c}_{i+} = \cos\theta_i \hat{a}_{i\uparrow} - e^{i\phi_i} \sin\theta_i \hat{a}_{i\downarrow}, \tag{7.25}$$

$$\hat{c}_{i-} = \cos\theta_i \hat{a}_{i\downarrow} + e^{-i\phi_i} \sin\theta_i \hat{a}_{i\uparrow} \tag{7.26}$$

For simplicity we assume all $\theta_i = \theta$, $\phi_i = \phi$. The trial state is a Slater determinant,

$$|\Psi_T\rangle = \prod_{i=1}^{N} \hat{c}_{i-}^\dagger |0\rangle , \tag{7.27}$$

which is automatically normalized. Now we want to find

$$E(\theta, \phi) = \langle \Psi_T | \hat{H} | \Psi_T \rangle \tag{7.28}$$

and minimize by varying the angles.

In order to compute the expectation value (7.28), we also transform our quasi-spin operators. For another approach, see section (10.3.2). We define

$$\hat{J}'_z = \frac{1}{2} \sum_{i=1}^{N} \left(\hat{c}_{i+}^\dagger \hat{c}_{i+} - \hat{c}_{i-}^\dagger \hat{c}_{i-} \right), \tag{7.29}$$

and similarly $\hat{J}'_\pm$. We do this because the expectation value (7.28) becomes easy in this representation; for example,

$$\left\langle \Psi_T \left| \hat{J}'_z \right| \Psi_T \right\rangle = -\frac{N}{2}, \tag{7.30}$$

$$\left\langle \Psi_T \left| \hat{J}'^2_z \right| \Psi_T \right\rangle = \frac{N^2}{4}, \tag{7.31}$$

$$\left\langle \Psi_T \left| \hat{J}'_- \hat{J}'_+ \right| \Psi_T \right\rangle = N; \tag{7.32}$$

all other expectation values are zero. before we get there, however, we must find the relationship between $\hat{J}_z, \hat{J}_\pm$ and $\hat{J}'_z, \hat{J}'_\pm$. While tedious, the result are

$$\hat{J}_z = \cos 2\theta \hat{J}'_z + \frac{1}{2} \sin 2\theta \cos\phi \left(\hat{J}'_+ + \hat{J}'_- \right), \tag{7.33}$$

$$\hat{J}_+ = \cos^2\theta \hat{J}'_+ - e^{-2i\phi} \sin^2\theta \hat{J}'_- - \sin 2\theta e^{-i\phi} \hat{J}'_z, \tag{7.34}$$

$$\hat{J}_- = \cos^2\theta \hat{J}'_- - e^{2i\phi} \sin^2\theta \hat{J}'_+ - \sin 2\theta e^{i\phi} \hat{J}'_z. \tag{7.35}$$

Inserting these into the Hamiltonian and taking the expectation value, we get the energy as a function of θ, ϕ is

$$\langle \Psi_T | \hat{H} | \Psi_T \rangle = E(\theta, \phi) = -\frac{N\epsilon}{2} \left(\cos 2\theta + \frac{1}{2} \chi \sin^2 2\theta \cos 2\phi \right), \tag{7.36}$$

where $\chi = (N-1)V/\epsilon$.

To find the minima, we take the derviatives:

$$\frac{\partial E}{\partial \theta} = N\epsilon \sin 2\theta(1 - \chi \cos 2\theta \cos 2\phi) = 0, \tag{7.37}$$

$$\frac{\partial E}{\partial \phi} = \frac{N\epsilon}{2}\chi \sin^2 2\theta \sin 2\phi = 0. \tag{7.38}$$

From the second equation, we must either have $\theta = 0, \pi/2$ or $\phi = 0, \pi/2$.

In order to be sure we have a minimum, we also need the second derivatives:

$$\frac{\partial^2 E}{\partial \theta^2} = 2N\epsilon(\cos 2\theta - \chi \cos 4\theta \cos 2\phi) > 0, \tag{7.39}$$

$$\frac{\partial^2 E}{\partial \phi^2} = N\epsilon\chi \sin^2 2\theta \cos 2\phi > 0. \tag{7.40}$$

In fact, for a minimum one needs the eigenvalues of the matrix of second derivatives to be positive, but by the condition (7.38) we find the cross-derivative $\partial^2/\partial\theta\partial\phi = 0$ always. We also find that when $\chi > 0$, $\phi = 0$ but when $\chi < 0$, $\phi = \pi/2$. In practice, however, this last just means we always replace χ by $|\chi|$, or, alternately, always require $\chi > 0$. I follow this last, for now.

Now we identify two cases:

Case A : $1 > \chi > 0$, $\theta = 0$, $E_{HF} = -N\epsilon/2$.

Case B : $\chi > 1$, $\cos 2\theta = 1/\chi$, $E_{HF} = -\frac{N\epsilon}{4}\left(\chi + \frac{1}{\chi}\right)$.

Note that these solutions agree at $\chi = 1$. Case A is often called "spherical" in the literature and Case B is often called "deformed," but those terms are misleading. In fact, Case A is better termed "symmetry-preserving," because the variational solution has good parity, which is an exact symmetry of the Hamiltonian, while case B is "symmetry-mixing," that is even though exact solutions of the Lipkin model have good parity, this variational state does not have good parity but mixes it. While breaking symmetries seems like a bad idea, in physics we often find that breaking symmetries in an approximation can often lead to a closer solution than keeping them. We'll see this again when we consider quasiparticles, where we crazily abandon having a fixed number of particles. In section 10.3 we'll consider 'variation after projection' where we start from a simple state, project out a state of good symmetry, and then vary the parameter(s) to get the lowest energy; while this yields very good results, at least for the Lipkin model, it is also considerably more difficult.

Fig. 7.2 compares the variational solution against the exact ground state energy for $N = 10$ particles. Note in particular:

• the variational energy is always above the exact ground state energy, as it should; and

• the variational solution exhibits a change from the constant solution for $\chi < 0$, the spherical or parity-conserving solution, with $\theta = 0$, to the deformed or parity-mixing solution, with $\theta \neq 0$, for $\chi > 0$.

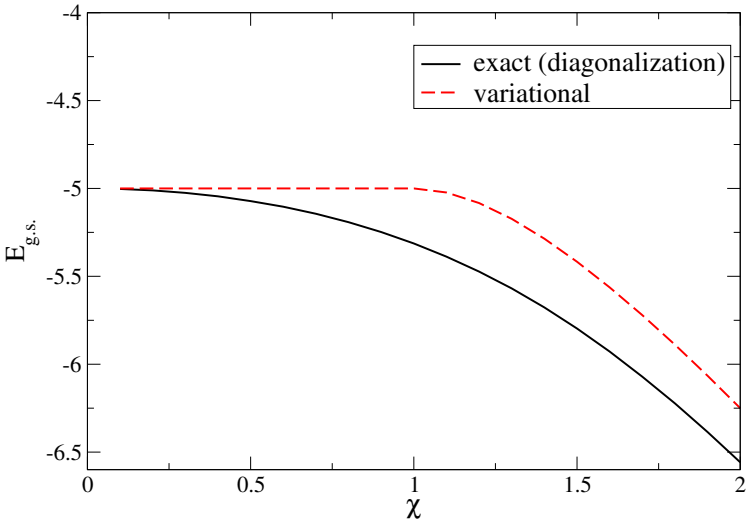

Figure 7.2: Ground state of the Lipkin model with $N = 10$, both though exact diagonalization of the Hamiltonian (solid black line) and through the variational approximation (dashed red line).

7.3.3 Moments and Transitions in the Lipkin model

Too often in studying many-body systems one focuses on the energy spectrum and ignores other observables that not only illuminate the wavefunction, but also are critical to interpreting and understanding experiments. In this section I briefly describe calculation of such observables, while noting we are still using the trick of quasi-spin operators to ease the calculation. Later chapters will tackle observables in more gory detai. (Despite their importance, however, this is an advanced topic that the reader may skip on the first go.)

A transition is when an operator, $\hat{\mathcal{O}}$, representing an external field, connects some initial state $|i\rangle$ to some final state $|f\rangle$, $f \neq i$, with a transition amplitude $\langle f|\hat{\mathcal{O}}|i\rangle$ or the transition strength or probability, $|\langle f|\hat{\mathcal{O}}|i\rangle|^2$. A moment is related, but is the expectation value of the operator for some state, often but not always the ground state. For example, one can talk about electric quadrupole (E2) or magnetic dipole (M1) transitions or moments. There is much more about moments and transitions that we will not discuss here.

For the Lipkin model, we have only a small handful of operators, basically $\hat{J}_z$ or $\hat{J}_\pm$. We can find the ground state moment of $\hat{J}_z$ in a straightforward fashion.

7.4 Generalizations of the Lipkin model

There are two generalizations of the Lipkin model. They are more challenging than the original Lipkin model, and the beginning can comfortably put this section aside, at least until she is more comfortable with manipulating operators.

7.4.1 The Lipkin model with isospin

Suppose we have A particles labeled by i, each of which can be in one of four states: $p_\uparrow, p_\downarrow, n^\uparrow, n_\downarrow$. Then, following Stoica, Mihut, and Suhonen (SMS), we introduce the operators

$$T_+^{(1)} = \sum_{i=1}^{A} p_{\uparrow i}^\dagger n_{\downarrow i},\ T_-^{(1)} = \sum_{i=1}^{A} n_{\downarrow i}^\dagger p_{\uparrow i},\quad T_z^{(1)} = \frac{1}{2}\sum_{i=1}^{A}(p_{\uparrow i}^\dagger p_{\uparrow i} - n_{\downarrow i}^\dagger n_{\downarrow i}) \quad (7.41)$$

$$T_+^{(2)} = \sum_{i=1}^{A} n_{\uparrow i}^\dagger p_{\downarrow i},\ T_-^{(2)} = \sum_{i=1}^{A} p_{\downarrow i}^\dagger n_{\uparrow i},\quad T_z^{(2)} = \frac{1}{2}\sum_{i=1}^{A}(n_{\uparrow i}^\dagger n_{\uparrow i} - p_{\downarrow i}^\dagger p_{\downarrow i}). \quad (7.42)$$

The Hamiltonian, as introduced by SMS, is

$$H = \epsilon(T_z^{(1)} + T_z^{(2)}) + V(T_+^{(1)}T_+^{(2)} + T_-^{(2)}T_-^{(1)}) + W(T_+^{(1)}T_-^{(1)} + T_+^{(2)}T_-^{(2)}) \quad (7.43)$$

By inspection this Hamiltonian conserves charge, so it must commute with

$$Z - N = 2(T_z^{(1)} - T_z^{(2)}) \quad (7.44)$$

We can also introduce charge-changing operators (to be done).

The $T^{(1)}$s and $T^{(2)}$s each generate commuting SU(2) algebras. In addition, by inspection, (7.43) commutes with $(\hat{T}^{(i)})^2$ but not $T_z^{(i)}$. The basis states we choose therefore is

$$|T^{(1)}M^{(1)}\rangle|T^{(2)}M^{(2)}\rangle, \quad (7.45)$$

where $T^{(i)}$ is the quantum number labeling the Casimir of the appropriate subalgebra. Ultimately, we want to express *everything* in terms of the quantum numbers of this basis, meaning in terms of $T^{(i)}, M^{(i)}$. In particular, ultimately we cannot compute the total number of particles $A = Z + N$. However we can use A to construct the basis.

To construct the basis, let us imagine putting A_1 particles into the states $p_\uparrow, n_\downarrow$, that is the first algebra, and $A_2 = A - A_1$ particles into the states $p_\downarrow, n_\uparrow$ or the second algebra. By inspection, one can deduce the maximal $M^{(i)}$ is $A^{(i)}/2$ and thus also the maximal values of $T^{(i)}$. Therefore for A particles we require $T^{(1)} + T^{(2)} \leq A/2$. Note that this is the maximal value; one can have values less than this.

Let me run through some examples. The case for $A = 1$ is trivial; the states are either p or n. Thus we have $T^{(i)} = 1/2$ and $M^{(i)} = \pm 1/2$.

For $A = 2$ we have 3 possible isospin states: pp, pn or nn, which correspond to $M^{(1)} - M^{(2)} = 1, 0, -1$. We have $T^{(1)} + T^{(2)} = 0, 1$ and each $T^{(i)} = 0, 1/2, 1$. We can directly list all the possible states of the form (7.45)

pp:

$$|1/2, 1/2\rangle|1/2, -1/2\rangle, \quad |0,0\rangle|1,-1\rangle, \quad |1,1\rangle|0,0\rangle$$

nn:

$$|1/2, -1/2\rangle|1/2, 1/2\rangle, \quad |0,0\rangle|1,1\rangle, \quad |1,-1\rangle|0,0\rangle$$

pn:

$$|0,0\rangle|0,0\rangle, \quad |0,0\rangle|1,0\rangle, \quad |1,0\rangle|0,0\rangle,$$
$$|1/2,1/2\rangle|1/2,1/2\rangle, \quad |1/2,-1/2\rangle|1/2,-1/2\rangle$$

States with the same $T^{(i)}$ but different $M^{(i)}$ belong to the same multiplet. So, for example, $|0,0\rangle|0,0\rangle$ is a multiplet all by itself. More interesting is the multiplet $|1/2,M^{(1)}\rangle|1/2,M^{(2)}\rangle$ which has 4 states. Below, when we solve for the eigenstates, we will diagonalize the Hamiltonian in a multiplet with a further restriction to states with fixed $M^{(1)}-M^{(2)}$. So, for example, for *pn*, $|1/2,1/2\rangle|1/2,1/2\rangle$ and $|1/2,-1/2\rangle|1/2,-1/2\rangle$, or, more trivially, for *pp* $|1/2,1/2\rangle|1/2,-1/2\rangle$ and for nn $|1/2,-1/2\rangle|1/2,1/2\rangle$. When we get to charge-changing transitions, we will stay within a multiple but change $M^{(1)}-M^{(2)}$.

Note also that there is a symmetry when we switch $T^{(1)} \leftrightarrow T^{(2)}$. This will ultimately be another degeneracy.

In case you are counting, notice that we ought to have $2^4 = 16$ states, but only found above 11 independent states. What happens is that some of the representations have multiple copies. We can even identify these by hand. For *pp*, there should be 4 states. Clearly $|0,0\rangle|1,1\rangle$ and $|1,1\rangle|0,0\rangle$ are unique, so that $|1/2,1/2\rangle|1/2,1/2\rangle$ must have two copies. An entire multiplet must be copied, so we now have accounted for 15 states. We therefore deduce that $|0,0\rangle|0,0\rangle$ must also have an additional copy. This won't affect any of our calculations. This also happens in the original Lipkin model.

In the exercises at the end of the chapter you are encouraged to find all the basis states for $A = 3, 4$. If you do so you will find the the state $|0,0\rangle|0,0\rangle$, for example, represents both *pn* and *ppnn*. This state will appear for all $Z = N$ cases and will always have the same energy (=0). This degeneracy, and others, is commonplace for Lipkin models.

To find the matrix elements of the Hamiltonian in this basis, one simply uses

$$\hat{T}_z|T,M\rangle = M|T,M\rangle, \tag{7.46}$$
$$\hat{T}_\pm|T,M\rangle = \sqrt{(T\mp M)(T\pm M+1)}|T,M\pm 1\rangle. \tag{7.47}$$

For the Hamiltonian there are only two kinds of matrix elements: the diagonal matrix elements

$$\langle T^{(1)}M^{(1)},T^{(2)}M^{(2)}|\hat{H}|T^{(1)}M^{(1)},T^{(2)}M^{(2)}\rangle = \epsilon(M^{(1)}+M^{(2)})$$
$$+W\left(\sqrt{\left(\left(T^{(1)}\right)^2-\left(M^{(1)}\right)^2\right)\left(\left(T^{(1)}+1\right)^2-\left(M^{(1)}\right)^2\right)}\right. \tag{7.48}$$
$$\left.+\sqrt{\left(\left(T^{(2)}\right)^2-\left(M^{(2)}\right)^2\right)\left(\left(T^{(2)}+1\right)^2-\left(M^{(2)}\right)^2\right)}\right) \tag{7.49}$$

and the off-diagonal matrix elements

$$\langle T^{(1)}M^{(1)}+1,T^{(2)}M^{(2)}+1|\hat{H}|T^{(1)}M^{(1)},T^{(2)}M^{(2)}\rangle =$$
$$V\sqrt{\left(T^{(1)}-M^{(1)}\right)\left(T^{(1)}+M^{(1)}+1\right)\left(T^{(2)}-M^{(2)}\right)\left(T^{(2)}+M^{(2)}+1\right)} \tag{7.50}$$

From this it is clear that if one chooses $V = 0$ then the solutions are nearly trivial, and possibly uninteresting. My feeling is one should focus on cases with $W = 0$ first, and then later try $W \neq 0$ to see if there is significant qualitative difference. I suspect not.

To give some starter solutions, for $A = 2$ there is only one nontrivial case, *pn* with $(T^{(1)}, T^{(2)}) = (1/2, 1/2)$; the basis states are

$$|1/2, 1/2\rangle|1/2, 1/2\rangle$$
$$|1/2, -1/2\rangle|1/2, -1/2\rangle$$

Then the matrix is

$$\begin{pmatrix} \epsilon & V \\ V & -\epsilon \end{pmatrix} \tag{7.51}$$

which has a ground state energy of $-\sqrt{\epsilon^2 + V^2}$.

$A = 3$ also has the following nontrivial cases from *ppn* (with mirror solutions in textitpnn): for $(T^{(1)}, T^{(2)}) = (1, 1/2)$:

$$\begin{pmatrix} \frac{3}{2}\epsilon & \sqrt{2}V \\ \sqrt{2}V & -\frac{1}{2}\epsilon \end{pmatrix} \tag{7.52}$$

with eigenvalues $\frac{1}{2}\epsilon - \sqrt{\epsilon^2 + 2V^2}$ and for $(T^{(1)}, T^{(2)}) = (1/2, 1)$:

$$\begin{pmatrix} \frac{1}{2}\epsilon & \sqrt{2}V \\ \sqrt{2}V & -\frac{3}{2}\epsilon \end{pmatrix} \tag{7.53}$$

with eigenvalues $-\frac{1}{2}\epsilon - \sqrt{\epsilon^2 + 2V^2}$.

7.4.2 Three-Level Lipkin Model

7.5 Summary

This chapter describes several simple toy models which nonetheless give good practice in working with fermion operators:

• the pairing or seniority model, which is a paradigm for pairing in many-body systems and which can be solved by invoking *quasi-spin*, that is, writing the problem in terms of operators which follow the SU(2) commutation relations and thus can be tackled with our knowledge of angular momentum algebra; and

• the Lipkin model and its variants, the calculation of which can also be simplified and illuminated by the use of quasi-spin techniques.

In addition to giving good practice in working with fermion operators, these two models will allow us to look at various standard approximations. Already in this chapter we looked at variational solutions to the Lipkin model. In future chapters we will tackle the problem of pairing plus non-degenerate single-particle energies, which cannot be easily solved analytically (there is the Richardson method, but that is beyond the scope of this book), but which we will approximate using *quasi-particles* in the Bardeen-Cooper-Schriefer or BCS method; and we will apply both quasi-particles and the random phase approximation to the Lipkin model and its variants. So stay tuned!

7.6 Exercises

(7.1) Prove (7.5).

(7.2) Show the operators (7.17) satisfy the usual SU(2) commutation relations.

(7.3) Find the energy spectrum for the Lipkin model for $N = 2$.

(7.4) Write a computer code to numerically solve for the energy spectrum for the Lipkin model for any reasonable N. Confirm the results for $N = 10$ as shown in Fig. 7.2.

(7.x) For the Lipkin model with isospin (section 7.4.1, for $A = 3$, find the four independent *ppp* states and the eight independent *ppn* states. What about *pnn* and *nnn*?

(7.y) For the Lipkin model with isospin (section 7.4.1, for $A = 4$, find the five independent *pppp* states, the eleven independent *pppn* states, and the fourteen independent *ppnn* states. What about *pnnn* and *nnnn*?

Chapter 8

Quasiparticles

> Your theory is crazy, but it's not crazy enough to be true. –*Niels Bohr.*

We previously looked at pairing with the seniority Hamiltonian, which can be solved exactly using quasispin. If one changes the Hamiltonian, for example by adding nondegenerate single-particle energies, the Hamiltonian is no longer exactly solvable. Instead a new trick can be invoked, that of quasi*particles*, one of the oddest and yet most powerful ideas we will encounter in this text.

8.1 The Bogoliubov transformation

Exact symmetries are often important in many-body systems: invariance under translation, rotation, and parity inversion. Yet many times in nuclear physics we break these exact symmetries with an approximate ansatz; in particular for mean-field (Hartree-Fock) calculations we almost always break translational symmetry and we frequently break rotational symmetry. This was illustrated in section (7.3.2) when we approximated the ground state of the Lipkin model by a Slater determinant, and found for some values of the parameters, a Slater determinant mixing parity yielded a better result than a symmetry-preserving determinant.

In a similar vein, starting from a pair of time-reversed fermion operators, $\hat{a}_k^\dagger, \hat{a}_{-k}^\dagger$, we boldly introduce the *Bogoliubov transformation*:

$$\begin{aligned} \hat{c}_k &= u_k \hat{a}_k - v_k \hat{a}_{-k}^\dagger, \\ \hat{c}_{-k} &= u_k \hat{a}_{-k} + v_k \hat{a}_k^\dagger, \\ \hat{c}_k^\dagger &= u_k \hat{a}_k^\dagger - v_k \hat{a}_{-k}, \\ \hat{c}_{-k}^\dagger &= u_k \hat{a}_{-k}^\dagger + v_k \hat{a}_k, \end{aligned} \tag{8.1}$$

where we take u_k, v_k to be real. Now if we further asssume $u_k^2 + v_k^2 = 1$, then we can prove

$$\{\hat{c}_k, \hat{c}_{-k}\} = \left\{\hat{c}_k, \hat{c}_{-k}^\dagger\right\} = \left\{\hat{c}_k^\dagger, \hat{c}_{-k}^\dagger\right\} = \left\{\hat{c}_{-k}, \hat{c}_k^\dagger\right\} = 0 \qquad (8.2)$$
$$\left\{\hat{c}_k, \hat{c}_k^\dagger\right\} = \left\{\hat{c}_{-k}, \hat{c}_{-k}^\dagger\right\} = 1.$$

(Later I will discuss generalization that do not depend upon "time-reversed" pairs.) This is an interesting result. The quasiparticle creation and annihilation operators are a mixture of particle creation and annihilation operators. But they have exactly the same anticommutation relations as any other fermion creation and annihilation operators, so in the same way we applied SU(2) algebra to abstract systems (seniority, the Lipkin model) that have nothing to do with angular momentum, we can apply our techniques for maniupulating fermion operators to quasiparticles. The 'symmetry' broken is conservation of the number of particles, and often a simple state that mixes particle number is nonetheless a better approximation to the ground state.

8.2 The quasiparticle vacuum

The next step is to define a new 'vacuum' state, that is, a state $|\tilde{0}\rangle$ such that

$$\hat{c}_k|\tilde{0}\rangle = \hat{c}_{-k}|\tilde{0}\rangle = 0. \qquad (8.3)$$

Having such a state will complete the analogy with ordinary fermion operators, where $\hat{a}_\pm|0\rangle = 0$. But with quasiparticles we'll get unexpected results.

It turns out that the unnormalized state

$$|\tilde{0}\rangle = \prod_k \left(u_k + v_k \hat{a}_k^\dagger \hat{a}_{-k}^\dagger\right)|0\rangle, \qquad (8.4)$$

satisfies (8.3). Let's assume the product is ordered:

$$|\tilde{0}\rangle = \left(u_1 + v_1 \hat{a}_1^\dagger \hat{a}_{-1}^\dagger\right)\left(u_2 + v_2 \hat{a}_2^\dagger \hat{a}_{-2}^\dagger\right)\ldots|0\rangle.$$

Now let's show $\hat{c}_m|\tilde{0}\rangle = 0$. We do this as usual by moving $\hat{c}_m$ rightward using anticommutation relations. Because we move either past a number or *two* fermion operators, where two minus signs give us a + overall, we actually are commuting. If $k \neq m$, then easily

$$\hat{c}_m\left(u_k + v_k \hat{a}_k^\dagger \hat{a}_{-k}^\dagger\right) = \left(u_m \hat{a}_m - v_m \hat{a}_{-m}^\dagger\right)\left(u_k + v_k \hat{a}_k^\dagger \hat{a}_{-k}^\dagger\right)$$
$$= \left(u_k + v_k \hat{a}_k^\dagger \hat{a}_{-k}^\dagger\right)\hat{c}_m;$$

commuting past u_k is trivial, and anticommuting first past $\hat{a}_k^\dagger$ and then $\hat{a}_{-k}^\dagger$ we pick up two minus signs which cancel.

We commute $\hat{c}_m$ past $k = 1, 2, 3, \ldots$, until we reach $k = m$. Then we have:

$$\hat{c}_m|\tilde{0}\rangle = \prod_{k<m}\left(u_k + v_k\hat{a}_k^\dagger\hat{a}_{-k}^\dagger\right)\hat{c}_m\left(u_m + v_m\hat{a}_m^\dagger\hat{a}_{-m}^\dagger\right)\prod_{k>m}\left(u_k + v_k\hat{a}_k^\dagger\hat{a}_{-k}^\dagger\right)|0\rangle \quad (8.5)$$

So now we have to consider

$$\begin{aligned}\hat{c}_m\left(u_m + v_m\hat{a}_m^\dagger\hat{a}_{-m}^\dagger\right) &= \left(u_m\hat{a}_m - v_m\hat{a}_{-m}^\dagger\right)\left(u_m + v_m\hat{a}_m^\dagger\hat{a}_{-m}^\dagger\right)\\ &= \left(u_m^2\hat{a}_m - u_m v_n\hat{a}_{-m}^\dagger + u_m v_m\hat{a}_m\hat{a}_m^\dagger\hat{a}_{-m}^\dagger - v_m^2\hat{a}_{-m}^\dagger\hat{a}_m^\dagger\hat{a}_{-m}^\dagger\right). \quad (8.6)\end{aligned}$$

The last term $\hat{a}_{-m}^\dagger\hat{a}_m^\dagger\hat{a}_{-m}^\dagger$ immediately gives $-\hat{a}_m^\dagger\hat{a}_{-m}^\dagger\hat{a}_{-m}^\dagger = 0$. The next to last term $\hat{a}_m\hat{a}_m^\dagger\hat{a}_{-m}^\dagger$ gives, using the anticommutators, $(1 - \hat{a}_m^\dagger\hat{a}_m)\hat{a}_{-m}^\dagger$ which $= \hat{a}_{-m}^\dagger + \hat{a}_m^\dagger\hat{a}_{-m}^\dagger\hat{a}_m$, so we have overall

$$\begin{aligned}&\left(u_m^2\hat{a}_m - u_m v_n\hat{a}_{-m}^\dagger + u_m v_m\hat{a}_{-m}^\dagger + u_m v_n\hat{a}_m^\dagger\hat{a}_{-m}^\dagger\hat{a}_m\right)\\ &\qquad = \left(u_m^2 + u_m v_n\hat{a}_m^\dagger\hat{a}_{-m}^\dagger\right)\hat{a}_m.\end{aligned}$$

Inserting this back where we were, we have

$$\prod_{k<m}\left(u_k + v_k\hat{a}_k^\dagger\hat{a}_{-k}^\dagger\right)\left(u_m^2 + u_m v_n\hat{a}_m^\dagger\hat{a}_{-m}^\dagger\right)\hat{a}_m\prod_{k>m}\left(u_k + v_k\hat{a}_k^\dagger\hat{a}_{-k}^\dagger\right)|0\rangle. \quad (8.7)$$

But we now can continue to march $\hat{a}_m$ leftward, as it has no impediment (because all the operators it now encounters have $k \neq m$), until it finally encounters the vacuum and $\hat{a}_m|0\rangle$ gives zero, thus proving $\hat{c}_m|\tilde{0}\rangle = 0$. In the exercises at the end of the chapter you will have the opportunity to gently modify this and prove $\hat{c}_{-m}|\tilde{0}\rangle = 0$ as well.

The appeal of the quasiparticle vacuum may not be obvious at first. But it is not a *particle* vacuum. We can show this by computing the expectation value of the number operator $\hat{N}$,

$$\hat{N} = \sum_{k>0}\hat{a}_k^\dagger\hat{a}_k + \hat{a}_{-k}^\dagger\hat{a}_{-k}.$$

In order to do this, we first rewrite N in terms of quasiparticle operators, so we need to invert the Bogoliubov transformation (8.1):

$$\begin{aligned}\hat{a}_k &= u_k\hat{c}_k + v_k\hat{c}_{-k}^\dagger,\\ \hat{a}_{-k} &= u_k\hat{c}_{-k} - v_k\hat{c}_k^\dagger, \quad (8.8)\end{aligned}$$

and the Hermitian conjugate, and with this we get

$$\begin{aligned}\hat{N} = \sum_{k>0}\Big\{&u_k^2\left(\hat{c}_k^\dagger\hat{c}_k + \hat{c}_{-k}^\dagger\hat{c}_{-k}\right) + v_k^2\left(\hat{c}_k\hat{c}_k^\dagger + \hat{c}_{-k}\hat{c}_{-k}^\dagger\right)\\ &u_k v_k\left(\hat{c}_{-k}\hat{c}_k - \hat{c}_k\hat{c}_{-k} + \hat{c}_k^\dagger\hat{c}_{-k}^\dagger - \hat{c}_{-k}^\dagger\hat{c}_k^\dagger\right)\Big\}. \quad (8.9)\end{aligned}$$

Now this we simplify by using anticommutation relations, and in particular by trying to put it into *normal order*, that is, all the creation operators to the left and all the annihilation operators to the right:

$$\hat{N} = \sum_{k>0} \Big\{ 2v_k^2 + (u_k^2 - v_k^2) \left(\hat{c}_k^\dagger \hat{c}_k + \hat{c}_{-k}^\dagger \hat{c}_{-k} \right) + 2u_k v_k \left(\hat{c}_k^\dagger \hat{c}_{-k}^\dagger + \hat{c}_{-k} \hat{c}_k \right) \Big\}. \tag{8.10}$$

Now when we have $\langle \tilde{0} | \hat{N} | \tilde{0} \rangle$, because $\hat{c}_{\pm k} | \tilde{0} \rangle = 0$ and also $\langle \tilde{0} | \hat{c}_{\pm k}^\dagger = 0$, the terms vanish, except for the constants, so that

$$\langle \hat{N} \rangle = \langle \tilde{0} | \hat{N} | \tilde{0} \rangle = 2 \sum_k v_k^2. \tag{8.11}$$

So the quasiparticle vacuum has quite a few particles in it! But the situation is even stranger. Compute $\langle N^2 \rangle$; I won't do this in detail (see the exercises), but when one writes down $\hat{N}^2$ and put into normal order, the constant term is now

$$\left(\sum_k 2v_k^2 \right)^2 + 4 \sum_k u_k^2 v_k^2;$$

so that

$$\langle \hat{N}^2 \rangle = \left(\sum_k 2v_k^2 \right)^2 + 4 \sum_k u_k^2 v_k^2 \tag{8.12}$$

and so the *fluctuation* or uncertainty in the number of particles is

$$\Delta N = \sqrt{\langle \hat{N}^2 \rangle - \langle \hat{N} \rangle^2} = 2 \sqrt{\sum_{k>0} u_k^2 v_k^2}. \tag{8.13}$$

In other words, while the average number of particles is nonzero, the number itself is not fixed; the quasiparticle vacuum $|\tilde{0}\rangle$ is not an eigenstate of the number operator.

It might seem having a state with an indefinite number of particles would be a bad situation. Nonetheless, for decades physicists have found the advantages outweight the disadvantages, as we will see.

Before going on, however, let's consider the *one-quasiparticle* state, $\hat{c}_m^\dagger | \tilde{0} \rangle$. If we calculate the average number of particles in this state,

$$\langle \tilde{0} | \hat{c}_m \hat{N} \hat{c}_m^\dagger | \tilde{0} \rangle = u_m^2 - v_m^2 + \sum_{k>0} 2v_k. \tag{8.14}$$

To interpret this, look at limits. If $u_m \approx 1$ then $v_m \approx 0$, so then $\hat{c}_m^\dagger \approx \hat{a}_m^\dagger$, and indeed by simple counting we have *added* one particle to the quasiparticle 'vacuum.' Conversely, if $u_m \approx 0$, $v_m \approx 1$, then $\hat{c}_m^\dagger \approx -\hat{a}_{-m}$ and we have one *less* particle.

For an ordinary Slater determinant, we can consider we have a sharp division, either $u_k = 0, v_k = 1$ for occupied states (paradoxically called 'hole' states, because $\hat{c}_k$ creates a hole by destroying a particle), or $u_k = 1, v_k = 0$, so-called 'particle' states. In such an either-or situation, we cannot have both u_k and v_k nonzero and the uncertainty in the number of particles is zero.

8.3 BCS theory

We now turn to the Bardeen-Cooper-Schrieffer (BCS) approach, used for superconductivity. We modify the seniority Hamiltonian by adding single-particle energies:

$$\hat{H} = \sum_{k>0} \epsilon_k \left(\hat{a}_k^\dagger \hat{a}_k + \hat{a}_{-k}^\dagger \hat{a}_{-k} \right) - G \sum_{k>0,k'>0} \hat{a}_k^\dagger \hat{a}_{k'}^\dagger \hat{a}_{k'} \hat{a}_k, \tag{8.15}$$

and convert to quasiparticle operators in normal order. This is left as an exercise to you, but the end result is:

$$\hat{H} = \hat{H}_{00} + \hat{H}_{11} + \hat{H}_{22} + \hat{H}_{20} + \hat{H}_{02} + \hat{H}_{40} + \hat{H}_{04} \tag{8.16}$$

where:

$$\hat{H}_{00} = \sum_{k>0} \left(2\epsilon_k v_k^2 - G v_k^4 \right) - G\Delta^2; \tag{8.17}$$

$$\hat{H}_{11} = \sum_{k>0} \left\{ \epsilon_k (u_k^2 - v_k^2) + G \left(v_k^4 + 2\Delta u_k v_k \right) \right\} \hat{N}_k - G \left(\sum_{k>0} u_k v_k \hat{N}_k \right)^2; \tag{8.18}$$

$$\hat{H}_{22} = -G \sum_{k>0,k'>0} \left(u_k^2 u_{k'}^2 + v_k^2 v_{k'}^2 \right) \hat{c}_k^\dagger \hat{c}_{-k}^\dagger \hat{c}_{-k'} \hat{c}_{k'}; \tag{8.19}$$

$$\hat{H}_{20} = -G \sum_{k>0} \left\{ \Delta u_k^2 \hat{c}_k^\dagger \hat{c}_{-k}^\dagger + \sum_{k'>0} v_k^2 u_{k'} v_{k'} \hat{N}_{k'} \hat{c}_k^\dagger \hat{c}_{-k}^\dagger - u_k^2 u_{k'} v_{k'} \hat{N}_{k'} \right\}; \tag{8.20}$$

$$\hat{H}_{40} = +G \sum_{k,k'>0} u_k^2 v_{k'}^2 \hat{c}_k^\dagger \hat{c}_{k'}^\dagger \hat{c}_{-k'}^\dagger \hat{c}_{-k}^\dagger, \tag{8.21}$$

where I've introduced the following conventions:

$$\Delta = \sum_k u_k v_k, \tag{8.22}$$

$$\hat{N}_k = \hat{c}_k^\dagger \hat{c}_k + \hat{c}_{-k}^\dagger \hat{c}_{-k}, \tag{8.23}$$

and

$$\hat{H}_{02} = \hat{H}_{20}^\dagger, \tag{8.24}$$

etc..

The labeling of the pieces of the Hamiltonian are as follows: the vacuum or $|\tilde{0}\rangle$ is a *zero*-quasiparticle state; states of the form $\hat{c}_m^\dagger |\tilde{0}\rangle$ are *one*-quasiparticle

states; states of the form $\hat{c}_m^\dagger \hat{c}_n^\dagger |\tilde{0}\rangle$ are *two*-quasiparticle states, etc.. Then: $\hat{H}_{00}$ is nonzero for the vacuum (zero-quasiparticle state); $\hat{H}_{11}$ and $\hat{H}_{22}$ must be between one- and two-quasiparticle states, respectively, to yield a nonzero result; $\hat{H}_{20}$ acts on a state with n quasiparticles and connects it with a state with $n+2$ quasiparticles; and similarly for $\hat{H}_{40}$.

For the standard BCS we take the expectation value in the

$$\langle\tilde{0}|\hat{H}|\tilde{0}\rangle = \sum_{k>0} 2\epsilon_k v_k^2 - G\left[\left(\sum_{k>0} u_k v_k\right)^2 + \sum_{k>0} v_k^4\right].$$

We solve by minimizing the energy, but we also must use a constraint on the average number of particles; the way to do this is to minimize

$$\langle\tilde{0}|\hat{H} - \lambda\hat{N}|\tilde{0}\rangle = \sum_{k>0} 2(\epsilon_k - \lambda) v_k^2 - G\left[\left(\sum_{k>0} u_k v_k\right)^2 + \sum_{k>0} v_k^4\right], \tag{8.25}$$

where λ is the *Langrange multiplier*. The general strategy of using a Lagrange multiplier is:

Choose some value λ;
Minimize $\langle\hat{H} - \lambda\hat{N}\rangle$;
Compute $\langle\hat{N}\rangle$; if high or low, adjust

We find the minimum in the usual way, but first we must rewrite using $u_k = \sqrt{1 - v_k^2}$ and then take the derivative with respect to v_m:

$$\frac{\partial}{\partial v_m} \sum_{k>0} 2(\epsilon_k - \lambda) v_k^2 - G\left[\left(\sum_{k>0} v_k \sqrt{1 - v_k^2}\right)^2 + \sum_{k>0} v_k^4\right] \tag{8.26}$$

$$= 4(\epsilon_m - \lambda) v_m - 4G v_m^3 + 2\left(\sum_k u_k v_k\right)\left(\frac{u_m^2 - v_m^2}{u_m}\right) = 0 \tag{8.27}$$

where I reinserted u_k where I could. Defining the "gap"

$$\Delta \equiv \sum_{k>0} u_k v_k, \tag{8.28}$$

we can rewrite this as

$$2(\epsilon_m - G v_m^2 - \lambda) u_m v_m = G\Delta(u_m^2 - v_m^2) \tag{8.29}$$

8.3.1 Numerical examples

8.3.2 Approximate diagonalization

In this section we preview Chapter 9 on diagonalization; you can skip this on a first pass.

8.4 Isospin Lipkin model

We can illustrate some of the ideas of quasi-particles by returning to the Lipkin model with isospin.

Now I want to concern myself with the HF and RPA approximations. We introduce for each subalgebra 1 and 2 mixing parameters:

$$\hat{\pi}_+ = \cos\theta_1 \hat{p}_\uparrow - e^{i\phi_1}\sin\theta_1 \hat{n}_\downarrow, \tag{8.30}$$
$$\hat{\nu}_- = \cos\theta_1 \hat{n}_\downarrow + e^{-i\phi_1}\sin\theta_1 \hat{p}_\uparrow \tag{8.31}$$

and

$$\hat{\nu}_+ = \cos\theta_2 \hat{n}_\uparrow - e^{i\phi_2}\sin\theta_2 \hat{p}_\downarrow, \tag{8.32}$$
$$\hat{\pi}_- = \cos\theta_2 \hat{p}_\downarrow + e^{-i\phi_2}\sin\theta_2 \hat{n}_\uparrow \tag{8.33}$$

These we invert to get

$$\hat{p}_\uparrow = \cos\theta_1 \hat{\pi}_+ + e^{i\phi_1}\sin\theta_1 \hat{\nu}_-, \tag{8.34}$$
$$\hat{n}_\downarrow = \cos\theta_1 \hat{\nu}_- - e^{-i\phi_1}\sin\theta_1 \hat{\pi}_+ \tag{8.35}$$

etc.

From these we get the same transformations as in the single-species Lipkin:

$$T_z^{(1)} = \cos 2\theta_1 \tilde{T}_z^{(1)} + \frac{1}{2}\sin 2\theta_1 e^{i\phi_1}\tilde{T}_+^{(1)} + \frac{1}{2}\sin 2\theta_1 e^{-i\phi_1}\tilde{T}_-^{(1)}, \tag{8.36}$$
$$T_+^{(1)} = \cos^2\theta_1 \tilde{T}_+^{(1)} - e^{-2i\phi_1}\sin^2\theta_1 \tilde{T}_-^{(1)} - \sin 2\theta_1 e^{-i\phi_1}\tilde{T}_z^{(1)}, \tag{8.37}$$
$$T_-^{(1)} = \cos^2\theta_1 \tilde{T}_-^{(1)} - e^{2i\phi_1}\sin^2\theta_1 \tilde{T}_+^{(1)} - \sin 2\theta_1 e^{i\phi_1}\tilde{T}_z^{(1)}. \tag{8.38}$$

where

$$\tilde{T}_+^{(1)} = \pi_+^\dagger \nu_- \tag{8.39}$$

etc, and similarly for the $T^{(2)}$s.

Now the trial ground state is just a product of these operators

$$|\Psi_T\rangle = \prod_{i=1}^{Z_0} \pi_{-,i}^\dagger \prod_{j=1}^{N_0} \nu_{-,j}^\dagger |0\rangle \tag{8.40}$$

We will consider the case where $Z_0 \neq Z$, $N_0 \neq N$ because we will have indefinite charge anyway. We do fix $Z + N = Z_0 + N_0 = A$.

One can compute the expectation values

$$\langle\Psi_T|\tilde{T}_z^{(1)}|\Psi_T\rangle = -\frac{N_0}{2} \tag{8.41}$$
$$\langle\Psi_T|\tilde{T}_z^{(2)}|\Psi_T\rangle = -\frac{Z_0}{2} \tag{8.42}$$
$$\langle\Psi_T|\tilde{T}_-^{(1)}\tilde{T}_+^{(1)}|\Psi_T\rangle = N_0 \tag{8.43}$$
$$\langle\Psi_T|\tilde{T}_-^{(2)}\tilde{T}_+^{(2)}|\Psi_T\rangle = Z_0 \tag{8.44}$$

Now we can start computing. First, we work out the expectation value of the Hamiltonian (taking W = 0)

$$\langle H\rangle = -\frac{1}{2}\epsilon(N_0\cos 2\theta_1 + Z_0\cos 2\theta_2) + \frac{1}{2}V\times N_0 Z_0 \sin 2\theta_1 \sin 2\theta_2 \cos(\phi_1+\phi_2) \tag{8.45}$$

Now, while $Z+N$ is fixed, we also need to fix, at least on average, $Z-N$. So we compute the average value

$$\langle Z-N\rangle = 2\langle T_z^{(1)} - T_z^{(2)}\rangle = Z_0\cos 2\theta_2 - N_0\cos 2\theta_1 \tag{8.46}$$

We require that the average of $Z-N$ be fixed. There are two ways to do this.

The first way (which I don't think really works out, but I include it now for completeness) is to to derive a relation between θ_1 and θ_2 for a choice of Z_0. For example, suppose $Z_0 = Z$ (and thus automatically $N_0 = N$). Then with the help of trig identities we have

$$Z\sin^2\theta_2 = N\sin^2\theta_1 \tag{8.47}$$

Here's where it gets a bit tricky. We must have $\sin^2\theta \leq 1$, so if $Z \leq N$ we can choose to vary θ_2 and constrain

$$\sin^2\theta_1 = \frac{Z}{N}\sin^2\theta_2 \tag{8.48}$$

On the other hand, if $Z > N$ we would chose to vary θ_1 and constrain

$$\sin^2\theta_2 = \frac{N}{Z}\sin^2\theta_1 \tag{8.49}$$

In either case we would then substitute into the Hamiltonian and then minimize. But experience seems to show that is too clunky. So we turn to another method which is actually very similar to what we do in HFB: use a Lagrange multiplier. We simply minimize $\langle H\rangle - \lambda\langle T_z^{(1)} - T_z^{(2)}\rangle$, that is,

$$-\frac{1}{2}\epsilon(N_0\cos 2\theta_1 + Z_0\cos 2\theta_2) + \frac{1}{2}V\times N_0 Z_0 \sin 2\theta_1 \sin 2\theta_2 \cos(\phi_1+\phi_2) - \frac{1}{2}\lambda\left(Z_0\cos 2\theta_2 - N_0\cos 2\theta_1\right) \tag{8.50}$$

What you do is: fix λ and then minimize with respect to the angles $\theta_1, \theta_2, \phi_1, \phi_2$. Then compute $\langle Z-N\rangle$. If it isn't what you want, change λ and then compute again. This is what one does in an HFB calculation.

Taking the derivatives with respect to the θs, we get remarkably simple equations:

$$VZ_0\sin 2\theta_2\cos(\phi_1+\phi_2) = -(\epsilon-\lambda)\tan 2\theta_1, \tag{8.51}$$

$$VN_0\sin 2\theta_1\cos(\phi_1+\phi_2) = -(\epsilon+\lambda)\tan 2\theta_2 \tag{8.52}$$

You need to work out the derivatives with respect to the ϕs, which look to yield simple solutions similar to the simple Lipkin model (although I am not sure).

Taking the ratio of these two equations and assuming $\cos(\phi_1 + \phi_2) \neq 0$ we get

$$Z_0(\epsilon - \lambda)\cos 2\theta_1 = N_0(\epsilon + \lambda)\cos 2\theta_2 \tag{8.53}$$

which may or may not be helpful. You can use this to eliminate, say, θ_2 and get some complicated expression for θ_1 in terms of V and Z_0, N_0. You will probably have to solve numerically at this point. Good luck!

It is interesting also to calculate the fluctuation, that is,

$$4\langle (T_z^{(1)} - T_z^{(2)})^2\rangle - 4\langle T_z^{(1)} - T_z^{(2)}\rangle^2 = Z_0 \sin^2 2\theta_2 + N_0 \sin^2 2\theta_1 \tag{8.54}$$

8.5 Generalization

I initially followed the standard development, where one identifies "time-reverse partner" states labeled by $\pm k$; these may be states with opposite linear momentum, as in $\pm\vec{p}$, or states with time-reverse angular momentum, labeled by $j, \pm m_j$. (In the latter case there is actually a phase: the time-reverse state is $(-1)^{j+m}\hat{a}^\dagger_{j,-m}$. This is the historical development, introduced to simplify the solution. One can have more general mixing, however.

If we no longer divide up states by their time-reverse partners, we can consider

$$\hat{c}_k = \sum_i u_{ki}\hat{a}_i + v_{ki}\hat{a}_i^\dagger, \tag{8.55}$$
$$\hat{c}_k^\dagger = \sum_i v_{ki}^*\hat{a}_i + u_{ki}^*\hat{a}_i^\dagger,$$

or

$$\begin{pmatrix} \vec{c} \\ \vec{c}^\dagger \end{pmatrix} = \begin{pmatrix} \mathbf{u} & \mathbf{v} \\ \mathbf{v}^* & \mathbf{u}^* \end{pmatrix} \begin{pmatrix} \vec{a} \\ \vec{a}^\dagger \end{pmatrix} \tag{8.56}$$

where the matrix

$$\begin{pmatrix} \mathbf{u} & \mathbf{v} \\ \mathbf{v}^* & \mathbf{u}^* \end{pmatrix}$$

is unitary, which implies

$$\mathbf{u}^\dagger\mathbf{u} + \mathbf{v}^T\mathbf{v}^* = \mathbf{1}, \tag{8.57}$$
$$\mathbf{v}^\dagger\mathbf{u} + \mathbf{u}^T\mathbf{v}^* = 0. \tag{8.58}$$

I leave it as an exercise to prove the anti-commutation relations are still preserved.

8.6 Summary

What you should get from this chapter:

• Somewhat counterintuitively, we can get an good approximation to the many-body problem by introducing the concept of *quasiparticles*, operators

which have fermion anti-commutation relations (and so we can use all our tools on them) but which mix creation and annihilation of particles. The resulting wavefunction do not have a fixed number of particles; nonetheless, this is often a very useful approximation.

• We applied quasiparticles to two example problems: the Bardeen-Cooper-Schrieffer model, which is the old pairing Hamiltonian with non-degenerate energy levels, as a model of superconductivity; and to the isospin Lipkin model.

8.7 Exercises

(8.1) Prove the anticommutation relations (8.2).

(8.2) Derive the form of $\hat{N}^2$ in quasiparticles and thus Eq. (8.12).

(8.3) Show that for the one-quasiparticle state $|\tilde{m}\rangle = \hat{c}^\dagger_m|\tilde{0}\rangle$

(a) $\langle\tilde{m}|\hat{N}|\tilde{m}\rangle - \langle\tilde{0}|\hat{N}|\tilde{0}\rangle = u_m^2 - v_m^2$, which we interpret as meaning that far above the Fermi surface, where $u_m \approx 1$ we have a particle, while deep beneath the Fermi surface, where $v_m \approx 1$ we have a hole; and

(b)

(8.4) Derive (8.16) from (8.15).

(8.5) Compute the expectation value of the BCS Hamiltonian (8.16) for the one-quasiparticle state and show that

$$\langle\tilde{0}|\hat{c}_m\hat{H}\hat{c}^\dagger_m|\tilde{0}\rangle = \dots$$

(8.6) As a preview of diagonalization methods in Chapter 9, compute the Hamiltonian matrix elements between different one-quasiparticles states, as well as matrix elements of the number operator. Choose some values for G and for the single-particle spectrum. Do you get a decrease in N^2?

Do the same for the two-quasiparticle states.

Chapter 9

Diagonalization: the configuration-interaction method

> The purpose of computing is insight, not numbers. – *Richard Hamming.*

One major use of the occupation representation in quantum many-body calculations is the technique called *configuration interaction* or CI (sometimes also called in nuclear physics the interacting shell model). CI is really nothing more than diagonalization of the Hamiltonian in a many-body basis, much as our practice problems in Chapters 1 and 3.

In this Chapter I will broadly outline CI calculations, although different codes have significantly different algorithms. I will finish up with a simple yet detailed case study, of three interacting fermions; if you have time on your hands, you are encouraged to write a code, really only a few hundred lnes, that reproduces those results

The basic idea of CI is very simple: expand in a generate a basis of many-body states, $|\alpha\rangle$, that is,

$$|\Psi\rangle = \sum_{\alpha} c_{\alpha}|\alpha\rangle \tag{9.1}$$

compute the matrix elements of the Hamiltonian between these states,

$$H_{\alpha\beta} = \langle\alpha|\hat{H}|\beta\rangle,$$

and then find the eigenvalues and eigenvectors of the matrix $\mathbf{H}$. In general we choose orthonormal basis states,

$$\langle\alpha|\beta\rangle = \delta_{\alpha,\beta}. \tag{9.2}$$

As you might imagine, this is easier said than done.

9.1 Basis

In principle one could choose any many-body basis, but some bases are more convenient than others. The *many-body* basis states are, ultimately built as Slater determinants, so one must start with a finite set of *single-particle* states, $\{\phi_a\}$. Suppose there are N_s states. From these we build N-particle states.

There are a couple of ways to represent such states in a computer program. One can list the occupied single-particle states; alternately, one can represent a Slater determinant as a string of N_s bits with 0 for occupied and 1 for unoccupied. So, if we have six single-particle states, some possible 3-particle states are

$$\begin{aligned} \hat{a}_1^\dagger \hat{a}_2^\dagger \hat{a}_3^\dagger |0\rangle &= |1,2,3\rangle = |111000\rangle, \\ \hat{a}_1^\dagger \hat{a}_2^\dagger \hat{a}_6^\dagger |0\rangle &= |1,2,6\rangle = |110001\rangle, \\ \hat{a}_2^\dagger \hat{a}_4^\dagger \hat{a}_4^\dagger |0\rangle &= |2,4,5\rangle = |010110\rangle, \end{aligned} \tag{9.3}$$

and so on.

If every possible combination of occupied single-particle states is chosen, the dimension of the basis is

$$\left(\begin{array}{c} N_s \\ N \end{array} \right) = \frac{N_s!}{N!(N_s - N)!}$$

which means, generally, as either N_s or N increases, the basis dimension can grow exponentially. Often, however, one truncates the basis.

If the Hamiltonian is rotationally invariant, for example for atomic nuclei or the electronic structure of single atoms, then both total angular momentum J and the z-component M are good quantum numbers (see Appendix for a deeper discussion; if you are not familiar with angular momentum algebra you can skip over this discussion). A consequence is that the Hamiltonian will not connect states with different J or different M, and one can without loss choose a basis of states with a fixed M, also called an M-scheme calculation, or with fixed J, called a J-scheme calculation. A fixed M-scheme basis has smaller dimension than the entire combinatoric basis, and a fixed J-scheme basis is smaller still.

To give you an example, consider a simplified case where one has a single-particle states with $j = 7/2$. There are a total of 8 single-particle states, and if one has 4 particles, the total number of possible basis states is $\left(\begin{array}{c} 8 \\ 4 \end{array} \right) = 70$, but there are only 8 states with $M = 0$ and and only one state with $J = 0$.

While a J-scheme basis is smaller, it also requires more work to construct. M is a simply additive quantum number. If one chooses a single-particle basis where each single-particle state has good m, then M for a Slater determinant is simply the sum of the ms of the occupied states. This means that it is easy to construct an m-scheme basis with Slater determinants. In general a J-scheme basis state, however, must be a superposition of Slater determinants, a highly nontrivial problem beyond the scope of these notes. The trade-off between the simplicity of the M-scheme and the smaller dimension of the J-scheme is a difficult choice, and both kinds of schemes are used in codes.

9.1.1 Truncations, shells, and configurations

There are additional kinds of truncations, which because they generally do not involve conserved quantities, do affect the results. These truncations center around energies of single particles or of aggregates of particles. One is n-particle, n-hole, discussed in Chapter 10, relative to the Fermi surface and Fermi energy. Another, for rotationally invariant systems, is truncation on "configurations," which is the origin of the name "configuration-interaction," which makes it worth explaining in some detail.

As discussed above, if our many-body Hamiltonian is rotationally invariant, it is often convenient to use for our Slater determinants single-particle states that have good j and m, in particular because it allows us to easily create states that have fixed total M. Additional quantum numbers allow us to further characterize the single-particle states, in particular spin s, orbital angular momentum l, and in order to characterize the radial part of the wavefunction, either the radial nodal quantum number n or the principal quantum number N. The nodal quantum number n counts the number of nodes in the radial wavefunction, with 0 being the lowest, while the principal quantum number refers to the single-particle energy.

(The principal quantum number is mostly useful for cases with an algebraic relation between the quantum numbers and the energy of a one-particle system. For example, in the case of the Coulomb interaction, $N = n + l + 1$ and the energy is $\propto N^{-2}$, while for the three-dimensional harmonic oscillator, $N = 2n + l$ and the energy is $\propto N + 3/2$. Most potentials do not yield such simple algebraic formulas for the energy; they arise for Coulomb and harmonic oscillator potentials because there have conserved quantities beyond angular momentum, a property which requires a discussion of group theory beyond the scope of this text.)

Depending on the system, we label *orbits* or *orbitals* by these quantum numbers. Almost always we use spectroscopic notation for orbital angular momentum l: s for $l = 0$, p for $l = 1$, d for $l = 2$, f for $l = 3$, and thereafter in alphabetical order. In atomic physics we list orbits by the the principal quantum number N and by the orbital angular momentum: $1s, 2s, 2p, 3s, 3p, 3d$, etc. In nuclear physics we typically label orbits by the nodal quantum number, orbital angular momentum, and total angular momentum j, hence $0s_{1/2}, 0p_{1/2}, 0p_{3/2}, 1s_{1/2}, 0d_{3/2}, 0d_{5/2}$, etc.. (Sometimes the number starts with 1 rather than 0; one has to determine this by context.) Note that an orbit differs from a state, which also includes the magnetic quantum number m, so that an orbit is composed of several degenerate states.

Orbits can be organized by single-particle energies, often reflecting a mean-field picture or some approximation to it. Sometimes an orbit is also called a shell, though alternately a shell may be a set of orbits with similar single-particle energies. Hence, in nuclear physics one can group the $1s_{1/2}, 0d_{3/2}$ and $0d_{5/2}$ orbits into the *sd*-shell. You should be keep in mind that different people use orbit and shell in slightly different ways.

A *configuration* usually refers to the occupation of orbits or shells without

specific reference to states. For example, one may have $(1s)^2(2s)^2(2p)^1$ which means there are 2 electrons each in the $1s$ and $2s$ orbits, filling them, and 1 electron in the $2p$ orbit. A configuration can contain multiple many-body states, all of which are degenerate in energy if one considers only single-particle energies and ignores interparticle interactions (or the residual interaction, in the parlance of nuclear physics), although if they are coupled to fixed total J or total L and S, there may be only one unique many-body state. These then lead to the many-body basis states, and is the origin of the term 'configuration-interaction.'

9.2 Matrix elements

The heart of configuration-interaction calculations is computing the matrix elements $H_{\alpha\beta} = \langle\alpha|\hat{H}|\beta\rangle$. In this chapter I will briefly outline calculation of these matrix elements, assuming orthonormal M-scheme Slater determinants. Even most J-scheme matrix elements generally are compiled from intermediate M-scheme matrix elements. (In section 10.3 I'll discuss a more general scheme where one does not assume orthogonality; this is useful, for example, if one is projecting out states of good angular momentum.)

The M-scheme Hamiltonian is generally *sparse*, that is, most matrix elements are zero. (J-scheme Hamiltonians are, conversely, generally *dense*, that is mostly nonzero.) It is straightforward to see why. The Hamiltonian is a one-plus two-body operator (one can extend to three-body operators and beyond, but that discussion is beyond the scope of this text). As you learned back in Chapter 6, you can think of a two-body operator $\hat{a}_a^\dagger\hat{a}_b^\dagger\hat{a}_d\hat{c}$, when acting on a Slater determinant, as *moving* two particles from states c and d to states a and b. So, for example,

$$\hat{a}_7^\dagger\hat{a}_5^\dagger\hat{a}_1\hat{a}_3|1234\rangle = \hat{a}_7^\dagger\hat{a}_5^\dagger\hat{a}_1\hat{a}_3\hat{a}_4^\dagger\hat{a}_3^\dagger\hat{a}_2^\dagger\hat{a}_1^\dagger|0\rangle = \hat{a}_7^\dagger\hat{a}_5^\dagger\hat{a}_4^\dagger\hat{a}_2^\dagger|0\rangle = |2457\rangle \tag{9.4}$$

(the ordering does not matter as long as one is always consistent, in order to pick out any relative phases that arise). But the final Slater determinant, $|2457\rangle$, is orthogonal to any other Slater determinant except itself. Therefore,

$$\langle abcd|\hat{a}_7^\dagger\hat{a}_5^\dagger\hat{a}_1\hat{a}_3|1234\rangle = 0 \tag{9.5}$$

unless $abcd = 2457$. Try a few more examples if you like, and you'll see that most matrix elements must be zero; furthermore, in general the matrix element $\langle\alpha|\hat{H}|\beta\rangle$ between two Slater determinants must be zero unless $|\alpha\rangle$ and $|\beta\rangle$ differ by no more than two occupied states.

9.3 Diagonalization

Suppose you now have the Hamiltonian matrix, either explicitly or implicitly. If the dimensions are relatively small, say under a few thousand, you can readily compute all the eigenpairs. A common and relatively efficient algorithm for fully

diagonalizing Hermitian matricians is Householder, which carries out a series of orthogonal transformations to reduce the original matrix to tridiagonal form, i.e., zero everywhere except for along the diagonal and the first immediate off-diagonal. A tridiagonal matrix is then relatively easy to solve, and there exist robust black-box routines to do so (see, e.g., Numerical Recipes or LAPACK).

But the dimensions are very large, say 10^4 to 10^10, then finding all the eigenpairs is difficult and indeed usually unnecessary, as one typically only wants the ground state energy and a few excited states. In that case it is more efficient to go to partial diagonalization algorithm, such as Lanczos (commonly used in nuclear physics) or Davidson-Liu (used in atomic physics) or related algorithm.

9.4 The seniority model, redux

As a second illustration of configuration-interaction methods, we return to the seniority Hamiltonian. Although we used quasi-spin methods to arrive algebraically at the exact spectrum, we will treat this system naively, and consider both the basis and the Hamiltonian matrix in microscopic detail.

For the seniority model, we have Ω pairs of single-particles states, labeled by $m, \bar{m}$. To begin, consider the simple case of $\Omega = 2$, in which case there are four single-particle states, labeled as $1, 2, \bar{1}, \bar{2}$, and with two particles, $N = 2$. For our many-body states, each single-particle state is either occupied or unoccupied. If we have two particles $N = 2$, there are $\begin{pmatrix} 4 \\ 2 \end{pmatrix} = 6$ states, which we can represent using either creation operators or bit occupation, e.g.:

$$
\begin{aligned}
|1\rangle &= \hat{a}_1^\dagger \hat{a}_2^\dagger |0\rangle = |1100\rangle, \\
|2\rangle &= \hat{a}_1^\dagger \hat{a}_{\bar{1}}^\dagger |0\rangle = |1010\rangle, \\
|3\rangle &= \hat{a}_1^\dagger \hat{a}_{\bar{2}}^\dagger |0\rangle = |1001\rangle, \\
|4\rangle &= \hat{a}_2^\dagger \hat{a}_{\bar{1}}^\dagger |0\rangle = |0110\rangle, \\
|5\rangle &= \hat{a}_2^\dagger \hat{a}_{\bar{2}}^\dagger |0\rangle = |0101\rangle, \\
|6\rangle &= \hat{a}_{\bar{1}}^\dagger \hat{a}_{\bar{2}}^\dagger |0\rangle = |0011\rangle,
\end{aligned}
$$

The ordering and thus the label of the many-body states is arbitrary. Only the many-body states $|2\rangle$ and $|5\rangle$ have "paired" particles, that is a state i and its partner $\bar{\imath}$ occupied, hence the seniority Hamiltonian will have nonzero matrix elements only among these states. By hand the matrix element between those states is $-G$, and so using the above ordering for the many-body basis, the many-body Hamiltonian matrix is

$$
\mathbf{H} = -G \begin{pmatrix}
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix}
$$

which has one eigenvalue $-2G$ and five eigenvalues 0.

Now let's take a larger case: $\Omega = 4$, so eight single-particle states labeled $1, 2, 3, 4, \bar{1}, \bar{2}, \bar{3}, \bar{4}$, and $N = 4$ particles, for a total of $\begin{pmatrix} 8 \\ 4 \end{pmatrix} = 70$ many-body states. I won't enumerate them all here, but even without writing them all down we can classify them and quickly recover the eigenenergy spectrum.

To classify them, let's introduce some semi-informal terminology. When both a state i and its partner $\bar{\imath}$ are occupied, we'll call that a simple pair (I use that terminology to differentiate from the coherent superposition

$$\sum_i \hat{a}_i^\dagger \hat{a}_{\bar{\imath}}^\dagger$$

which forms part of the algebraic solution). There are six states with two simple pairs each, which for convenience I write with bit-occupation notation

$$|11001100\rangle, |10101010\rangle, |10011001\rangle, |01100110\rangle, |01010101\rangle, |00110011\rangle.$$

There are also 48 states with exactly one simple pair each, and 16 states with no simple pairs, all of which add up to 70 many-body states.

The seniority Hamiltonian essentially moves one 'simple pair' to another (or the same) simple pair; hence it cannot connect states between these different groups. Taking the two simple pair states in the order above, the sub-Hamiltonian can be worked out by hand:

$$\mathbf{H} = -G \begin{pmatrix} 2 & 1 & 1 & 1 & 1 & 0 \\ 1 & 2 & 1 & 1 & 0 & 1 \\ 1 & 1 & 2 & 0 & 1 & 1 \\ 1 & 1 & 0 & 2 & 1 & 1 \\ 1 & 0 & 1 & 1 & 2 & 1 \\ 0 & 1 & 1 & 1 & 1 & 2 \end{pmatrix}$$

Eigenvalues are less obvious, but they are $-6G$, $-2G$ (with degeneracy of 3) and 0 (degeneracy of 2).

The states with a single 'simple pair' each have two unpaired spectators; because they are unpaired (that is, their partner is not occupied), the seniority Hamiltonian cannot touch them. For example, consider the state $|11100010\rangle$; the single-particle states 1 and 2 are unpaired, and states 3 and $\bar{3}$ are paired. If we think about the action of the Hamiltonian on this state, it cannot move the pair $\hat{a}_3^\dagger \hat{a}_{\bar{3}}^\dagger$ to either $\hat{a}_1^\dagger \hat{a}_{\bar{1}}^\dagger$ or $\hat{a}_2^\dagger \hat{a}_{\bar{2}}^\dagger$, because the single-particle states 1 and 2 are already occupied. It can only move to $\hat{a}_4^\dagger \hat{a}_{\bar{4}}^\dagger$, and thus to the many-body state $|11010001\rangle$. Thus we get another subblock of the Hamiltonian for the states $|11100010\rangle, |11010001\rangle$, which is

$$\mathbf{H} = -G \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}.$$

The eigenvalues are $-2G, 0$. This pattern repeats throughout the subspace of states with a single 'simple pair,' and so we get 24 eigenvalues $-2G$ and 24

eigevalues of 0. In some cases we pick up a phase via anticommuting past an occupied state, so for example

$$\langle 11100100|\hat{H}|10110001\rangle = +G,$$

but for us it only affects the wavefunction, not the eigenvalue; such phases are critical, however, for more complicated, messier systems.

Finally, the 16 states with no simple pairs cannot have any nonzero Hamiltonian matrix elements among them, and so we have 16 additional eigenvalues of 0.

While this is an extremely simple system, and one we already solved using the algebraic 'trick' of quasi-spin operators, it is a useful beginning illustration of how one approaches more general problems, not solvable by tricks, via configuration-interaction.

9.5 The Lipkin Model, redux

As a second illustration of configuration-interaction methods, we return to the Lipkin model of section 7.3. Rather than using the trick of quasi-spin, however, we will tackle the Lipkin model naively.

9.6 Case study

To illustrate what we have learned, I will go over a detailed example: three fermions in a harmonic oscillator well, with a quartic interaction between particles:

$$\hat{H} = \sum_{i=1}^{3} \frac{\hat{p}_i^2}{2m} + \frac{1}{2}m\omega^2 x_i^2 + V_0 \sum_{i<j} (x_i - x_j)^4. \tag{9.6}$$

You are encouraged to create your own code to solve this problem and to reproduce the results given in this chapter. This will give you an idea of how a configuration-interaction code works. It will also form the basis for testing other approximations, such as Hartree-Fock and the random phase approximation.

In principle one can write a code that allow for a flexible number of particles. To do so efficiently is far from trivial, and the implementation I discuss here is far from the most efficient manner possible.

9.6.1 Basis

In principle fermions have spin, but we assume all three have the same z-component. Therefore the basis can be written as

$$|n_1 < n_2 < n_3\rangle. \tag{9.7}$$

The first task, given some $n_{\max}$ is to enumerate and create the basis in some array.

[give dimensions of the basis as a function of $n_{\max}$.]

9.7 Summary

What you should get out of this chapter:
• One way to solve the many-particle Schrödinger equation is by diagonalizing the Hamiltonian in a basis.
• Specific examples of how many-body Hamiltonian matrices are constructed and how they look.

9.8 Exercises

Exercise 1: Consider the seniority Hamiltonian with $\Omega = 3$, that is, six single-particle states, but with 3 particles. One particle will be unpaired. To compare against the algebraic result, v will be a positive odd integer.

Exercise: Write a computer program to solve the seniority Hamiltonian for general values of Ω and N using Slater determinants and compare against the algebraic result.

Exercise: If you feel up to it, do the same as our "case study," but for bosons.

Chapter 10

General Slater determinants and Thouless' theorem

> One cannot really argue with a mathematical theorem. – *Stephen Hawking*

The definition of an N-particle Slater determinant in occupation space is fairly simple: given a set of creation operators $\{\hat{a}^\dagger_\alpha\}$ representing single-particle wavefunctions $\{\phi_\alpha(\vec{r})\}$, Slater determinants have the form

$$\prod_{i=1}^{N} \hat{a}^\dagger_{\alpha_i}|0\rangle.$$

But of course, in principle the original choice of single-particle wavefunction $\{\phi_\alpha(\vec{r})\}$ is arbitrary. One can always redefine the states through a unitary transformation:

$$\phi'_a(\vec{r}) = \sum_{\alpha=1}^{N_s} U^*_{\alpha a}\phi_\alpha(\vec{r}), \tag{10.1}$$

(here N_s is the number of single-particle states in the space) which automatically leads to a redefinition of the creation and annihilation operators:

$$\hat{c}^\dagger_a = \sum_{\alpha=1}^{N_s} U^*_{\alpha a}\hat{a}^\dagger_\alpha. \tag{10.2}$$

Although I used $\hat{c}^\dagger_a$ previously to indicate quasiparticle operators, I also use it here for general mixing of operators. One should keep in mind our mantra: there is no physically special or 'true' single-particle states $\{\phi_\alpha(\vec{r})\}$, although one set may be more convenient than another.

If one uses all possible Slater determinants, for example as described in Chapter 9, then one might as well use the most convenient set of single-particle

states. On the other hand, many approximations, such as Hartree-Fock, the random phase approximation, and so on, depending critically upon starting from a single optimal (in some well-defined sense) Slater determinant, the choice is key.

First, an important and ubiquitous convention. Suppose we have fixed a set of single-particle states, and we choose to fill the first N states, so that the starting Slater determinant is

$$|\Psi_0\rangle = \hat{c}_1^\dagger \hat{c}_2^\dagger \dots \hat{c}_N^\dagger |0\rangle.$$

We then use the letters i, j to label the occupied states $1, 2, \dots, N$, and we use the letters m, n to label the unoccupied states $N+1, N+2, \dots$. (I use the letters a, b, c to label either kind of state, if unspecified.)

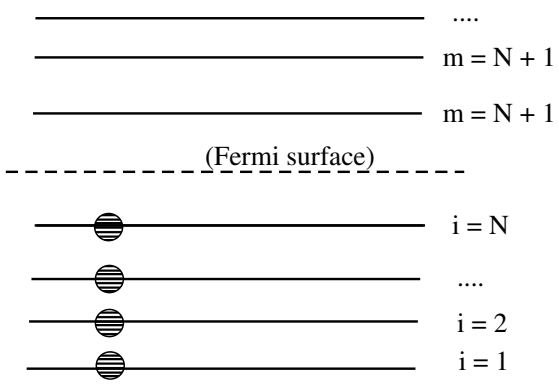

Figure 10.1: Illustration of the Fermi surface dividing occupied and unoccupied states in a given Slater determinant.

The division between the occupied states and the unoccupied states is called the *Fermi surface*. In many applications there are energies associated with each single-particle states, with the occupied states having lower energies than the unoccupied states. The *Fermi energy* can be thought of as the highest energy of the occupied states; later on I [may] give a more specific interpretations in terms of a chemical potential.

This convention is the basis for the *particle-hole* notation, which we will be using extensively in later chapters. The particle-hole picture can be thought of as a redefinition of the vacuum, for

$$\hat{c}_i^\dagger |\Psi_0\rangle = \hat{c}_m |\Psi_0\rangle = 0 \tag{10.3}$$

for any choice of i or m, while

$$\hat{c}_i |\Psi_0\rangle \neq 0, \hat{c}_m^\dagger |\Psi_0\rangle \neq 0. \tag{10.4}$$

In other words the operators for the unoccupied states m have the 'usual' effect, while the creation and annihilation operators for the occupied states i

have the opposite effect. Therefore these states are given the names, which at first glance appear paradoxical, *particle* and *hole* states respectively, because $\hat{c}_m^\dagger$ creates a particle (as usual) while $\hat{c}_i$ creates a hole. Note that this is *only* true relative to a specific Slater determinant.

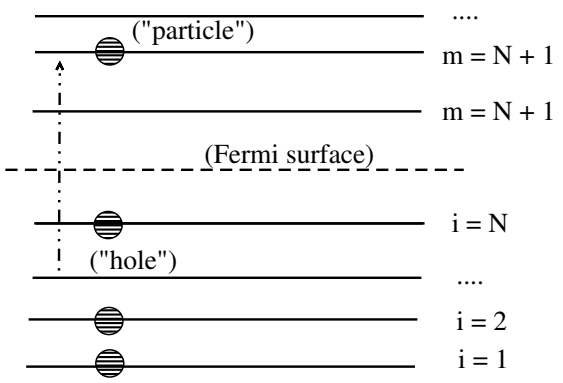

Figure 10.2: Illustration of a one-particle, one-hole state (relative to the Slater determinant in Fig. 10.1).

The state $\hat{c}_m^\dagger c_i|\Psi_0\rangle$ is called a *one-particle, one-hole* state because we have created a hole (destroyed one of the originally occupied states) and also created a particle (in an originally unoccupied state). You can think of this as moving a particle from an occupied state up to an unoccupied state, leaving behind a hole. Often one uses the shorthand notation $|mi^{-1}\rangle$ for such a particle-hole state. One can obviously also have *two-particle, two-hole* states, $|mni^{-1}j^{-1}\rangle = \hat{c}_m^\dagger \hat{c}_n^\dagger c_i c_j|\Psi_0\rangle$, etc. We will use this notation heavily for developments later on.

10.1 Density matrices and idempotency

While, given *any* set of single-particle states, we can construct a Slater determinant many-body wavefunction, the inverse question is more subtle: given a wavefunction, can it be represented by a single Slater determinant?

To answer this, we have to introduce the idea of a *density matrix*, and in particular a one-body density matrix.

Given a wavefunction $|\Psi\rangle$ and a set of single-particle wavefunctions and their corresponding creation/annihilation operators $\{\hat{c}_a^\dagger\}$, the one-body density matrix is

$$\rho_{ab} = \langle\Psi|\hat{c}_a^\dagger \hat{c}_b|\Psi\rangle / \langle\Psi|\Psi\rangle \tag{10.5}$$

(Elsewhere [TBD] I will introduce generalizations, for example two-body density matrices, and transition densities where the initial and final states are different. Density matrices are important and powerful tools for computing observables.)

Now, there is a simple concept that determines whether or not $|\Psi\rangle$ can be

written as a single Slater determinant: ρ must be *idempotent*, that is,

$$\rho^2 = \rho. \tag{10.6}$$

The only way ρ can be idempotent is if its eigenvalues are either 0 or 1. That idempotency is both a necessary and sufficient condition is easily proved. This can be easily proved by noting that the density matrix (10.5) is Hermitian.

10.2 Thouless' theorem

Thouless' theorem is an extremely important result upon which many later developments will depend.

First I will state Thouless' theorem, and [maybe] later prove it.

Thouless' theorem Let $|\Psi\rangle$ be a single Slater determinant. Let $\hat{Z}^\dagger = \sum_{ab} z^*_{ab}\hat{c}^\dagger_a\hat{c}_b$ be a general one-body operator. Then

$$\exp(\hat{Z}^\dagger)|\Psi\rangle$$

is also a single Slater determinant, which is not orthogonal to the original Slater determinant.

Before [maybe] proving Thouless' theorem, let's make note of a couple of useful ideas.

First, we don't need the most general one-body operator $\hat{Z}^\dagger$. Any Slater determinant is defined by the division between occupied and unoccupied states. A tranformation just among the occupied states, given by terms such as $\hat{c}^\dagger_i\hat{c}_j$,or a transformation just among the unoccupied states, given by terms such as $\hat{c}^\dagger_m\hat{c}_n$, do not change the Slater determinant in any fundamental way. Hence the only meaningful terms are $\hat{c}^\dagger_m\hat{c}_i$ (and possibly $\hat{c}^\dagger_i\hat{c}_m$); we call these particle-hole operators.

Second, even if $|\Psi\rangle$ is normalized, $\exp(\hat{Z}^\dagger)|\Psi\rangle$ will not be normalized. However, this can be readily addressed. You can show (see Exercise 12.1)

$$\exp\left(\sum_{mi} Z^*_{mi}\hat{c}^\dagger_m\hat{c}_i\right)|\Psi\rangle \tag{10.7}$$

is normalized, up to second order in Z_{mi}. Furthermore, for *any* one-body operator $\hat{Z}^\dagger$, unrestricted in the sum,

$$\exp(\hat{Z}^\dagger - \hat{Z})|\Psi\rangle \tag{10.8}$$

is normalized. This is because $\hat{Z}^\dagger - \hat{Z}$ is an anti-Hermitian operator, and the exponential of an anti-Hermitian operator is a rigorously unitary operator, preserving norms.

10.3 Non-orthogonal Slater determinants and their matrix elements

When used in configuration interaction calculations, Slater determinants are typically orthonormal to each other. For many applications, such as the derivation of Hartree-Fock, the random phase approximation, and generator-coordinate method, it is useful to consider Slater determinants which are non-orthogonal, or oblique. Thus in what follows we want to calculate the following:
• Overlap $\langle\Psi|\Psi'\rangle$ between two non-orthogonal Slater determinants;
• Matrix elements of one- and two-body operators $\hat{\mathcal{O}}$ between two non-orthogonal Slater determinants;
• How to project out states of good angular momentum and parity from a single Slater determinant; this will require rotating an arbitrary Slater determinant;
• Finally, we will want to learn how to drive or evolve a Slater determinant with a one-body operator, in order to form a generator-coordinate basis.

We suppose have N_s single-particle states. Thus, any single-particle wavefunction can be represented by a vector of length N_s as in (10.2). If we have N_p particles, the Slater determinant can represented by a N_s (rows) by N_p (columns) matrix $\mathbf{\Psi}$, whose columns are exactly those vectors defining the 'new' single-particle states, that is, we represent $\hat{c}_a^\dagger = \sum_{\alpha=1}^{N_s} U_{a\alpha}\hat{a}_\alpha^\dagger$ by the vector

$$\begin{pmatrix} U_{1a} \\ U_{2a} \\ U_{3a} \\ \vdots \\ U_{N_s a} \end{pmatrix}$$

and the entire Slater determinant by

$$\mathbf{\Psi} = \begin{pmatrix} \begin{pmatrix} U_{11} \\ U_{21} \\ U_{31} \\ \vdots \\ U_{N_s 1} \end{pmatrix} & \begin{pmatrix} U_{12} \\ U_{22} \\ U_{32} \\ \vdots \\ U_{N_s 2} \end{pmatrix} & \cdots & \begin{pmatrix} U_{1\,N_p} \\ U_{2\,N_p} \\ U_{3\,N_p} \\ \vdots \\ U_{N_s\,N_p} \end{pmatrix} \end{pmatrix} \tag{10.9}$$

The matrix $\mathbf{\Psi}$ can be complex. (I'm being slightly sloppy and inconsistent above, needs to be fixed.) Although originally one conceives of this formalism with the column vectors being orthonormal, in fact it turns out it works even when they are not orthonormal.

I state a couple of lemmas without proof, although with some reflection they should appear reasonable to the reader.

Lemma 1: Given two Slater determinants $|\Psi\rangle$ and $\Psi'\rangle$, represented by the matrices $\mathbf{\Psi}$, $\mathbf{\Psi'}$ respectively, the overlap is given by

$$\langle\Psi|\Psi'\rangle = \det\left(\mathbf{\Psi}^\dagger\mathbf{\Psi'}\right). \tag{10.10}$$

Note that $\mathbf{\Psi}^\dagger\mathbf{\Psi}'$ is an $N_p \times N_p$ matrix. The reader can check the following: if the columns of $\mathbf{\Psi}$ are orthonormal vectors, then $\langle\Psi|\Psi\rangle = 1$. If any two columns of $\mathbf{\Psi}$ are identical (two particles in the same state), then $\langle\Psi|\Psi\rangle = 0$. Furthermore, if $\mathbf{\Psi}'$ is $\mathbf{\Psi}$ but with two columns interchanged, then $\langle\Psi|\Psi'\rangle = -1$. Also, if at least one column vector of $\mathbf{\Psi}'$ is orthogonal to every column vector of $\mathbf{\Psi}$, then $\langle\Psi|\Psi'\rangle = 0$. And so on.

Thouless' theorem: Let $\hat{\mathcal{O}}_1 = \sum_{ij} \Theta_{ij}\hat{a}_i^\dagger\hat{a}_j$ be a one-body operator. Then if $|\Psi\rangle$ is a Slater determinant, then $\exp(\hat{\mathcal{O}}_1)|\Psi\rangle = |\Psi'\rangle$ is also a Slater determinant, which is not orthogonal to $|\Psi\rangle$. NB: This does not hold for 2-body operators, that is, in general $\exp(\hat{\mathcal{O}}_2)|\Psi\rangle$ cannot be written as a single Slater determinant.

Lemma 2. (Matrix representation of Thouless' theorem). In matrix form we can represent $\exp(\hat{\mathcal{O}}_1)|\Psi\rangle = |\Psi'\rangle$ by

$$\mathbf{\Psi}' = \exp(\mathbf{\Theta})\mathbf{\Psi}. \tag{10.11}$$

This turns out to be incredibly useful.

We need a final theorem, frequently covered in mathematical methods courses:

$$\ln\det\mathbf{A} = \mathrm{tr}\ln\mathbf{A}. \tag{10.12}$$

10.3.1 Generalized Wick theorems

In this section, I derive a series of *generalized Wick theorems*, which are nothing more than rules for computing matrix elements of n-body operators. In particular, I want to compute matrix elements of the form

$$\left\langle \Psi \left| \hat{a}_i^\dagger\hat{a}_j\hat{a}_k^\dagger\hat{a}_l\ldots \right| \Psi' \right\rangle. \tag{10.13}$$

To do this, I introduce a *generating function*. Let

$$\hat{\Theta} = \sum_{ij} \eta_{ij}\hat{a}_i^\dagger\hat{a}_j. \tag{10.14}$$

So $\hat{\Theta}$ is a one-body operator and the η_{ij} are simply the matrix elements.

The generating function is a function of the η_{ij}. In operator form,

$$Z_{op}(\eta) = \left\langle \Psi \left| \exp(\hat{\Theta}) \right| \Psi' \right\rangle. \tag{10.15}$$

The key to deriving the desired matrix elements is that we can also write this in purely matrix form, in a useful albeit at first strange form. We write

$$\mathbf{\Theta} = \sum_{ij} \eta_{ij}\theta_{ij} \tag{10.16}$$

In matrix form the generating function is

$$Z_{mat}(\eta) = \det\left[\Psi^\dagger e^{\mathbf{\Theta}}\Psi\right]. \tag{10.17}$$

The formulation (10.16) may seem redundant at first. Again the η_{ij} are the *values* of the matrix elements, while the θ_{ij} are 'base' matrices, that is, θ_{ij} is an $N_s \times N_s$ matrix that is zero everywhere, except for a '1' at the location ij. The reason is derivatives. For operators,

$$\left.\frac{\partial \exp(\hat{\Theta})}{\partial \eta_{ij}}\right|_{\eta=0} = \hat{a}_i^\dagger \hat{a}_j, \tag{10.18}$$

while for matrices

$$\left.\frac{\partial \exp(\mathbf{\Theta})}{\partial \eta_{ij}}\right|_{\eta=0} = \theta_{ij}. \tag{10.19}$$

With that in hand we can begin. With the operator form of the generating function, we take the derivative of the logarithm,

$$\frac{\partial \ln Z_{op}}{\partial \eta_{ij}} = \frac{1}{\left\langle \Psi \left| \exp(\hat{\Theta}) \right| \Psi' \right\rangle} \left\langle \Psi \left| \hat{a}_i^\dagger \hat{a}_j \exp(\hat{\Theta}) \right| \Psi' \right\rangle, \tag{10.20}$$

so that

$$\left.\frac{\partial \ln Z_{op}}{\partial \eta_{ij}}\right|_{\eta=0} = \frac{\left\langle \Psi \left| \hat{a}_i^\dagger \hat{a}_j \right| \Psi' \right\rangle}{\langle \Psi | \Psi' \rangle} \tag{10.21}$$

Now we simply have to do the same for the matrix formulation of the generating function,

$$\frac{\partial \ln Z_{mat}}{\partial \eta_{ij}} = \frac{\partial}{\partial \eta_{ij}} \mathrm{tr} \ln \mathbf{\Psi}^\dagger e^{\mathbf{\Theta}} \mathbf{\Psi}' = \mathrm{tr} \left[\left(\mathbf{\Psi}^\dagger e^{\mathbf{\Theta}} \mathbf{\Psi}' \right)^{-1} \mathbf{\Psi}^\dagger \theta_{ij} e^{\mathbf{\Theta}} \mathbf{\Psi}' \right] \tag{10.22}$$

and then

$$\left.\frac{\partial \ln Z_{mat}}{\partial \eta_{ij}}\right|_{\eta=0} = \mathrm{tr} \left[\left(\mathbf{\Psi}^\dagger \mathbf{\Psi}' \right)^{-1} \mathbf{\Psi}^\dagger \theta_{ij} \mathbf{\Psi}' \right]. \tag{10.23}$$

Because the trace is cyclic, we can rewrite this:

$$\left.\frac{\partial \ln Z_{mat}}{\partial \eta_{ij}}\right|_{\eta=0} = \mathrm{tr} \left[\theta_{ij} \mathbf{\Psi}' \left(\mathbf{\Psi}^\dagger \mathbf{\Psi}' \right)^{-1} \mathbf{\Psi}^\dagger \right]. \tag{10.24}$$

Furthermore–and this is the clever bit (I can't take credit for it)–θ_{ij} is a simple matrix with a single, non-zero matrix element. You can convince yourself that

$$\mathrm{tr} \left(\theta_{ij} \mathbf{A} \right) = A_{ji},$$

that is, taking the trace of any matrix $\mathbf{A}$ with θ_{ij} picks out the jith matrix element of $\mathbf{A}$. Similarly,

$$\mathrm{tr} \left(\theta_{ij} \mathbf{A} \theta_{kl} \mathbf{B} \right) = A_{jk} B_{li}.$$

Hence,

$$\left.\frac{\partial \ln Z_{mat}}{\partial \eta_{ij}}\right|_{\eta=0} = \left[\mathbf{\Psi}' \left(\mathbf{\Psi}^\dagger \mathbf{\Psi}' \right)^{-1} \mathbf{\Psi}^\dagger \right]_{ji}. \tag{10.25}$$

That is,

$$\frac{\left\langle \Psi \left| \hat{a}_i^\dagger \hat{a}_j \right| \Psi' \right\rangle}{\langle \Psi | \Psi' \rangle} = \left[\mathbf{\Psi}' \frac{1}{\mathbf{\Psi}^\dagger \mathbf{\Psi}'} \mathbf{\Psi}^\dagger \right]_{ji} \equiv \rho_{ij}. \tag{10.26}$$

We call ρ the *density matrix*. It is an $N_s \times N_s$ matrix, and requires that $\mathbf{\Psi}'$ not be orthogonal to $\mathbf{\Psi}$.

In this way we can generate any arbitrary matrix element between two non-orthogonal Slater determinants, by (carefully) taking as many derivatives as we need. For now, however, we only need matrix elements of one- and two-body operators.

Continuing,

$$\left. \frac{\partial^2 \ln Z_{op}}{\partial \eta_{ij} \partial \eta_{kl}} \right|_{\eta=0} = \frac{\left\langle \Psi \left| \hat{a}_i^\dagger \hat{a}_j \hat{a}_k^\dagger \hat{a}_l \right| \Psi' \right\rangle}{\langle \Psi | \Psi' \rangle} - \frac{\left\langle \Psi \left| \hat{a}_i^\dagger \hat{a}_j \right| \Psi' \right\rangle}{\langle \Psi | \Psi' \rangle} \frac{\left\langle \Psi \left| \hat{a}_k^\dagger \hat{a}_l \right| \Psi' \right\rangle}{\langle \Psi | \Psi' \rangle} \tag{10.27}$$

and

$$\begin{aligned} \left. \frac{\partial^2 \ln Z_{mat}}{\partial \eta_{ij} \partial \eta_{kl}} \right|_{\eta=0} = & \\ \mathrm{tr} \left[\theta_{ij} \theta_{kl} \mathbf{\Psi}' \left(\mathbf{\Psi}^\dagger \mathbf{\Psi}' \right)^{-1} \mathbf{\Psi}^\dagger - \theta_{ij} \mathbf{\Psi}' \left(\mathbf{\Psi}^\dagger \mathbf{\Psi}' \right)^{-1} \mathbf{\Psi}^\dagger \theta_{kl} \mathbf{\Psi}' \left(\mathbf{\Psi}^\dagger \mathbf{\Psi}' \right)^{-1} \mathbf{\Psi}^\dagger \right] & \\ = \delta_{jk} \rho_{il} - \rho_{il} \rho_{kj}. & \end{aligned} \tag{10.28}$$

From this we derive

$$\frac{\left\langle \Psi \left| \hat{a}_i^\dagger \hat{a}_j \hat{a}_k^\dagger \hat{a}_l \right| \Psi' \right\rangle}{\langle \Psi | \Psi' \rangle} = \rho_{ij} \rho_{kl} - \rho_{il} \rho_{kj} + \delta_{jk} \rho_{il}. \tag{10.29}$$

Finally, for the usual normal ordering, $\hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_l \hat{a}_k = \hat{a}_i^\dagger \hat{a}_k \hat{a}_j^\dagger \hat{a}_l - \delta_{jk} \hat{a}_i^\dagger \hat{a}_l$, so that

$$\frac{\left\langle \Psi \left| \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_l \hat{a}_k \right| \Psi' \right\rangle}{\langle \Psi | \Psi' \rangle} = \rho_{ik} \rho_{jl} - \rho_{il} \rho_{jk}. \tag{10.30}$$

Although the derivation of these generalized Wick theorems is subtle, the basic result is straightforward: to compute *any* general matrix element between two non-orthogonal Slater determinants, we only need to compute the density matrix (10.26).

10.3.2 Application to the Lipkin model

TBD

10.4 Summary

What you should learn from this chapter:

•: Although the basic structure of a Slater determinant is simple, you can get different Slater determinants simply by a transformation of the single-particle basis. Note that this transformation does not affect the full many-body basis nor any 'full' solution, but can and does affect approximations. (Indeed, in the next chapter we'll use this as the basis for the Hartree-Fock approximation.)

•: Two different Slater determinants that are not orthogonal can be related to each other through *Thouless' theorem.*

10.5 Exercises

12.1 . Prove that (10.7) is normalized, up to second-order in Z_{mi}.

Chapter 11

Mean-field theory: Hartree-Fock

> Research consists in seeing what everyone else has seen, but thinking what no one else has thought. *Albert Szent-Gyorgyi*

Though much of physics, including the quantum theory of many-body systems, is couched in the language of partial differential equations, we humans are bad at solving such equations. The fewer the variables, the better we are able to solve it: one variable is easiest, and even three variables is challenging.

And so one approach to many-body physics is to approximate it by an effective *one*-body system, using the variational theorem. This leads us into *mean-field* theory. The first example of mean-field theory I will treat is Hartree-Fock theory. In the next chapter I discuss the generalization Hartree-Fock-Bogoliubov.

I will derive Hartree-Fock theory in two ways [maybe more]. In both cases we assume for our trial many-body wavefunction $|\Psi_T\rangle$ a single Slater determinant, and then find the Slater determinant which minimizes the expectation value of the energy,

$$\frac{\langle\Psi_T|\hat{H}|\Psi_T\rangle}{\langle\Psi_T|\Psi_T\rangle}. \tag{11.1}$$

The denominator simply means we haven't assumed the trial wavefunction is normalized.

For the first, more transparent derivation, we assume a standard Hamiltonian with local potentials,

$$\hat{H} = \sum_i -\frac{\hbar^2\nabla_i^2}{2m} + \frac{1}{4}\sum_{i\neq j} V(\vec{r}_i - \vec{r}_j),$$

and ignore spin and other labels. (These limiting assumptions are partly, but not exclusively, why I'll go through other, more general derivations.) Using the

tools from previous chapters, we can write down the expectation value for N particles:

$$\langle\Psi_T|\hat{H}|\Psi_T\rangle = \sum_{i=1}^{N}\int \phi_i^*(\vec{r}_1)\left(-\frac{\hbar^2\nabla^2}{2m}\right)\phi_i(\vec{r}_1)d^3r_1 \quad (11.2)$$

$$+\frac{1}{2}\sum_{i,j=1}^{N}\int\int \phi_i^*(\vec{r}_1)\phi_j^*(\vec{r}_2)V(\vec{r}_1-\vec{r}_2)\left(\phi_i(\vec{r}_1)\phi_j(\vec{r}_2)-\phi_j(\vec{r}_1)\phi_i(\vec{r}_2)\right)d^3r_1\,d^3r_2.$$

Now we want to apply the variational principle, but before that you may have cleverly noticed I haven't kept the denominator from (11.1). Instead, I employ a Lagrange multiplier,

$$\lambda\sum_{i=1}^{N}\int \phi_i^*(\vec{r}_1)\phi_i(\vec{r}_1)d^3r_1.$$

What we want to vary now are the single-particle wavefunctions, or more specifically, $\phi_a^*(\vec{r})$, that is, take

$$\frac{\partial}{\partial\phi_a^*(\vec{r})}\left(\sum_{i=1}^{N}\int \phi_i^*(\vec{r}_1)\left(-\frac{\hbar^2\nabla^2}{2m}\right)\phi_j(\vec{r}_1)d^3r_1+\right. \quad (11.3)$$

$$\frac{1}{2}\sum_{i,j=1}^{N}\int\int \phi_i^*(\vec{r}_1)\phi_j^*(\vec{r}_2)V(\vec{r}_1-\vec{r}_2)\left(\phi_i(\vec{r}_1)\phi_j(\vec{r}_2)-\phi_j(\vec{r}_1)\phi_i(\vec{r}_2)\right)d^3r_1\,d^3r_2$$

$$\left.-\lambda\sum_{i=1}^{N}\int \phi_i^*(\vec{r}_1)\phi_i(\vec{r}_1)d^3r_1\right)=0$$

The reason I use the labels r_1, r_2 is that when I take the functional derivative, r can equal either r_1 or r_2. Taking the derivative (and renaming the leftover variable of integration as r', the result is

$$-\frac{\hbar^2\nabla^2}{2m}\phi_a(\vec{r})+\sum_{j=1}^{N}\int \phi_j^*(\vec{r}')V(\vec{r}-\vec{r}')\left(\phi_a(\vec{r})\phi_j(\vec{r}')-\phi_j(\vec{r})\phi_a(\vec{r}')\right)d^3r'=\lambda\phi_a(\vec{r}). \quad (11.4)$$

We can reorganize it into a slightly more illustrative form, recognizable as the fabled Hartree-Fock equation:

$$-\frac{\hbar^2\nabla^2}{2m}\phi_a(\vec{r})+V_{\rm dir}(\vec{r})\phi_a(\vec{r})-\int V_{\rm exc}(\vec{r},\vec{r}')\phi_a(\vec{r}')d^3r'=\lambda\phi_a(\vec{r}). \quad (11.5)$$

The *direct* or *Hartree* potential is exactly what one might naively imagine classically:

$$V_{\rm dir}(\vec{r})=\int V(\vec{r}-\vec{r}')\rho(\vec{r}')d^3r', \quad (11.6)$$

$$\rho(\vec{r}')=\sum_{j=1}^{N}|\phi_j(\vec{r}')|^2$$

that is, the potential generated by interacting with the density of particles of the system. Of course, this overcounts; taken by itself, one has a particle interacting with itself, which at this level at least is unphysical. (There is such as thing as self-energy but that is beyond the scope of this work.)

This overcounting is fortuitously corrected for by the *exchange* or *Fock* potential,

$$V_{\rm exc}(\vec{r},\vec{r}') = V(\vec{r}-\vec{r}')\sum_{j=1}^{N}\phi_j^*(\vec{r}')\phi_j(\vec{r}) \tag{11.7}$$

which arises from the antisymmetry of many-fermion wavefunctions. Note that, unless V is a zero-range interaction, the exchange potential is inherently nonlocal, which causes all sorts of headaches.

What have we gained? The original many-body Schrödinger equation is linear, which means one finds the eigenpairs of either a linear partial differential equation or (as discussed in Chapter 9) a large matrix. The problem is the partial differential equation or the matrix may be so large as to be numerically intractable. The Hartree-Fock equation, by contrast, is a much simpler differential (or, as derived below, matrix) equation. As always, there is a price to be paid. For one, the Hartree-Fock equation is an approximation. Moreover, it is a *nonlinear* equation which must be solved self-consistently.

I will not go into detail into methods of solving the Hartree-Fock equation, but the basic scheme is as follows:

1. Make a starting guess for the occupied single-particle wavefunctions ϕ_a;
2. Compute the direct and exchange potentials $V_{\rm dir}, V_{\rm exc}$ which depend on the occupied ϕ_a;
3. Solve the Hartree-Fock equations for a new set of ϕ'_a;
4. If the old and new solutions agree within some tolerance, then declare a converged solution; if not, replace (but see below) ϕ_a with ϕ'_a and go to step 2. Note the comparison is not trivial: does one compare energies or wavefunctions? For example, although I will not go into detail, for an odd number of particles it is converge in energy, but jump back and forth between time-reversed states. It is also possible to cycle between two (or more) solutions without having found the local minimum. For this reason, often may take a linear combination of new and old potentials; this procedure often breaks accidental symmetries that hinder convergence.

In other words, part of the price one pays is to solve a simpler set of equations but *multiple times*.

11.1 Hartree-Fock in occupation space

Another, useful way to derive the Hartree-Fock equations is in occupation space, using Thouless' theorem from Chapter 10. Suppose we are starting with a given Slater determinant,

$$|\Psi_T\rangle = \prod_i \hat{c}_i^\dagger|0\rangle, \tag{11.8}$$

where the product is only over occupied states in the m, i representation from Chapter 10. For convenience we can assume this Slater determinant is normalized. Now introduce a general particle-hole operator,

$$\hat{Z}^\dagger = \sum_{mi} z^*_{mi} \hat{c}^\dagger_m \hat{c}_i. \tag{11.9}$$

One thing to note is, since $\hat{c}_m|\Psi_T\rangle = 0$, then

$$\hat{Z}|\Psi_T\rangle = \langle\Psi_T|\hat{Z}^\dagger = 0. \tag{11.10}$$

Now we parameterize a set of Slater determinants by the particle-hole amplitudes z_{mi}:

$$|\Psi(\vec{z})\rangle = \exp\left(\hat{Z}^\dagger\right)|\Psi_T\rangle \tag{11.11}$$

and we can introduce the energy:

$$E(\vec{z}) = \frac{\langle\Psi(\vec{z})|\hat{H}|\Psi(\vec{z})\rangle}{\langle\Psi(\vec{z})|\Psi(\vec{z})\rangle}. \tag{11.12}$$

This is sometimes called the *energy landscape*. Now let's expand to first order in the z_{mi}s. We already know that to first order $|\Psi(\vec{z})\rangle$ is normalized. Therefore, to first order, the energy is

$$\begin{aligned} E(\vec{z}) = \langle\Psi(\vec{z})|\hat{H}|\Psi(\vec{z})\rangle = \langle\Psi_T|e^{\hat{Z}}\hat{H}e^{\hat{Z}^\dagger}|\Psi_T\rangle \\ = \langle\Psi_T|\hat{H}|\Psi_T\rangle + \langle\Psi_T|\hat{H}\hat{Z}^\dagger|\Psi_T\rangle + \langle\Psi_T|\hat{Z}\hat{H}|\Psi_T\rangle. \end{aligned} \tag{11.13}$$

But from (11.10) we can subtract without change

$$\langle\Psi_T|\hat{Z}^\dagger\hat{H}|\Psi_T\rangle + \langle\Psi_T|\hat{H}\hat{Z}|\Psi_T\rangle$$

because both terms are zero. This leaves us with

$$\begin{aligned} E(\vec{z}) = \langle\Psi_T|\hat{H}|\Psi_T\rangle + \langle\Psi_T|\left[\hat{H}, \hat{Z}^\dagger\right]|\Psi_T\rangle + \langle\Psi_T|\left[\hat{Z}, \hat{H}\right]|\Psi_T\rangle = \\ \langle\Psi_T|\hat{H}|\Psi_T\rangle + \sum_{mi}\langle\Psi_T|\left[\hat{H}, \hat{c}^\dagger_m\hat{c}_i\right]|\Psi_T\rangle z^*_{mi} + \langle\Psi_T|\left[\hat{H}, \hat{c}^\dagger_m\hat{c}_i\right]|\Psi_T\rangle^* z_{mi}. \end{aligned} \tag{11.14}$$

Now setting

$$\frac{\partial E(\vec{z})}{\partial z^*_{mi}} = 0,$$

we obtain

$$\langle\Psi_T|\left[\hat{H}, \hat{c}^\dagger_m\hat{c}_i\right]|\Psi_T\rangle = 0. \tag{11.15}$$

This is the *Hartree-Fock condition* for $|\Psi_T\rangle$ to be at a local minimum of the energy landscape.

We can make this more precise by evaluating the commutators. I've left some of the details to problems 12.1 and 12.2; using the results from there, one can see that

$$\left\langle HF\left|\left[\sum_{abcd} T_{ab}\hat{c}^\dagger_a\hat{c}_b, \hat{c}^\dagger_m\hat{c}_i\right]\right|HF\right\rangle = T_{im}, \tag{11.16}$$

and

$$\left\langle HF \left| \left[\sum_{ab} V_{abcd} \hat{c}_a^\dagger \hat{c}_b^\dagger \hat{c}_d \hat{c}_c, \hat{c}_m^\dagger \hat{c}_i \right] \right| HF \right\rangle = \sum_j V_{ijmj} \tag{11.17}$$

where one must use the antisymmetry of the matrix elements, $V_{abcd} = -V_{bacd} = -V_{abdc} = +V_{badc}$. If we introduce the effective *Hartree-Fock Hamiltonian*,

$$h_{ab} = T_{ab} + \sum_j V_{ajbj} \tag{11.18}$$

then the Hartree-Fock condition is equivalent to saying

$$h_{im} = 0. \tag{11.19}$$

A sufficient, though not necessary, condition is that the Hartree-Fock Hamiltonian be diagonal:

$$h_{ab} = \delta_{ab} \epsilon_a. \tag{11.20}$$

The ϵ_a are the Hartree-Fock single-particle energies.

Note that the Hartree-Fock Hamiltonian is one-body in character, and also depends upon a reference state. There is a straightforward matrix representation for this, as discussed in Chapter 10 [Need to insert this discussion], we can conveniently represent a Slater determinant by a rectangular matrix Ψ, which has N_p columns, one for each occupied state, and N_s rows, one for each single-particle basis state. In this case the density matrix is easy to compute:

$$\rho(\Psi) = \mathbf{\Psi}\mathbf{\Psi}^\dagger. \tag{11.21}$$

Therefore, as with the coordinate-space version, one starts by guessing a Slater determinant $\mathbf{\Psi}$, computing the density matrix ρ. From this one can easily generate the Hartree-Fock Hamiltonian

$$h_{ab} = T_{ab} + \sum_{cd} V_{acbd} \rho_{dc} \tag{11.22}$$

and then diagonalize

$$\sum_b h_{ab} \psi_b = \epsilon \psi_a. \tag{11.23}$$

The new Ψ is then formed by filling its columns with the vectors corresponding to the N_p lowest energies, and repeating.

This methodology is *not* guaranteed to converge. If one has an odd number of particles, for example, one often bounces back and forth between two 'time-reversed' states. Nonetheless, it is a starting point for most Hartree-Fock calculations. Alternately, one can use 'gradient descent,' which is guaranteed to find the local minimum, but which in practice can be slower than iterated diagonlization.

11.2 Summary

What you should learn from this chapter:

•: The fabled Hartree-Fock equation is a lesson in trade-offs: instead of an linear but dimensionally intractable many-body Schrödinger equation, which in principle has to be solved just once, one instead

11.3 Exercises

12.1 Using the particle-hole notation, confirm

$$\left[\hat{c}_a^\dagger \hat{c}_b, \hat{c}_m^\dagger \hat{c}_i\right] = \delta_{mb}\hat{c}_a^\dagger \hat{c}_i - \delta_{ia}\hat{c}_m^\dagger \hat{c}_b$$

and

$$\left[\hat{c}_a^\dagger \hat{c}_b^\dagger \hat{c}_d \hat{c}_c, \hat{c}_m^\dagger \hat{c}_i\right] = \delta_{mc}\hat{c}_a^\dagger \hat{c}_b^\dagger \hat{c}_d \hat{c}_i + \delta_{md}\hat{c}_a^\dagger \hat{c}_b^\dagger \hat{c}_i \hat{c}_c + \delta_{ia}\hat{c}_m^\dagger \hat{c}_b^\dagger \hat{c}_d \hat{c}_c + \delta_{ib}\hat{c}_a^\dagger \hat{c}_m^\dagger \hat{c}_d \hat{c}_c.$$

12.2 Now take the expectation value of the commutations from problem (12.1) for the Hartree-Fock state. This means using $\langle HF|\hat{c}_m^\dagger = 0$. You should find

$$\langle HF|\left[\hat{c}_a^\dagger \hat{c}_b, \hat{c}_m^\dagger \hat{c}_i\right]|HF\rangle = \delta_{mb}\delta_{ai}$$

and

$$\langle HF|\left[\hat{c}_a^\dagger \hat{c}_b^\dagger \hat{c}_d \hat{c}_c, \hat{c}_m^\dagger \hat{c}_i\right]|HF\rangle = \delta_{mc}(\delta_{ai}\delta_{bd\in j} - \delta_{ib}\delta_{ad\in}) + \delta_{md}(\delta_{ac\in j}\delta_{ib} - \delta_{ia}\delta_{bc\in j})$$

where the notation $\in j$ means not only the two states must be equal, but must be occupied states.

Chapter 12

More mean-field theory: Hartree-Fock-Bogoliubov

All science is either physics or stamp collecting – *Ernest Rutherford.*

The idea of quasi-particles, while astounding at first, leads to a very powerful formalism, a generalization of Hartree-Fock using quasi-particles, or the Hartree-Fock-Bogoliubov (HFB) method. This method does not have a definite particle number, which may seem like a drawback, but it is in accord with ordinary Hartree-Fock where deformed states, without a definite angular momentum, lead to a superior description. Most commonly HFB helps to encode pairing phenomena, which are important in heavy nuclei.

We denote our original fermion creation operators by $\{\hat{a}_m^\dagger\}$, while our quasi-particles we write as $\{\hat{\alpha}_\mu^\dagger\}$. Then introduce a general Bogoliubov transformation:

$$\hat{\alpha}_\mu^\dagger = \sum_m U_{n\mu}\hat{a}_m^\dagger + V_{n\mu}\hat{a}_m. \tag{12.1}$$

By taking the adjoint we get

$$\hat{\alpha}_\mu = \sum_m U_{m\mu}^*\hat{a}_n + V_{m\mu}^*\hat{a}_m^\dagger. \tag{12.2}$$

It is important to note that here the matrices $\mathbf{U}$ and $\mathbf{V}$ are *not* unitary! We can represent this succinctly in a supermatrix form: if $\vec{\alpha}^\dagger$ is the column vector of quasi-particle creation operators, and so on, we write

$$\begin{pmatrix} \vec{\alpha} \\ \vec{\alpha}^\dagger \end{pmatrix} = \begin{pmatrix} \mathbf{U}^\dagger & \mathbf{V}^\dagger \\ \mathbf{V}^T & \mathbf{U}^T \end{pmatrix} \begin{pmatrix} \vec{a} \\ \vec{a}^\dagger \end{pmatrix}. \tag{12.3}$$

The matrices $\mathbf{U}$ and $\mathbf{V}$ are not arbitrary, however. Because we want the quasi-particles to satisfy the usual fermion anticommutation relations,

$$\left\{\hat{\alpha}_\mu, \hat{\alpha}_\nu^\dagger\right\} = \delta_{\mu\nu}, \quad \left\{\hat{\alpha}_\mu, \hat{\alpha}_\nu\right\} = \left\{\hat{\alpha}_\mu^\dagger, \hat{\alpha}_\nu^\dagger\right\} = 0, \tag{12.4}$$

one can arrive at the following equations:

$$\mathbf{U}^\dagger\mathbf{U} + \mathbf{V}^\dagger\mathbf{V} = \mathbf{1}; \quad \mathbf{U}\mathbf{U}^\dagger + \mathbf{V}^*\mathbf{V}^T = \mathbf{1} \tag{12.5}$$

$$\mathbf{U}^T\mathbf{V} + \mathbf{V}^T\mathbf{U} = \mathbf{0}; \quad \mathbf{U}\mathbf{V}^\dagger + \mathbf{V}^*\mathbf{U}^T = \mathbf{0}. \tag{12.6}$$

(We leave this as an excellent exercise for the reader.) This can be rewritten in supermatrix form:

$$\begin{pmatrix} \mathbf{U}^\dagger & \mathbf{V}^\dagger \\ \mathbf{V}^T & \mathbf{U}^T \end{pmatrix}^\dagger \begin{pmatrix} \mathbf{U}^\dagger & \mathbf{V}^\dagger \\ \mathbf{V}^T & \mathbf{U}^T \end{pmatrix} = \begin{pmatrix} \mathbf{U}^\dagger & \mathbf{V}^\dagger \\ \mathbf{V}^T & \mathbf{U}^T \end{pmatrix} \begin{pmatrix} \mathbf{U}^\dagger & \mathbf{V}^\dagger \\ \mathbf{V}^T & \mathbf{U}^T \end{pmatrix}^\dagger = \begin{pmatrix} \mathbf{1} & \mathbf{0} \\ \mathbf{0} & \mathbf{1} \end{pmatrix} \tag{12.7}$$

This in turn allows us to invert and represent particle operators as quasiparticles:

$$\hat{a}_m^\dagger = \sum_\mu U_{m\mu}^* \hat{\alpha}_\mu^\dagger + V_{m\mu}\hat{\alpha}_\mu, \tag{12.8}$$

$$\hat{a}_m = \sum_\mu U_{m\mu}\hat{\alpha}_\mu + V_{m\mu}^*\hat{\alpha}_\mu^\dagger. \tag{12.9}$$

12.1 Transforming the Hamiltonian

Consider a general two-body Hamiltonian,

$$\hat{H} = \sum_{mn} T_{mn}\hat{a}_m^\dagger\hat{a}_n + \frac{1}{4}\sum_{ijmn} V_{ijmn}\hat{a}_i^\dagger\hat{a}_j^\dagger\hat{a}_n\hat{a}_m. \tag{12.10}$$

Keep in mind the antisymmetry of the two-body term:

$$V_{ijmn} = -V_{jimn} = -V_{ijnm} = +V_{jinm}.$$

In general one can also assume the time-reversal symmetry, that is, $V_{ijmn} = V_{mnij}$.

We now want to transform this into a anti-normal-ordered quasiparticle formalism. The results are somewhat complicated, so we break the answer into pieces.

$$\begin{aligned} \hat{H} = H^0 + \sum_{\mu\nu}\tilde{T}_{\mu\nu}\hat{\alpha}_\mu^\dagger\hat{\alpha}_\nu + \frac{1}{4}\sum_{\alpha\beta\mu\nu}\tilde{V}_{\alpha\beta\mu\nu}\hat{\alpha}_\alpha^\dagger\hat{\alpha}_\beta^\dagger\hat{\alpha}_\nu\hat{\alpha}_\mu \\ + \sum_{\mu\nu}\tilde{H}_{\mu\nu}^{20}\hat{\alpha}_\mu^\dagger\hat{\alpha}_\nu^\dagger + \tilde{H}_{\mu\nu}^{20*}\hat{\alpha}_\nu\hat{\alpha}_\mu \\ + \frac{1}{4}\sum_{\alpha\beta\mu\nu}\tilde{H}_{\alpha\beta\mu\nu}^{31}\hat{\alpha}_\alpha^\dagger\hat{\alpha}_\beta^\dagger\hat{\alpha}_\mu^\dagger\hat{\alpha}_\nu + \tilde{H}_{\alpha\beta\mu\nu}^{31*}\hat{\alpha}_\nu^\dagger\hat{\alpha}_\mu\hat{\alpha}_\beta\hat{\alpha}_\alpha \\ + \frac{1}{4}\sum_{\alpha\beta\mu\nu}\tilde{H}_{\alpha\beta\mu\nu}^{40}\hat{\alpha}_\alpha^\dagger\hat{\alpha}_\beta^\dagger\hat{\alpha}_\mu^\dagger\hat{\alpha}_\nu^\dagger + \tilde{H}_{\alpha\beta\mu\nu}^{40*}\hat{\alpha}_\nu\hat{\alpha}_\mu\hat{\alpha}_\beta\hat{\alpha}_\alpha \end{aligned} \tag{12.11}$$

Here we've ordered the terms in decreasing importance. Like the above, deriving the transformed Hamiltonian is an excellent, if slightly complicated exercise for the novice. Some useful quantities along the way will be the density matrix or the normal density

$$\rho = \mathbf{V}^* \mathbf{V}^T, \tag{12.12}$$

(so that ρ is Hermitian) and the pairing density or abnormal density

$$\kappa = \mathbf{V}^* \mathbf{U}^T = -\mathbf{U}\mathbf{V}^\dagger \tag{12.13}$$

(and thus skew-symmetric), We will have occasion to use the density ρ. We can also introduce the Hartree-Fock potential,

$$\Gamma_{im} = \sum_{jn} V_{ijmn} \rho_{nj} \tag{12.14}$$

which in turn leads to the Hartree-Fock effective single-particle Hamiltonian,

$$\mathbf{H} = \mathbf{T} + \frac{1}{2}\mathbf{\Gamma} \tag{12.15}$$

and the pairing potential

$$\Delta_{ij} = \frac{1}{2} \sum_{mn} V_{ijmn} \kappa_{mn} \tag{12.16}$$

To illustrate how one carries out such a derviation, begin with the original one-body part, and introduce the quasiparticles

$$\begin{aligned}
\sum_{mn} T_{mn} \hat{a}_m^\dagger \hat{a}_n = \\
\sum_{mn} T_{mn} \sum_{\mu} (U_{m\mu}^* \hat{\alpha}_\mu^\dagger + V_{m\mu} \hat{\alpha}_\mu) \sum_{\nu} (U_{n\nu} \hat{\alpha}_\nu + V_{n\nu}^* \hat{\alpha}_\nu^\dagger) \\
= \sum_{mn} T_{mn} \sum_{\mu\nu} \big(U_{m\mu}^* U_{n\nu} \hat{\alpha}_\mu^\dagger \hat{\alpha}_\nu + V_{m\mu} V_{n\nu}^* \hat{\alpha}_\mu \hat{\alpha}_\nu^\dagger \\
+ U_{m\mu} V_{n\nu}^* \hat{\alpha}_\mu^\dagger \hat{\alpha}_\nu^\dagger + V_{m\mu} U_{n\nu}^* \hat{\alpha}_\mu \hat{\alpha}_\nu \big) \\
= \sum_{mn} T_{mn} \sum_{\mu\nu} \big(\delta_{\mu\nu} V_{m\mu} V_{n\nu}^* + U_{m\mu}^* U_{n\nu} \hat{\alpha}_\mu^\dagger \hat{\alpha}_\nu - V_{m\mu} V_{n\nu}^* \hat{\alpha}_\nu^\dagger \hat{\alpha}_\mu \\
+ U_{m\mu} V_{n\nu}^* \hat{\alpha}_\mu^\dagger \hat{\alpha}_\nu^\dagger + V_{m\mu} U_{n\nu}^* \hat{\alpha}_\mu \hat{\alpha}_\nu \big)
\end{aligned} \tag{12.17}$$

The first term of this last expression, which has no operators, simplifies to

$$\sum_{mn} T_{mn} \sum_{\mu} V_{m\mu} V_{n\mu}^* = \sum_{mn} T_{mn} (\mathbf{V}^* \mathbf{V}^T)_{nm} = \sum_{mn} T_{mn} \rho_{nm} = \operatorname{tr} \mathbf{T}\rho. \tag{12.18}$$

The next two terms of (12.17), which are one-quasiparticle operators, become, with suitable swapping of indices,

$$\sum_{\mu\nu} (\mathbf{U}^\dagger \mathbf{T} \mathbf{U} - \mathbf{V}^\dagger \mathbf{T}^T \mathbf{V})_{\mu\nu} \hat{\alpha}_\mu^\dagger \hat{\alpha}_\nu. \tag{12.19}$$

The final two terms of (12.17) create and destroy, respectively, two quasiparticles, and contribute to $\hat{H}^{20}$.

The potential energy can also be rewritten in the same way, although it requires quite a bit more work to get through. We just put the final results here, and encourage the reader to reproduce them.

To begin with, the 'vacuum' energy, which is really the ground state energy, is

$$\langle\tilde{0}|\hat{H}|\tilde{0}\rangle = H^0 = \mathrm{tr}\,\mathbf{h}\rho - \frac{1}{2}\mathrm{tr}\,\mathbf{\Delta}\kappa^*. \tag{12.20}$$

In the next section we will discuss how to minimize H^0 through the Hartree-Fock-Bogoliubov equations.

The other terms are

$$\tilde{\mathbf{T}} = \mathbf{U}^\dagger\mathbf{h}\mathbf{U} - \mathbf{V}^\dagger\mathbf{h}^T\mathbf{V} + \mathbf{U}^\dagger\mathbf{\Delta}\mathbf{V} - \mathbf{V}^\dagger\mathbf{\Delta}^*\mathbf{U}, \tag{12.21}$$

$$\tilde{\mathbf{H}}^{20} = \mathbf{U}^\dagger\mathbf{h}\mathbf{V}^* + \frac{1}{2}\left(\mathbf{U}^\dagger\mathbf{\Delta}\mathbf{U}^* - \mathbf{V}^\dagger\mathbf{\Delta}^*\mathbf{V}^*\right), \tag{12.22}$$

and, finally, assuming time-reversal symmetry,

$$\tilde{V}_{\alpha\beta\mu\nu} = \sum_{ijmn} V_{ijmn}\left(U^*_{i\alpha}U^*_{j\beta}U_{n\nu}U_{m\mu} + V^*_{i\alpha}V^*_{j\beta}V_{n\nu}V_{m\mu} + 4U^*_{i\alpha}V^*_{n\beta}U_{m\nu}V_{j\mu}\right). \tag{12.23}$$

We leave H^{31} and H^{40} as exercises for the reader to find.

12.2 The Hartree-Fock-Bogoliubov equations

12.3 General Thouless transformation

The ground state in HFB is *defined* as the quasiparticle vacuum state:

$$\hat{\alpha}_\mu|\tilde{0}\rangle = 0. \tag{12.24}$$

This is, on the surface, unlike a Slater determinant, but as discussed (?) previously, a Slater determinant is annihilated by particle destruction operators $\hat{c}_m$ and by hole creation operator $\hat{c}^\dagger_i$. Instead of a sharp bifurcation, quasiparticle dial smoothly between particles and hole.

The general Thouless transformation is thus

$$\exp\left(\sum_{\mu\nu} Z_{\mu\nu}\hat{\alpha}^\dagger_\mu\hat{\alpha}^\dagger_\nu\right)|\tilde{0}\rangle. \tag{12.25}$$

We can make this explicitly unitary:

$$\exp\left(\sum_{\mu\nu} Z_{\mu\nu}\hat{\alpha}^\dagger_\mu\hat{\alpha}^\dagger_\nu - Z^*_{\mu\nu}\hat{\alpha}_\nu\hat{\alpha}_\mu\right)|\tilde{0}\rangle = |\mathbf{Z}\rangle \tag{12.26}$$

so that the transformed state $|\mathbf{Z}\rangle$ is always normalized.

We can then carry out a variational calculation. To first order in $\mathbf{Z}$,

$$\frac{\langle \mathbf{Z}|\hat{H}|\mathbf{Z}\rangle}{\langle \mathbf{Z}|\mathbf{Z}\rangle} = \sum_{\mu\nu} Z_{\mu\nu}\langle\tilde{0}|\hat{H}\hat{\alpha}^\dagger_\mu\hat{\alpha}^\dagger_\nu|\tilde{0}\rangle - Z^*_{\mu\nu}\langle\tilde{0}|\hat{\alpha}_\nu\hat{\alpha}_\mu\hat{H}|\tilde{0}\rangle \tag{12.27}$$

Using the vacuum condition (12.24) and its adjoint, we can rewrite this in terms of commutators:

$$= \sum_{\mu\nu} Z_{\mu\nu}\langle\tilde{0}|\left[\hat{H},\hat{\alpha}^\dagger_\mu\hat{\alpha}^\dagger_\nu\right]|\tilde{0}\rangle - Z^*_{\mu\nu}\langle\tilde{0}|\left[\hat{\alpha}_\nu\hat{\alpha}_\mu,\hat{H}\right]|\tilde{0}\rangle \tag{12.28}$$

By taking

$$\frac{\partial}{\partial Z_{\mu\nu}}\frac{\langle \mathbf{Z}|\hat{H}|\mathbf{Z}\rangle}{\langle \mathbf{Z}|\mathbf{Z}\rangle} = \langle\tilde{0}|\left[\hat{H},\hat{\alpha}^\dagger_\mu\hat{\alpha}^\dagger_\nu\right]|\tilde{0}\rangle = 0, \tag{12.29}$$

we gain the HFB generalization of the Hartree-Fock condition.

12.4 Exercises

Show

$$\tilde{H}^{40}_{\alpha\beta\mu\nu} = \sum_{ijmn} U^*_{i\alpha}U^*_{j\beta}V_{ijmn}V^*_{n\nu}V^*_{m\mu} \tag{12.30}$$

Chapter 13

Beyond the mean field: the Tamm-Dancoff and random phase approximations

> Research is the process of going up alleys to see if they are blind.– *Marston Bates.*

13.1 Introduction: particle-hole states

Mean field theory is a very useful approximation, but it is only the starting point, not the end. Mean field theory generally only gives you the ground state. It also, by design, does not handle correlations between particles very well. We therefore turn to one of the most common *beyond mean field* approximations, particle-hole approximations. This will allow is to generate a subspace of Slater determinants which is more than just the Hartree-Fock (or HFB) state, but still much smaller than the full space.

To be specific, following on Chapter 11, we assume we start with some Slater determinant which is usually a product of the Hartree-Fock method. For convience we call this the "vacuum' state, $|\tilde{0}\rangle$, even though it is not empty; the $\tilde{}$ signifies this is a redefinition. We label the occupied states by i, j, which are below the Fermi surface, and the unoccupied states by m, n, above the Fermi surface. Then we have the same rules, that

$$\hat{c}_i^\dagger|\tilde{0}\rangle = \hat{c}_m|\tilde{0}\rangle = 0.$$

But $\hat{c}_i|\tilde{0}\rangle$ and $\hat{c}_m^\dagger|\tilde{0}\rangle$ are both nonzero. Since i, j and m, n operate in completely different single-particle subspaces, they have simple anticommutation rules, namely, $\{\hat{c}_m^\dagger, \hat{c}_i\} = 0$, and so on.

This allows us to introduce *particle-hole* states. In essence, we move particles from below to above the Fermi surface. The simplest are one-particle, one-hole

states, which we write with this notation:

$$\hat{c}_m^\dagger \hat{c}_i |\tilde{0}\rangle \equiv |mi^{-1}\rangle, \tag{13.1}$$

with the $^{-1}$ signifying we've removed a particle from the previously occupied state i. This is still a Slater determinant, and retains all the nice properties of a Slater determinant: it is normalized, it is orthogonal to the HF vacuum state $|\tilde{0}\rangle$, and the one-particle, one-hole states have simple orthogonality relations, namely,

$$\langle nj^{-1}|mi^{-1}\rangle = \delta_{m,n}\delta_{i,j}. \tag{13.2}$$

(Exercise: show this explicitly.) Thus we get a convenient orhonormal set that spans a subspace of the full Hilbert space.

You probably already see how to generalize. In the section 13.3 below, we will use *two-particle, two-hole* states,

$$|mn, i^{-1}j^{-1}\rangle = \hat{c}_m^\dagger \hat{c}_n^\dagger \hat{c}_i \hat{c}_j |\tilde{0}\rangle. \tag{13.3}$$

These, too, have straightforward orthonormality relations.

Because the particle (unoccupied) and hole (occupied) single particle spaces are separate, some authors use distinct notation, for example,

$$\hat{c}_m^\dagger \to \hat{p}_m^\dagger, \tag{13.4}$$

$$\hat{c}_i \to \hat{h}_i. \tag{13.5}$$

Note that we map a creation operator to the *particle* creation operator, but an annihilation operator to the *hole* **creation** operator. This way the Hartree-Fock "vacuum" state truly looks like a vacuum, being destroyed by both kinds of annihilation operators

$$\hat{p}_i |\tilde{0}\rangle = \hat{h}_m |\tilde{0}\rangle = 0 \tag{13.6}$$

One then has the usual anticommutation relations,

$$\{\hat{p}_i, \hat{p}_j^\dagger\} = \delta_{ij}, \;\; \{\hat{h}_m, \hat{h}_n^\dagger\} = \delta_{mn}, \tag{13.7}$$

$$\{\hat{p}_i, \hat{h}_m\} = \{\hat{p}_i^\dagger, \hat{h}_m^\dagger\} = \{\hat{p}_i, \hat{h}_m^\dagger\} = \{\hat{p}_i^\dagger, \hat{h}_m\} = 0 \tag{13.8}$$

and so on. Although such notation can be useful pedagogically, because there is not a widely used standard, if it is not carefully and explicitly defined it can be confusing for the casual user. This is particularly true if, instead of using $\hat{p}$ and $\hat{h}$ one uses arbitrary symbols, e.g. $\hat{A}$ and $\hat{B}$.

13.2 The Tamm-Dancoff approximation

Now let's put these particle-hole states to good use. Back in Chapter 11 we had, in Eq. (11.15), the *Hartree-Fock condition*, which we write in slightly variant form,

$$\langle \tilde{0}|[\hat{H}, \hat{c}_m^\dagger \hat{c}_i]|\tilde{0}\rangle = 0. \tag{13.9}$$

We can expand the commutator

$$0 = \langle\tilde{0}|\hat{H}\hat{c}_m^\dagger\hat{c}_i|\tilde{0}\rangle - \langle\tilde{0}|\hat{c}_m^\dagger\hat{c}_i\hat{H}|\tilde{0}\rangle = \langle\tilde{0}|\hat{H}\hat{c}_m^\dagger\hat{c}_i|\tilde{0}\rangle = \langle\tilde{0}|\hat{H}|mi^{-1}\rangle \tag{13.10}$$

where we used the fact that $\langle\tilde{0}|\hat{c}_m^\dagger = 0$. (The reason we have the commutator in the first place is not just because physicists are enamored of commutators, although they are, but because it makes the calculation easier, which is why physicists are enamored of commutators.) Colloquially, we say the Hamiltonian does not connect one-particle, one-hole states to the Hartree-Fock state. This is not true of two-particle, two-hole states, a fact that will play a role in Section 13.3.

The Tamm-Dancoff matrix is just the matrix elements of the Hamiltonian between particle-hole states, specifically

$$A_{nj,mi} = \langle nj^{-1}|\hat{H}|mi^{-1}\rangle. \tag{13.11}$$

In the Hartree-Fock basis, one can show (this will be an exercise) that

$$A_{nj,mi} = \delta_{mn}\delta_{ij}(\epsilon_m - \epsilon_i) + V_{nj,mi} \tag{13.12}$$

(NOTE: I have to check this).

Then solving the Tamm-Dancoff equation is just solving the eigenvalue equation,

$$\mathbf{A}v_\lambda = E_\lambda v_\lambda, \tag{13.13}$$

where E_λ is the excitation energy of the λth excited state, which has a wave function

$$|\lambda\rangle = \sum_{m,i} v_{\lambda,mi}|mi^{-1}\rangle \tag{13.14}$$

.

13.3 The random phase approximation

The Tamm-Dancoff approximation, by design, does not include any correlations in the ground state. This is because, by definition, all matrix elements of the Hamiltonian between the Hartree-Fock ground state and any one-particle, one-hole excitation is zero. The next step, then, is to include two-particle, two-hole excitations, which will connect via the Hamiltonian to the ground state, that is, the matrix element $\langle 0|\hat{H}|mn, i^{-1}j^{-1}\rangle$ is generally not zero.

The naive thing to do would be to diagonalize the Hamiltonian in a basis consisting of the ground state, all one-particle, one-hole states, and all two-particle, two-hole states. But that will be quite large: if N_p is the number of particle states and N_h the number of hole states, the dimensions will be $N_p^2 N_h^2$.

The *random phase* approximation folds in the role of two-particle, two-hole correlations, without diagonalizing in the full two-particle, two-hole basis, instead finding eigenpairs of a non-Hermitian matrix that is merely twice the dimension of the Tamn-Dancoff matrix. Although it will at first seem nonintuitive, one can arrive at the random phase approximation, or RPA, multiple

ways; one of the earliest, which we will not cover, assumes a certain phase is random and therefore certain matrix elements can be averaged to zero (thus, unlike the Tamm-Dancoff approximation, the random phase approximation was not proposed by Professor Random and Doctor Phase),

The matrix form of the RPA equation are very similar to the TDA equation. There is a Green's function form, but that is within the scope of this book. The matrix RPA equation is

$$\begin{pmatrix} \mathbf{A} & \mathbf{B} \\ -\mathbf{B}^* & -\mathbf{A}^* \end{pmatrix} \begin{pmatrix} \vec{x}_\lambda \\ \vec{y}_\lambda \end{pmatrix} = E_\lambda \begin{pmatrix} \vec{x}_\lambda \\ \vec{y}_\lambda \end{pmatrix} \tag{13.15}$$

Here the matrix $\mathbf{A}$ is exactly the same matrix as in TDA, while

$$B_{nj,mi} = -V_{mn,ij} \tag{13.16}$$

(CHECK!) Thus the RPA matrix has just twice the dimensions of the TDA matrix.

Like Hartree-Fock, we will give several derivations. While the equations will seem strange at first glance, one can understand RPA as follows: the Hartree-Fock equations lead to a (local) minimum in an energy surface, while the RPA approximates the energy surface around the HF minimum as quadratic, and the excited states as the lowest harmonic oscillator excitations.

13.4 More on RPA

13.4.1 Gradient descent

Begin with a trial Slater determinant wavefunction, $|\Psi\rangle$. Let's consider a very specific Thouless transformation. Define the Thouless particle-hole creation operator,

$$\hat{Z}^\dagger = \sum_{mi} Z^*_{mi} c^\dagger_m c_i \tag{13.17}$$

Then define a new state by

$$|\Psi'\rangle = \exp(\hat{Z}^\dagger - \hat{Z})|\Psi\rangle. \tag{13.18}$$

Because $\hat{Z}^\dagger - \hat{Z}$ is manifestly anti-Hermitian, the transformation is unitary and the Slater determinant retains its normalization. Of course, in the computer we represent Ψ by a rectangular $N_s \times N_f$ matrix $\mathbf{\Psi}$ and and both the Thouless particle-hole operator $\hat{Z}$ and the unitary transformation $\hat{U}$ by square $N_s \times N_s$ matrices $\mathbf{Z}$ and $\mathbf{U}$. (In appendices I describe how to compute the unitary transformation from $\mathbf{Z}$).

Although for application to Ψ we treat $\hat{Z}$ as a matrix, in order to actually compute $\hat{Z}$ we have to treat it as a vector. In the former case, we have the matrix $Z_{\alpha,\beta}$, where α, β are distinct indices, where for the latter, $\{\alpha\beta\}$ (more properly $\{mi\}$) is treated as a single index.

Expanding the energy functional to second order in Z,

$$E(Z) = \left\langle \Psi \left| \hat{H} \right| \Psi \right\rangle + \left\langle \Psi \left| [\hat{H}, \hat{Z}^\dagger] - [\hat{H}, \hat{Z}] \right| \Psi \right\rangle \quad (13.19)$$
$$+\frac{1}{2} \left\langle \Psi \left| [\hat{Z}^\dagger, [\hat{H}, \hat{Z}]] + [\hat{Z}, [\hat{H}, \hat{Z}^\dagger]] - [\hat{Z}, [\hat{H}, \hat{Z}]] - [\hat{Z}^\dagger, [\hat{H}, \hat{Z}^\dagger]] \right| \Psi \right\rangle$$

Consider the coefficients $\{Z_{mi}\}$ to form a vector $\vec{z}$. Then

$$E(\vec{z}) = E_0 + \begin{pmatrix} \vec{h}^*, & \vec{h} \end{pmatrix} \cdot \begin{pmatrix} \vec{z} \\ \vec{z}^* \end{pmatrix} \quad (13.20)$$
$$+\frac{1}{2} \begin{pmatrix} \vec{z}^*, & \vec{z} \end{pmatrix} \cdot \begin{pmatrix} \mathbf{A}, & \mathbf{B} \\ \mathbf{B}^*, & \mathbf{A}^* \end{pmatrix} \cdot \begin{pmatrix} \vec{z} \\ \vec{z}^* \end{pmatrix}$$

where $E_0 = \left\langle \Psi \left| \hat{H} \right| \Psi \right\rangle$, and

$$h_{mi} \equiv \left\langle \Psi \left| [\hat{H}, \hat{c}_m^\dagger \hat{c}_i] \right| \Psi \right\rangle, \quad (13.21)$$
$$A_{nj,mi} \equiv \left\langle \Psi \left| \left[\hat{c}_j^\dagger \hat{c}_n, [\hat{H}, \hat{c}_m^\dagger \hat{c}_i] \right] \right| \Psi \right\rangle, \quad (13.22)$$
$$B_{nj,mi} \equiv \left\langle \Psi \left| \left[[\hat{H}, \hat{c}_n^\dagger \hat{c}_j], \hat{c}_m^\dagger \hat{c}_i \right] \right| \Psi \right\rangle \quad (13.23)$$

Note: $\mathbf{A}$ is Hermitian and $\mathbf{B}$ symmetric.

In the particle-hole basis define $h_{ab} = T_{ab} + \sum_k V_{ak,bk}$, where k only runs over occupied states. Then

$$A_{nj,mi} = \delta_{ij} h_{mn} - \delta_{mn} h_{ij} - V_{ni,mj}, \quad (13.24)$$
$$B_{nj,mi} = V_{nm,ji} \quad (13.25)$$

At the Hartree-Fock minimum, $\mathbf{h}$ is diagonal in the p-h basis (but not in the fundamental basis): $h_{ab} = \delta_{ab} e_a$, with the eigenvalues e interpreted as single-particle energies. Or, to be more precise, $h_{mi} = h_{im} = 0$, and one can easily diagonalize separately in the particle and hole basis.

In general one can allow all the coefficient to be complex. Often we will only deal with real coefficients.

$$E(\vec{z}) = E_0 + 2\begin{pmatrix} \mathrm{Re}\,\vec{h}, & \mathrm{Im}\,\vec{h} \end{pmatrix} \cdot \begin{pmatrix} \mathrm{Re}\,\vec{z} \\ \mathrm{Im}\,\vec{z} \end{pmatrix} \quad (13.26)$$
$$+\begin{pmatrix} \mathrm{Re}\,\vec{z}, & \mathrm{Im}\,\vec{z} \end{pmatrix} \cdot \begin{pmatrix} \mathrm{Re}\,(\mathbf{A}+\mathbf{B}), & -\mathrm{Im}\,(\mathbf{A}-\mathbf{B}) \\ \mathrm{Im}\,(\mathbf{A}-\mathbf{B}), & \mathrm{Re}\,(\mathbf{A}-\mathbf{B}) \end{pmatrix} \cdot \begin{pmatrix} \mathrm{Re}\,\vec{z} \\ \mathrm{Im}\,\vec{z} \end{pmatrix}$$

If all the coefficients are real, the curvatures for Re $\vec{z}$ are eigenvalues of $(\mathbf{A}+\mathbf{B})$ and for Im $\vec{z}$ are eigenvalues of $(\mathbf{A}-\mathbf{B})$. Consider, for example, rotations, which are of the form $\exp(i\hat{J}_i\theta_i)$, where $i = x, y, z$. Because the matrices for $\hat{J}_{x,z}$ are real, the corresponding Thouless matrices are imaginary and the zeroes ought to be found in $(\mathbf{A}-\mathbf{B})$. Rotations about the y-axis ought to be found in the real sector, that is, zeroes of $(\mathbf{A}+\mathbf{B})$.

13.4.2 Boson mapping

There are many ways to derive the RPA equations. I'll start with a crude approximation, but do it more carefully later on starting in section 13.4.4

The particle-hole creation operators $\hat{c}_m^\dagger \hat{c}_i$ have the commutation relations:

$$\left[\hat{c}_m^\dagger \hat{c}_i, \hat{c}_n^\dagger \hat{c}_j\right] = 0, \ \left[\hat{c}_i^\dagger \hat{c}_m, \hat{c}_n^\dagger \hat{c}_j\right] = \delta_{mn}\delta_{ij} - \delta_{ij}\hat{c}_m^\dagger \hat{c}_n + \delta_{mn}\hat{c}_j^\dagger \hat{c}_i. \tag{13.27}$$

If we map the fermion particle-hole creation operator $\hat{c}_m^\dagger \hat{c}_i$ onto a boson creation operator $\hat{b}_{mi}^\dagger$, we get a nearly, but not quite, identical commutator:

$$[\hat{b}_{mi}, \hat{b}_{nj}^\dagger] = \delta_{mi,nj}, \tag{13.28}$$

Therefore we map the fermion Hamiltonian onto the boson image

$$\hat{H}_B = E_{\rm HF} + \vec{h}\cdot(\vec{b}^\dagger + \vec{b}) + \vec{b}^\dagger \mathbf{A}\vec{b} + \frac{1}{2}(\vec{b}^\dagger \cdot \mathbf{B}\cdot \vec{b}^\dagger + \vec{b}\cdot\mathbf{B}\cdot\vec{b}), \tag{13.29}$$

which has the parallel result

$$h_{mi} \equiv \left(0\left|[\hat{H}_B, \hat{b}_{mi}^\dagger]\right|0\right), \tag{13.30}$$

$$A_{nj,mi} \equiv \left(0\left|\left[\hat{b}_{jn}, [\hat{H}_B, \hat{b}_{mi}^\dagger]\right]\right|0\right), \tag{13.31}$$

$$B_{nj,mi} \equiv \left(0\left|\left[[\hat{H}_B, \hat{b}_{nj}^\dagger], \hat{b}_{mi}^\dagger\right]\right|0\right) \tag{13.32}$$

Because this has the same commutation relations as the fermion Hamiltonian, we say this is the boson image to RPA order. (For now I'll keep the linear part even though it disappears for the Hamiltonian at the HF minimum.)

We rewrite this into matrix form, which induces an additional constant term:

$$\hat{H}_B = E_{\rm HF} - \frac{1}{2}{\rm tr}\mathbf{A} + \frac{1}{2}\begin{pmatrix} \vec{b}^\dagger, & \vec{b} \end{pmatrix}\cdot\begin{pmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{B} & \mathbf{A} \end{pmatrix}\cdot\begin{pmatrix} \vec{b} \\ \vec{b}^\dagger \end{pmatrix}. \tag{13.33}$$

We diagonalize the quadratic part by a boson Bogoliubov transformation. Let

$$\begin{pmatrix} \vec{b} \\ \vec{b}^\dagger \end{pmatrix} = \begin{pmatrix} \mathbf{X} & \mathbf{Y} \\ \mathbf{Y} & \mathbf{X} \end{pmatrix}\begin{pmatrix} \vec{\beta} \\ \vec{\beta}^\dagger \end{pmatrix}. \tag{13.34}$$

I will refer to $\hat{\beta}_\lambda$ as the *collective boson creation operator*. We can assume that the transformation is real (and if $\mathbf{A}, \mathbf{B}$ are, and the stability matrix is positive-definite, so will be $\mathbf{X}, \mathbf{Y}$). By insisting on the commutation relation (13.28), we get the completeness relations

$$\mathbf{X}\mathbf{X}^T - \mathbf{Y}\mathbf{Y}^T = \mathbf{1}, \ \mathbf{X}\mathbf{Y}^T - \mathbf{Y}\mathbf{X}^T = 0. \tag{13.35}$$

One can also invert the transformation,

$$\begin{pmatrix} \vec{\beta} \\ \vec{\beta}^\dagger \end{pmatrix} = \begin{pmatrix} \mathbf{X}^T & -\mathbf{Y}^T \\ -\mathbf{Y}^T & \mathbf{X}^T \end{pmatrix}\begin{pmatrix} \vec{b} \\ \vec{b}^\dagger \end{pmatrix}, \tag{13.36}$$

and the orthonormality relations

$$\mathbf{X}^T\mathbf{X} - \mathbf{Y}^T\mathbf{Y} = \mathbf{1},\ \mathbf{X}^T\mathbf{Y} - \mathbf{Y}^T\mathbf{X} = 0. \tag{13.37}$$

Applying the Bogoliubov transformation (13.34) to the boson Hamiltonian (14.6), we get

$$\hat{H}_B = E_{\rm HF} - \frac{1}{2}{\rm tr}\mathbf{A} + \frac{1}{2}\sum_\lambda \Omega_\lambda(\hat{\beta}^\dagger_\lambda\hat{\beta}_\lambda + \hat{\beta}_\lambda\hat{\beta}^\dagger_\lambda) \tag{13.38}$$

if we satisfy the classic RPA equation,

$$\begin{pmatrix} \mathbf{A} & \mathbf{B} \\ -\mathbf{B} & -\mathbf{A} \end{pmatrix}\begin{pmatrix} \mathbf{X} & \mathbf{Y} \\ \mathbf{Y} & \mathbf{X} \end{pmatrix} = \begin{pmatrix} \mathbf{X} & \mathbf{Y} \\ \mathbf{Y} & \mathbf{X} \end{pmatrix}\begin{pmatrix} \mathbf{\Omega} & 0 \\ 0 & -\mathbf{\Omega} \end{pmatrix}. \tag{13.39}$$

If we rewrite Eqn (13.38) in normal order,

$$\hat{H}_B = E_{\rm HF} - \frac{1}{2}{\rm tr}\mathbf{A} + \frac{1}{2}{\rm tr}\mathbf{\Omega} + \sum_\lambda \Omega_\lambda\hat{\beta}^\dagger_\lambda\hat{\beta}_\lambda \tag{13.40}$$

we get the RPA correlation energy,

$$E^{\rm RPA}_{\rm corr} = -\frac{1}{2}{\rm tr}\mathbf{A} + \frac{1}{2}\sum_\lambda \Omega_\lambda. \tag{13.41}$$

If we use $\mathbf{A} = \mathbf{X}\mathbf{\Omega}\mathbf{X}^\dagger + \mathbf{Y}^*\mathbf{\Omega}\mathbf{Y}^T$ as well as the completeness relation, we can then write

$$E^{\rm RPA}_{\rm corr} = -\sum_\lambda \Omega_\lambda \sum_{mi} |Y_{mi,\lambda}|^2. \tag{13.42}$$

There is a problem. Equations (13.41) and (13.42) are equal if and only if the RPA frequencies $\Omega_\lambda > 0$, that is, there are no zero modes. But often there are zero modes. In that case one cannot solve the RPA equations with normalizable vectors, and so the Bogoliubov transformation (13.34) *does not exist*. Another way to express it is that the representation of $\mathbf{A}$ used to derive (13.42) no longer holds. Hence we must modify our approach to deal with zero or very soft modes.

13.4.3 Generalized collective coordinates

We follow Marshalak and Weneser and introduce generalized collective coordinates $\hat{\mathcal{Q}}_\lambda$ and their conjugate momenta $\hat{\mathcal{P}}_\lambda$, with the usual commutation relations,

$$\left[\hat{\mathcal{Q}}_\lambda, \hat{\mathcal{Q}}_\mu\right] = \left[\hat{\mathcal{P}}_\lambda, \hat{\mathcal{P}}_\mu\right] = 0,\ \ \left[\hat{\mathcal{Q}}_\lambda, \hat{\mathcal{P}}_\mu\right] = i\delta_{\lambda\mu}, \tag{13.43}$$

as well as the equations of motion

$$\left[\hat{H}_B, \hat{\mathcal{P}}_\lambda\right] = i\Omega^2_\lambda M_\lambda \hat{\mathcal{Q}}_\lambda,\ \ \left[\hat{H}_B, \hat{\mathcal{Q}}_\lambda\right] = -\frac{i}{M_\lambda}\hat{\mathcal{P}}_\lambda. \tag{13.44}$$

For nonzero modes we can write down the relation between the collective boson creation and annihilation operators and the colllective coordinates in the usual way,

$$\hat{\beta}^\dagger_\lambda = \sqrt{\frac{M_\lambda \Omega_\lambda}{2}}\hat{\mathcal{Q}}_\lambda + i\sqrt{\frac{1}{2M_\lambda\Omega_\lambda}}\hat{\mathcal{P}}_\lambda, \tag{13.45}$$

$$\hat{\beta}_\lambda = \sqrt{\frac{M_\lambda \Omega_\lambda}{2}}\hat{\mathcal{Q}}_\lambda - i\sqrt{\frac{1}{2M_\lambda\Omega_\lambda}}\hat{\mathcal{P}}_\lambda \tag{13.46}$$

Substituting into (13.40), we get a form in obvious analogy with the harmonic operator:

$$\hat{H}_B = E_{\mathrm{HF}} - \frac{1}{2}\mathrm{tr}\,\mathbf{A} + \sum_\lambda \frac{\hat{\mathcal{P}}^2}{2M_\lambda} + \frac{1}{2}M_\lambda\Omega^2\hat{\mathcal{Q}}^2_\lambda \tag{13.47}$$

This form is more general and works even for $\Omega_\lambda = 0$, which corresponds to cases with a symmetry, in which case there is only a dependence on the 'momentum' and not on the generalized coordinate (for example, rotational energy does not depend on the angle of rotation). The additional terms in the correlation energy come about from the zero-point energy of the different generalized oscillators.

Now we need to find a way to deal with zero-frequency modes, because there are no collective bosons and one cannot find a normalizable X, Y vectors. Let

$$\hat{\mathcal{Q}}_\lambda = \sum_{mi} Q_{mi,\lambda}\hat{b}^\dagger_{mi} + Q^*_{mi,\lambda}\hat{b}_{mi}, \tag{13.48}$$

$$\hat{\mathcal{P}}_\lambda = \sum_{mi} P_{mi,\lambda}\hat{b}^\dagger_{mi} + P^*_{mi,\lambda}\hat{b}_{mi}. \tag{13.49}$$

We can no longer assume that the coefficients $Q_{mi,\lambda}$, $P_{mi,\lambda}$ are real. From the commutation relation we get

$$\sum_{mi} Q^*_{mi,\lambda}P_{mi,\mu} - Q_{mi,\lambda}P^*_{mi,\mu} = i\delta_{\lambda,\mu} \tag{13.50}$$

If we treat $\vec{P}_\lambda$ as a vector with components $P_{mi,\lambda}$, then the equations of motion (13.44) become

$$\begin{pmatrix} \mathbf{A} & \mathbf{B} \\ -\mathbf{B} & -\mathbf{A} \end{pmatrix}\begin{pmatrix} \vec{P}_\lambda \\ -\vec{P}^*_\lambda \end{pmatrix} = i\Omega^2_\lambda M_\lambda \begin{pmatrix} \vec{Q}_\lambda \\ -\vec{Q}^*_\lambda \end{pmatrix}, \tag{13.51}$$

$$\begin{pmatrix} \mathbf{A} & \mathbf{B} \\ -\mathbf{B} & -\mathbf{A} \end{pmatrix}\begin{pmatrix} \vec{Q}_\lambda \\ -\vec{Q}^*_\lambda \end{pmatrix} = -\frac{i}{M_\lambda}\begin{pmatrix} \vec{P}_\lambda \\ -\vec{P}^*_\lambda \end{pmatrix}. \tag{13.52}$$

For zero modes this becomes

$$\mathbf{A}\vec{P}_\lambda - \mathbf{B}\vec{P}^*_\lambda = 0, \tag{13.53}$$

$$\mathbf{A}\vec{Q}_\lambda - \mathbf{B}\vec{Q}^*_\lambda = -\frac{i}{M_\lambda}\vec{P}_\lambda. \tag{13.54}$$

The zero modes can be identified with the zero eigenvalues of the stability matrix discussed earlier. Assume $\vec{P}_\lambda$ is purely real. Then it is a zero of $\mathbf{A}-\mathbf{B}$, which, as we discussed earlier, can be found for Im $\vec{z}$, such as rotations about the x- or z-axis. In this case $\vec{Q}_\lambda$ is purely imaginary, $\vec{Q}_\lambda = -i\vec{q}_\lambda$ and $(\mathbf{A}+\mathbf{B})\vec{q}_\lambda = M_\lambda^{-1}\vec{P}_\lambda$.

Conversely, if $\vec{P}_\lambda = i\vec{p}_\lambda$ is purely imaginary, it is a zero of $(\mathbf{A}+\mathbf{B})$ and $(\mathbf{A}-\mathbf{B})\vec{Q}_\lambda = M_\lambda^{-1}\vec{p}_\lambda$. One can then find P, Q, subject to the normalization condition

$$2\vec{q}_\lambda \cdot \vec{p}_\lambda = 1, \tag{13.55}$$

which helps to define M_λ.

Now combining (13.34) and (13.45), (13.46), I get

$$\hat{b}_{mi} = -i\sum_\lambda \left(P_{mi,\lambda}\hat{\mathcal{Q}}_\lambda - Q_{mi,\lambda}\hat{\mathcal{P}}_\lambda\right), \tag{13.56}$$

$$\hat{b}^\dagger_{mi} = i\sum_\lambda \left(P^*_{mi,\lambda}\hat{\mathcal{Q}}_\lambda - Q^*_{mi,\lambda}\hat{\mathcal{P}}_\lambda\right). \tag{13.57}$$

We can now finally deal with the discrepancy that haunted us previously. One can find that

$$A_{mi,nj} = \sum_\lambda \frac{1}{M_\lambda} P_{mi,\lambda}P^*_{nj,\lambda} + M_\lambda\Omega_\lambda^2 Q_{mi,\lambda}Q^*_{nj,\lambda}, \tag{13.58}$$

$$B_{mi,nj} = \sum_\lambda \frac{1}{M_\lambda} P_{mi,\lambda}P_{nj,\lambda} + M_\lambda\Omega_\lambda^2 Q_{mi,\lambda}Q_{nj,\lambda}. \tag{13.59}$$

The difference between $\mathbf{A}$ and $\mathbf{B}$ is very subtle, but keep in mind that either P or Q is imaginary, but not both.

Most useful is the generalized Bogoliubov transformation,

$$\hat{b}_{mi} = \sum_{\lambda,\Omega_\lambda>0}\left(X_{mi,\lambda}\hat{\beta}_\lambda + Y_{mi,\lambda}\hat{\beta}^\dagger_\lambda\right) - i\sum_{\mu,\Omega_\mu=0}\left(P_{mi,\mu}\hat{\mathcal{Q}}_\mu - Q_{mi,\mu}\hat{\mathcal{P}}_\mu\right) \tag{13.60}$$

and its Hermitian conjugate. In that case one gets for the bosonized Hamiltonian

$$\hat{H}_B = E_{\rm HF} - \frac{1}{2}\mathrm{tr}\,\mathbf{A} + \frac{1}{2}\mathrm{tr}\,\mathbf{\Omega} + \sum_{\lambda,\Omega_\lambda>0}\Omega_\lambda\hat{\beta}^\dagger_\lambda\hat{\beta}_\lambda + \sum_{\mu,\Omega_\mu=0}\frac{\hat{\mathcal{P}}^2_\mu}{2M_\mu} \tag{13.61}$$

For the ground state, at least if it has zero angular momentum, we expect $\left\langle\hat{\mathcal{P}}^2_\mu\right\rangle = 0$ for zero modes.

Finally I can resolve the discrepancy between (13.41) and (13.42). The true representation of $\mathbf{A}$ is

$$A_{mi,nj} = \sum_{\lambda,\Omega_\lambda>0}\Omega_\lambda(X_{mi,\lambda}X_{nj,\lambda} + Y_{mi,\lambda}Y_{nj,\lambda}) + \sum_{\mu,\Omega_\mu=0}\frac{1}{M_\mu}P_{mi,\mu}P^*_{nj,\mu}. \tag{13.62}$$

Then we have the true identity,

$$-\frac{1}{2}\mathrm{tr}\,\mathbf{A} + \frac{1}{2}\mathrm{tr}\,\mathbf{\Omega} = -\sum_\lambda\Omega_\lambda\sum_{mi}|Y_{mi,\lambda}|^2 - \frac{1}{2}\sum_{\mu,\Omega_\mu=0}\frac{1}{M_\mu}\sum_{mi}|P_{mi,\mu}|^2. \tag{13.63}$$

13.4.4 More detailed derivation

Here I rederive RPA more carefully, using another, seldome used approach, from the generator coordinate method **?**. In these notes I will review the derviation from generator coordinates. Following I will then attempt to derive systematic extensions of RPA.

(Please note that I have merged together two documents so there may be inconsistencies!)

The generator coordinate method in brief assume the wavefunction can be written in integral form. Let $\{|\lambda\rangle\}$ be a set of "basis" wavefunction which depend upon a continuous parameter (or set of parameters) λ; these states are not necessarily orthogonal, may not be complete, or may be overcomplete. Then let

$$|\Psi\rangle = \int d\lambda f(\lambda) |\lambda\rangle . \tag{13.64}$$

If we introduce the following functions,

$$\mathcal{N}(\lambda', \lambda) = \langle \lambda' | \lambda \rangle , \tag{13.65}$$

$$\mathcal{H}(\lambda', \lambda) = \left\langle \lambda' | \hat{H} | \lambda \right\rangle , \tag{13.66}$$

we then get the Hill-Wheeler integral equation:

$$\int d\lambda \left(\mathcal{H}(\lambda', \lambda) - E\mathcal{N}(\lambda', \lambda) \right) f(\lambda) = 0. \tag{13.67}$$

Now I choose the actual form of the "basis." Let $|0\rangle$ be some starting state, almost always a Slater determinant and a Hartree-Fock minimum. Given a Hartree-Fock state, one can choose occupied states, for which I follow the tradition of labeling with i, j, and unoccupied states, which I also traditionally lable by m, n. This means that (pay close attention to creation $\hat{c}^\dagger$ versus annihilation $\hat{c}$):

$$\hat{c}_i^\dagger |0\rangle = \langle 0 | \hat{c}_i = \hat{c}_m |0\rangle = \langle 0 | \hat{c}_m^\dagger = 0. \tag{13.68}$$

Introduce the general particle-hole operator

$$\hat{Z}^\dagger = \sum_{mi} z_{mi}^* \hat{c}_m^\dagger \hat{c}_i \tag{13.69}$$

then let the general state be

$$|z\rangle = \exp(\hat{Z}^\dagger)|0\rangle; \tag{13.70}$$

by Thouless' theorem this is still a Slater determinant. In general the z_{mi} are complex numbers (more about this later).

From (13.68) we can deduce the useful relation

$$\hat{Z}|0\rangle = 0, \quad \langle 0 | \hat{Z}^\dagger = 0 \tag{13.71}$$

Finally, some simplified notation. All of what we do will be using expectation values of operators between a Slater determinant = "$|0\rangle$." Hence, for a general operator $\hat{X}$, I make the replacement

$$\langle \hat{X} \rangle \equiv \langle 0 | \hat{X} | 0 \rangle.$$

13.4.5 Expansion to second order

I begin by expanding to second order in z_{mi}; later, to generalize, I will expand to fourth order.

First expand to second order

$$\langle z'|z\rangle = \left\langle (1+\hat{Z}'+\frac{1}{2}\hat{Z}'^2)(1+\hat{Z}^\dagger+\frac{1}{2}\hat{Z}^{\dagger 2})\right\rangle = \left\langle 1+\hat{Z}'+\hat{Z}^\dagger+\hat{Z}'\hat{Z}^\dagger+\frac{1}{2}\hat{Z}'^2+\frac{1}{2}\hat{Z}^{\dagger 2}\right\rangle, \tag{13.72}$$

but using (13.71), all we are left with is

$$\langle z'|z\rangle = \langle (1+\hat{Z}'\hat{Z}^\dagger)\rangle, \tag{13.73}$$

which equals (using (13.68))

$$1+\sum_{mi}\sum_{nj} z'_{mi}z^*_{nj}\langle \hat{c}^\dagger_j\hat{c}_n\hat{c}^\dagger_m\hat{c}_i\rangle = 1+\sum_{mi} z'_{mi}z^*_{mi}. \tag{13.74}$$

Next, compute the Hamiltonian (or any operator for that matter) to second order,

$$\langle z'|\hat{H}|z\rangle = \langle \hat{H}\rangle + \langle \hat{Z}'\hat{H}+\hat{H}\hat{Z}^\dagger\rangle + \left\langle \hat{Z}'\hat{H}\hat{Z}^\dagger+\frac{1}{2}\hat{Z}'^2\hat{H}+\frac{1}{2}\hat{H}\hat{Z}^{\dagger 2}\right\rangle \tag{13.75}$$

We can take these term by term.

Zeroth order: $\langle \hat{H}\rangle = E_{HF}$, the Hartree-Fock energy.

First order: if we assume we are at a Hartree-Fock minimum, then by definition

$$\langle 0|\hat{Z}'\hat{H}|0\rangle = \langle 0|\hat{H}\hat{Z}^\dagger|0\rangle = 0. \tag{13.76}$$

Second order: again, using (13.71), one can show

$$\langle \hat{Z}'\hat{H}\hat{Z}^\dagger\rangle = \left\langle \left[\hat{Z}',\hat{H}\right]\hat{Z}^\dagger\right\rangle + \left\langle \hat{H}\hat{Z}'\hat{Z}^\dagger\right\rangle = \left\langle \left[\left[\hat{Z}',\hat{H}\right],\hat{Z}^\dagger\right]\right\rangle + \left\langle \hat{H}\hat{Z}'\hat{Z}^\dagger\right\rangle. \tag{13.77}$$

Because of the particular definition of $\hat{Z}$, one can show that *always*

$$\hat{Z}'\hat{Z}^\dagger|0\rangle = |0\rangle\sum_{mi} z'_{mi}z^*_{mi}. \tag{13.78}$$

Thus we get

$$\langle \hat{Z}'\hat{H}\hat{Z}^\dagger\rangle = \left\langle \left[\left[\hat{Z}',\hat{H}\right],\hat{Z}^\dagger\right]\right\rangle + E_{HF}\sum_{mi} z'_{mi}z^*_{mi}. \tag{13.79}$$

Going further,

$$\left\langle \left[\left[\hat{Z}',\hat{H}\right],\hat{Z}^\dagger\right]\right\rangle = \sum_{mi,nj} z'_{nj}z^*_{mi}\left\langle \left[\left[\hat{c}^\dagger_j\hat{c}_n,\hat{H}\right],\hat{c}^\dagger_m\hat{c}_i\right]\right\rangle. \tag{13.80}$$

Thus we define

$$A_{nj,mi} \equiv \left\langle \left[\left[\hat{c}_j^\dagger \hat{c}_n, \hat{H} \right], \hat{c}_m^\dagger \hat{c}_i \right] \right\rangle \tag{13.81}$$

The matrix $A_{nj,mi}$ is Hermitian, which I leave to the reader to prove.

As for the other second-order terms,

$$\left\langle \hat{Z}'^2 \hat{H} \right\rangle = \left\langle \hat{Z}' \left[\hat{Z}', \hat{H} \right] \right\rangle = \left\langle \left[\hat{Z}', \left[\hat{Z}', \hat{H} \right] \right] \right\rangle = \sum_{mi,nj} z'_{nj} z'_{mi} B_{nj,mi}, \tag{13.82}$$

where

$$B_{nj,mi} \equiv \left\langle \left[\hat{c}_i^\dagger \hat{c}_m, \left[\hat{c}_j^\dagger \hat{c}_n, \hat{H} \right] \right] \right\rangle \tag{13.83}$$

which is *symmetric* but not necessarily Hermitian. By taking the complex conjugate one gets also

$$\left\langle \hat{H} \hat{Z}^{\dagger 2} \right\rangle = \sum_{mi,nj} z^*_{nj} z^*_{mi} B^*_{nj,mi}. \tag{13.84}$$

Now we can combine the first- and second-order terms (the first order vanishing, recall):

$$\langle z' | \hat{H} | z \rangle = E_{HF} \left(1 + \sum_{mi} z'_{mi} z^*_{mi} \right) + \sum_{nj,mi} \left\{ A_{nj,mi} z'_{nj} z^*_{mi} + \frac{1}{2} B_{nj,mi} z'_{nj} z'_{mi} + \frac{1}{2} B^*_{nj,mi} z^*_{nj} z^*_{mi} \right\}. \tag{13.85}$$

or, consistent to second-order,

$$\langle z' | \hat{H} | z \rangle = \left(E_{HF} + \sum_{nj,mi} \left\{ A_{nj,mi} z'_{nj} z^*_{mi} + \frac{1}{2} B_{nj,mi} z'_{nj} z'_{mi} + \frac{1}{2} B^*_{nj,mi} z^*_{nj} z^*_{mi} \right\} \right) \langle z' | z \rangle. \tag{13.86}$$

13.4.6 Differential form of the Hill-Wheeler equation

To faciliate a generator-coordinate interpretation, we make the approximation

$$\langle z' | z \rangle = 1 + \sum_{mi} z'_{mi} z^*_{mi} \approx \exp \left(\sum_{mi} z'_{mi} z^*_{mi} \right). \tag{13.87}$$

Now we can rewrite the Hill-Wheeler equation (13.67)

$$\int \left[\sum_{nj,mi} \left\{ A_{nj,mi} z'_{nj} z^*_{mi} + \frac{1}{2} B_{nj,mi} z'_{nj} z'_{mi} + \frac{1}{2} B^*_{nj,mi} z^*_{nj} z^*_{mi} \right\} + (E_{HF} - E) \right] \exp \left(\sum_{mi} z'_{mi} z^*_{mi} \right) f(\vec{z}) d\vec{z} =$$

(13.88)

This integral equation can be replaced by a differential equation through a simple transformation: let

$$\phi(z') \equiv \int \exp \left(\sum_{mi} z'_{mi} z^*_{mi} \right) f(\vec{z}) d\vec{z}, \tag{13.89}$$

and note that

$$\int z^*_{nj} \exp\left(\sum_{mi} z'_{mi} z^*_{mi}\right) f(\vec{z}) d\vec{z} = \frac{\partial}{\partial z'_{nj}} \int \exp\left(\sum_{mi} z'_{mi} z^*_{mi}\right) f(\vec{z}) d\vec{z} = \frac{\partial}{\partial z'_{nj}} \phi(z'). \tag{13.90}$$

Then the Hill-Wheeler equation becomes

$$\left[\sum_{nj,mi} \left\{ A_{nj,mi} z'_{nj} \frac{\partial}{\partial z'_{mi}} + \frac{1}{2} B_{nj,mi} z'_{nj} z'_{mi} + \frac{1}{2} B^*_{nj,mi} \frac{\partial^2}{\partial z'_{nj} \partial z'_{mi}} \right\} + (E_{HF} - E)\right] \phi(z') = 0. \tag{13.91}$$

We can now drop the primes on the z.

13.4.7 Quasi-boson form

This differential form of the Hill-Wheeler equation (13.91) is *approximate* because it is only second order, especially in the overlap matrix $\langle z'|z\rangle$. Later, when we consider fourth-order terms we will see corrections for the Pauli exclusion principle.

Because (13.91) is quadratic in $z, \partial/\partial z$, we can interpret this as coupled harmonic oscillators, and we can explicitly write down the ladder (boson) operators.

Begin by noting the following (boson) commutation relation:

$$\left[\frac{\partial}{\partial z_{mi}}, z_{nj}\right] = \delta_{mi,nj}.$$

This suggests we make the following substitution:

$$z_{mi} \to \hat{b}^\dagger_{mi}, \quad \frac{\partial}{\partial z_{mi}} \to \hat{b}_{mi} \tag{13.92}$$

The fact that the zs are complex is not injurious (and in fact one can show it is necessary). With this substitution we have the boson eigenvalue equation

$$\hat{H}_B |0) = E|0),$$

where $|0)$ is a harmonic oscillator ground state, and the bosonized Hamiltonian is

$$\hat{H}_B = E_{HF} + \sum_{nj,mi} \left\{ A_{nj,mi} \hat{b}^\dagger_{nj} \hat{b}_{mi} + \frac{1}{2} B_{nj,mi} \hat{b}^\dagger_{nj} \hat{b}^\dagger_{mi} + \frac{1}{2} B^*_{nj,mi} \hat{b}_{nj} \hat{b}_{mi} \right\} \tag{13.93}$$

Before going on to the next section, we write the Hamiltonian in an explicitly quadratic form. First note that, using commutation relations and the fact that $\mathbf{A}$ is Hermitian

$$A_{nj,mi} \hat{b}^\dagger_{nj} \hat{b}_{mi} = \frac{1}{2} A_{nj,mi} \hat{b}^\dagger_{nj} \hat{b}_{mi} + \frac{1}{2} A_{nj,mi} \left(\hat{b}_{mi} \hat{b}^\dagger_{nj} - \delta_{mi,nj}\right) = \frac{1}{2} A_{nj,mi} \hat{b}^\dagger_{nj} \hat{b}_{mi} + \frac{1}{2} A^*_{mi,nj} \hat{b}_{mi} \hat{b}^\dagger_{nj} - \delta_{mi,nj} \frac{1}{2} A_{mi,mi}.$$

Armed with this, we rewrite

$$\hat{H}_B = E_{HF} - \frac{1}{2}\mathrm{tr}\mathbf{A} + \frac{1}{2}\begin{pmatrix} \vec{b}^\dagger & \vec{b} \end{pmatrix}\begin{pmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{B}^* & \mathbf{A}^* \end{pmatrix}\begin{pmatrix} \vec{b} \\ \vec{b}^\dagger \end{pmatrix} \tag{13.94}$$

From here on out, everything is the same as back in Eqn. (14.6).

13.4.8 Observables

13.4.9 Strength functions in "independent-particle" approximation and in TDA

Let $\hat{\mathcal{O}} = \sum_{\alpha\beta} O_{\alpha\beta}\hat{a}^\dagger_\alpha \hat{a}_\beta$ be some one-body transition operator, such as Gamow-Teller or E2. One is very interested in computing the strength function

$$S(E) = \sum_f \delta(E - E_f + E_{g.s.}) \left|\langle f|\hat{\mathcal{O}}|g.s.\rangle\right|^2 . \tag{13.95}$$

As usual, we transform to the p-h basis to get O_{ab}.

In the independent-particle approximation, excited states are just one-particle, one-hole states whose excitation energies are given by differences in single-particle energies:

$$S_{IPA}(E) = \sum_{mi} \delta(E - e_m + e_i) \left|O_{mi}\right|^2 . \tag{13.96}$$

In the TDA, or Tamm-Dancoff Approximation, one diagonalizes the matrix $\mathbf{A}$ at the Hartree-Fock minimum. This is equivalent to diagonalizing in a basis of particle states $|mi^{-1}\rangle$. Note from the expressions above that, at the Hartree-Fock minimum,

The eigenvalue equation for TDA is

$$\sum_{nj} A_{mi,nj} x_{nj,f} = \omega_f x_{mi,f}. \tag{13.97}$$

The TDA strength function is

$$S_{TDA}(E) = \sum_f \delta(E - \omega_f) \left|\sum_{mi} O_{mi} x_{mi,f}\right|^2 . \tag{13.98}$$

13.4.10 Strength functions in RPA

The RPA strength function is a straightforward extension of TDA. One solves the equation (which is a non-Hermitian eigenvalue equation and therefore non-trivial)

$$\begin{pmatrix} \mathbf{A} & \mathbf{B} \\ -\mathbf{B}^* & -\mathbf{A}^* \end{pmatrix}\begin{pmatrix} \vec{x}_f \\ \vec{y}_f \end{pmatrix} = \omega_f^{RPA}\begin{pmatrix} \vec{x}_f \\ \vec{y}_f \end{pmatrix} \tag{13.99}$$

Then the RPA strength function is

$$S_{RPA}(E) = \sum_f \delta(E - \omega_f^{RPA}) \left| \sum_{mi} O_{mi} x_{mi,f} + O_{im} y_{mi,f} \right|^2 . \qquad (13.100)$$

Chapter 14

Bosonic many-body theory

> I have not failed. I've just found 10,000 things that won't work.
> –*Thomas Edison*

Many-body theory for fermions is more widely used than for bosons, in large part because most of the fundamental building blocks of matter–electrons, protons, neutrons–are all fermions. Nonetheless one can develop many-body theory for bosons. Here I shall only scratch the surface.

For bosons I shall use $\hat{b^\dagger}_\alpha, \hat{b}_\alpha$ as the fumdamental creation and annihilation operators, using lower case Greek letters labeling them.

To warm up, let's consider a boson-conserving Hamiltonian. (One can have a boson non-conserving Hamiltonian, where one can create and destroy bosons, such as photons, gluons, pions, etc.. In general one must conserve fermions at some level; at most one can change fermions from one kind to another, or create or destroy *pairs* of fermions.) The trickiest part is the interaction term. As for fermions, we have to consider two-boson states, whether using *permanents* as introduced in Section 2.4,

$$\Phi_{\alpha,\beta}(r_1, r_2) = \frac{1}{\sqrt{2(1+\delta_{\alpha\beta})}} \left(\phi_\alpha(x_1)\phi_\beta(x_2) + \phi_\beta(x_1)\phi_\alpha(x_2)\right), \tag{14.1}$$

or with the occupation representation,

$$|\alpha\beta\rangle = \frac{1}{\sqrt{1+\delta_{\alpha\beta}}} \hat{b}^\dagger_\alpha \hat{b}^\dagger_\beta |0\rangle. \tag{14.2}$$

You should confirm for yourself these states are appropriately normalized. From the permanent, one can get the two-body matrix element

$$V_{\alpha\beta\gamma\delta} = \int \Phi^*_{\alpha\beta}(r_1, r_2) V(r_1, r_2) \Phi_{\gamma\delta}(r_1, r_2) dr_1 dr_2 =$$

$$\zeta^{-1}_{\alpha\beta}\zeta^{-1}_{\gamma\delta} \int \phi^*_\alpha(r_1)\phi^*_\beta(r_2) V(r_1, r_2) \left\{\phi_\gamma(r_1)\phi_\delta(r_2) + \phi_\delta(r_1)\phi_\gamma(r_2)\right\} dr_1 dr_2 \tag{14.3}$$

where as before $\zeta_{\alpha\beta} = \sqrt{1+\delta_{\alpha\beta}}$, and one assume $V(r_1, r_2) = V(r_2, r_2)$. It's pretty obvious then that $V_{\alpha\beta\gamma\delta}$ is symmetric, that is, $V_{\alpha\beta\gamma\delta} = +V_{\beta\alpha\gamma\delta} = +V_{\alpha\beta\delta\gamma}$. From this one can show that the operator

$$\hat{V} = \frac{1}{4}\sum_{\alpha\beta\gamma\delta} \zeta_{\alpha\beta}\zeta_{\gamma\delta} V_{\alpha\beta\gamma\delta} \hat{b}^\dagger_\alpha \hat{b}^\dagger_\beta \hat{b}_\gamma \hat{b}_\delta \tag{14.4}$$

has the correct matrix elements between two-body states, that is,

$$\langle \alpha\beta|\hat{V}|\gamma\delta\rangle = V_{\alpha\beta\gamma\delta}. \tag{14.5}$$

From this we can write down a general, boson-conserving, one+two-body Hamiltonian:

$$\hat{H} = \sum_{\alpha\beta} T_{\alpha\beta}\hat{b}^\dagger_\alpha \hat{b}_\beta + \frac{1}{4}\sum_{\alpha\beta\gamma\delta} \zeta_{\alpha\beta}\zeta_{\gamma\delta} V_{\alpha\beta\gamma\delta} \hat{b}^\dagger_\alpha \hat{b}^\dagger_\beta \hat{b}_\gamma \hat{b}_\delta. \tag{14.6}$$

14.1 Boson condensates

The simplest, and most common, bosonic many-body state is the *condensate*. Unlike fermions, many bosons can occupy the same state with the same quantum numbers; in fact, if one anthropomorphizes the bosons *like* to be in the same state. This is a condenstate: if we define

$$\hat{c}^\dagger = \sum_\alpha U_\alpha \hat{b}^\dagger_\alpha, \tag{14.7}$$

then a condensate of this boson is

$$|c^N\rangle = \frac{1}{\sqrt{N!}}\left(\hat{c}^\dagger\right)^N |0\rangle. \tag{14.8}$$

It's relatively straightforward to find a condensate which minimizes the energy of the Hamiltonian (14.6). First, we imagine the condensate boson (14.7) is just part of a more general unitary transformation,

$$\hat{c}^\dagger_i = \sum_\alpha U_{i\alpha}\hat{b}^\dagger_\alpha, \tag{14.9}$$

and it's inverse,

$$\hat{b}^\dagger_\alpha = \sum_i U^*_{i\alpha}\hat{c}^\dagger_i, \tag{14.10}$$

so that in this transformed basis the boson Hamiltonian is

$$\hat{H} = \sum_{ij} \tilde{T}_{ij}\hat{c}^\dagger_i \hat{c}_j + \frac{1}{4}\sum_{ijkl} \tilde{V}_{ijkl}\hat{c}^\dagger_i \hat{c}^\dagger_j \hat{c}_k \hat{c}_l, \tag{14.11}$$

with the transformed matrix elements

$$\tilde{T}_{ij} = \sum_{\alpha\beta} U^*_{i\alpha} T_{\alpha\beta} U_{j\beta} \tag{14.12}$$

and

$$\tilde{V}_{ijkl} = \sum_{\alpha\beta\gamma\delta} \zeta_{\alpha\beta}\zeta_{\gamma\delta}U^*_{i\alpha}U^*_{j\beta}V_{\alpha\beta\gamma\delta}U_{k\gamma}U_{l\delta}. \tag{14.13}$$

The energy of any N-boson condensate is

$$\langle c_i^N||\hat{H}|c_i^N\rangle = N\tilde{T}_{ii} + \frac{N^2-N}{4}\tilde{V}_{iiii}. \tag{14.14}$$

We can now carry out a variational calculation, but before doing that we need a Lagrange multiplier in order to fix the normalization of the unitary transformation, that is,

$$\frac{\partial}{\partial U^*_{i\alpha}}\left(\langle c_i^N||\hat{H}|c_i^N\rangle - \lambda\sum_\beta U^*_{i\beta}U_{i\beta}\right) = 0. \tag{14.15}$$

The result is a self-consistent eigenvalue equation, much like the fermionic Hartree-Fock equation from Chapter 11, except now it is called the Hartree-**Bose** equation:

$$\sum_\beta h_{\alpha\beta}(N,\rho)U_{i\beta} = \lambda U_{i\alpha} \tag{14.16}$$

where $\rho_{\gamma\delta} = U^*_{i\gamma}U_{i\delta}$ is the density matrix (it's important to note that there is *no* sum over i), and the density- and number-dependent effective one-body Hamiltonian is

$$h_{\alpha\beta}(N,\rho) = NT_{\alpha\beta} + \frac{N^2-N}{2}\sum_{\gamma\delta}\zeta_{\alpha\gamma}\zeta_{\beta\delta}\rho_{\gamma\delta}V_{\alpha\gamma\beta\delta}. \tag{14.17}$$

14.1.1 Sample application: Bosonic pairing

We can test out the Hartree-Bose equations against a toy model for which we know the exact results: the bosonic pairing model of Section 5.4. Then the only nonzero two-body matrix elements are $V_{\alpha,-\alpha,\beta,-\beta} = -G$. We can write this in pair-separble form, that is, write $V_{\alpha\beta\gamma\delta} = -G\delta_{\beta,-\alpha}\delta_{\delta,-\gamma}$. One solution for the Hartree-Bose equation is a constant vector, that is, $U_\alpha = (2\Omega)^{-1/2}$. Then $\tilde{V}_{iiii} = -G$, and our Hartree-Bose energy is $-\frac{1}{4}GN(N-1)$ which is above the exact answer of $-\frac{1}{4}GN(N-2+2\Omega)$; in fact, for $\Omega \gg N/2$ (which one would call a dilute boson gas) it is a very poor approximation. We will see if we can improve on this.

Part III

Putting a spin on things

Chapter 15

A whirlwind tour of the quantum theory of angular momentum

> If I were again beginning my studies, I would follow the advice of Plato and start with mathematics. –*Galileo Galilei*

Angular momentum is all around us: if the laws of physics are isotropic (a fancy way of saying they are the same no matter in which direction you look), then a necessary consequence is conservation of angular momentum. The quantum theory of angular momentum and the addition of angular momentum is extremely important in low-energy nuclear physics, and important in particle and atomic physics. It is generally less important in solid states physics, where one typically has discrete lattice symmetries instead.

While classically we think of angular momentum in terms of $\vec{L} = \vec{r} \times \vec{p}$, in quantum mechanics one can and must treat angular momentum more abstractly. The 'must' is because of intrinsic angular momentum or *spin* that elementary particles such as quarks and electrons carry. While it is very tempting to think of an electron as a little spinning ball of charge, in the Dirac equation, the relativistic successor to the Schrödinger equation, one finds spin arises without any substructure at all; in the Dirac equation it is only the combination of orbital ($\vec{r} \times \vec{p}$) angular momentum plus intrinsic spin which is conserved.

If it walks like angular momentum, talks like angular momentum, or, more importantly, if it satisfies the same commutation relations as angular momentum, i.e., the so-called SU(2) commutation relations as in Eq. (4.3), which I reproduce here but with trivially different notation

$$\left[\hat{J}_x, \hat{J}_y\right] = i\hbar\hat{J}_z, \quad \left[\hat{J}_y, \hat{J}_z\right] = i\hbar\hat{J}_x, \quad \left[\hat{J}_z, \hat{J}_x\right] = i\hbar\hat{J}_y, \tag{15.1}$$

it either *is* angular momentum, as in the case of intrinsic spin, or can be treated as if it were angular momentum, as in the case of isospin or quasispin (cf. section 7.1). This is a strategy typical of physicists: although we are comfortable with abstract concepts, we really like to make a new abstract concept look as much as possible like an old abstract concept we have already mastered.

In this and the remaining chapters I will discuss how to marry the quantum theory of angular momentum with the occupation representation, mostly in the calculation of matrix elements of various operators. Before doing that, let me review some of the basic results from Chapter 4. I do assume this is not the reader's first time at the angular momentum rodeo, and has had some exposure to spherical harmonics and the Pauli spin matrices. I will barely scratch the surface, and so the reader is encouraged to obtain a copy of one of the many fine references on angular momentum (although few are good as pedagogical introductions). One should be aware that there can be differences in definitions and conventions, such as phases and overall factors. I follow A. R. Edmond's excellent little book, *Angular momentum in quantum mechanics*, which contains 95% of what I need; for the remaining 5% turn to the thicker, even more detailed *Quantum theory of angular momentum* by Varshalovich, Moskalev, and Khersonskii.

Starting from the SU(2) commutation relations, we were able to establish the existence of a non-trivial operator $\hat{J}^2 = \hat{J}_x^2 + \hat{J}_y^2 + \hat{J}_z^2$ which commutes with the operators $\hat{J}_{x,y,z}$. (This is a *second-order Casimir operator*.) Because $\hat{J}^2$ and $\hat{J}_z$ commute (and we could have easily chosen $\hat{J}_y$ or $\hat{J}_x$, but the z-component is conventional), we know we can find simultaneous eigenstates of $\hat{J}^2$ and $\hat{J}_z$. Further we were able to establish the eigenvalues. In short we found there exist states $|j, m\rangle$ such that

$$\hat{J}^2|j,m\rangle = \hbar^2 j(j+1)|j,m\rangle; \tag{15.2}$$

$$\hat{J}_z|j,m\rangle = \hbar m|j,m\rangle, \tag{15.3}$$

with the restrictions that j must either be a nonzero integer or a positive half-integer (i.e., $1/2, 3/2, 5/2, \ldots$), and that for a given j the value of m can take on only one of $-j, -j+1, \ldots, j-1$, or j. All of this comes directly from the commutation relations, so if we have operators which satisfy those commutation relations, these results hold automatically. We used this idea to find analytic results via quasispin for the fermion pairing Hamiltonian and for the Lipkin model, two models which have nothing to do with angular momentum but which, by design, share the same mathematics.

Although the mathematics applies to any system of operators with the SU(2) commutation relations, I'll begin by discussing some fundamental systems exhibiting them.

15.1 Spherical Harmonics

Classically, angular momentum is $\vec{L} = \vec{r} \times \vec{p}$. In quantum mechanics, the coordinate-space representation of $\vec{p}$ is $\frac{\hbar}{i}\vec{\nabla}$. To compute the kinetic energy of a particle we need $p^2 = -\hbar^2\nabla^2$. In spherical coordinates, one can tediously show that

$$\nabla^2 = \frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\left(\vec{r} \times \vec{\nabla}\right)^2. \tag{15.4}$$

But this last term is proportional to the quantum $\hat{L}^2$. Thus spherical harmonics can arise even in purely classical situations, and can be seen as nothing more than the eigenfunctions of the angular part of the Laplacian ∇^2:

$$-(\vec{r} \times \vec{\nabla})^2 Y_{lm}(\theta\phi) = l(l+1)Y_{lm}(\theta\phi). \tag{15.5}$$

Because $\hat{L}^2$ and $\hat{L}_z$ commute, we construct the spherical harmonics to also be eigenfunctions of the latter:

$$\frac{1}{i}\frac{\partial}{\partial\phi}Y_{lm}(\theta\phi) = mY_{lm}(\theta\phi). \tag{15.6}$$

The spherical harmonics are orthonormal,

$$\int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta\, d\theta\, Y^*_{l'm'}(\theta,\phi)Y_{lm}(\theta,\phi) = \delta_{l'l}\delta_{m'm}, \tag{15.7}$$

and form a complete basis set for functions periodic in θ and ϕ. The complex conjugate of a spherical harmonic is given by $Y^*_{lm} = (-1)^m Y_{l\,-m}$, which we'll later see is a general property of *spherical tensors*. You can find full expressions for spherical harmonics in any decent introduction to quantum angular momentum. More important is how to calculate with them, as discussed below.

15.2 Spinors, Spin, and Pauli matrices

As we saw proved in Chapter 4, values of j can be either integers $0, 1, 2, 3, \ldots$ or half-integers $1/2, 3/2, \ldots$. The case with $j = 0, m = 0$ is trivial, so the smallest nontrivial case is $j = 1/2$ with $m = \pm 1/2$. The operators for this two-dimensional space are the spin matrices, already introduced in the Exercises for Chapter 4 (and taking $\hbar = 1$ for simplicity),

$$\mathbf{S}_x = \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},\ \mathbf{S}_y = \frac{1}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix},\ \mathbf{S}_z = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{15.8}$$

The eigenstates of $\mathbf{S}_z$ form a convenient basis for *spinors*,

$$\left|j = \frac{1}{2}, m = +\frac{1}{2}\right\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} = |\uparrow\rangle, \tag{15.9}$$

$$\left|j = \frac{1}{2}, m = -\frac{1}{2}\right\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} = |\downarrow\rangle, \tag{15.10}$$

where I've also introduced the notation for 'spin-up', $|\uparrow\rangle$ and 'spin-down' $|\downarrow\rangle$ states. Because

$$\mathbf{S}^2 = \mathbf{S}_x^2 + \mathbf{S}_y^2 + \mathbf{S}_z^2 = \frac{3}{4}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \tag{15.11}$$

all spinors are trivially eigenstates of $\mathbf{S}^2$.

15.2.1 Isospin

Protons and neutrons are very different particles: protons are charged, while neutrons are neutral; neutrons are slightly heavier than protons, and can beta decay to a proton, while protons, at least as far as we know, do not decay. (Some theories predict or require proton decay, and physicists have assiduously searched for proton decay; but to date we have never had a confirmed proton decay, which rules out certain otherwise appealing theories.)

Yet, they are not *very* different. They have the same mass to within 0.5%; they have the same spin. And because the nuclear force is roughly a hundred times stronger than the Coulomb force, one can quite reasonably argue that the fact that protons have electric charge and neutrons do not, is only a small effect on the order of a few percent.

This led Werner Heisenberg in 1932 to propose the concept of *isospin*. In the same way that electrons, or any spin-$\frac{1}{2}$ particle, can be in a "spin-up" $|\uparrow\rangle$ or a "spin-down" $|\downarrow\rangle$ state, which are two different quantum states of the same particle, Heisenberg imagined protons and neutrons as the "same" particle but with "isospin-up" (protons) or "isospin-down" (neutrons). We call this an isospin doublet, and we can represent it by an isospin spinor in exactly the same we do with spin.

Heisenberg's proposal works remarkably well. For example, mirror nuclides–nuclei with the numbers of protons and neutrons reverse (e.g., ^{12}B and ^{12}N) have very similar excitation spectra. To a large extent we can treat isospin as an approximately conserved quantum number.

15.3 Addition of angular momentum

We are now in the position to discuss the rules for adding or coupling angular momentum. These rules apply to any sort of angular momentum, be it orbital or intrinsic (spin) or composite. Therefore I will use the notation J to represent total angular momentum and M to represent the z-component.

The basic question we face is: given two initial angular momenta, $\vec{J}_1$ and $\vec{J}_2$, how do they combine to get $\vec{J}_{12}$?

Classically, one just adds the components of two angular momentum vectors:

$$\vec{J}_{12} = (J_{12x}, J_{12y}, J_{12z}) = \vec{J}_1 + \vec{J}_2 = (J_{1x} + J_{2x}, J_{1y} + J_{2y}, J_{1z} + J_{2z}). \tag{15.12}$$

But in quantum mechanics, we have only two numbers to describe angular momentum, the total angular momentum$J$ and by convention the z-component or 3rd component or magnetic quantum number M.

If we have two angular momenta, (J_1, M_1) and (J_2, M_2), the z-components add as usual:

$$M_{12} = M_1 + M_2. \tag{15.13}$$

It's the total angular momentum J_{12} that is tricky, because the x- and y-components are not determined.

It turns out that, unlike classical mechanics, there are multiple possible results for J_{12}. First we will look at the *possible* values, and then the *probabilities* for each possible outcome.

The possible outcomes are given by the *triangle rule*:

$$|J_1 - J_2| \leq J_{12} \leq J_1 + J_2, \tag{15.14}$$

with J_{12} taking units steps (actually steps of $\hbar$, which I've set $= 1$). The rules (15.13) and (15.14) are also called *selection rules*, because they select only certain outcomes as possible. (Other groups also have selection rules, but most of them are beyond our scope. One simple example, however, are matrix elements of x and p in a harmonic oscillator basis: they can only connect states which differ by exact one $\hbar\omega$. We will have occasion to see this selection rule in action later.)

Example. Suppose we add together angular momentum 7/2 with angular momentum 2. Then the possible total angular momenta are 3/2, 5/2,7/2, 9/2, or 11/2.

Example: Suppose we have $J_1 = 7/2, M_1 = -3/2$ and $J_2 = 3/2, M_2 = -3/2$. Then the total z-component is $M_{12} = -3$ and the possible total angular momenta are $J_{12} = 3, 4, 5$; although $|7/2 - 3/2| = 2$, we must have $J_{12} \geq |M_{12}|$.

Now that we have the possibilities, we have to consider the *probabilities*. It will help to recall some of the basic principles of quantum mechanics, as discussed in the first chapter. We can think of $|J_1, M_1; J_2 M_2\rangle$ as a state; sometimes it is written as $|J_1, M_1\rangle|J_2, M_2\rangle$ or even as a tensor product $|J_1, M_1\rangle \times |J_2, M_2\rangle$. At any rate we want to expand this state in terms of states with good total angular momentum J_{12}. That is, we write

$$|J_1, M_1; J_2 M_2\rangle = \sum_{J_{12}} c(J_{12}) |J_{12}, M_{12} = M_1 + M_2\rangle. \tag{15.15}$$

We call the states $|J_1, M_1; J_2 M_2\rangle$ the *uncoupled basis* and the states $|j_{12}, M_{12}\rangle$ the coupled basis; often to emphasize the coupling one writes $|(J_1, J_2) j_{12}, M_{12}\rangle$.

Now the coefficient $C(J_{12})$ represent a unitary transformation from the uncoupled basis and the coupled basis. To see this, it helps to realize that for a particular basis the dimensions of the uncoupled basis and the coupled basis are exactly the same.

Example: Consider adding two angular momenta, $j_1 = j_2 = 1/2$. The possible values of $m_{1,2}$ are $\pm 1/2$. Therefore there are four states in the uncoupled

basis:

j_1	m_1	j_2	m_2
$\frac{1}{2}$	$+\frac{1}{2}$	$\frac{1}{2}$	$+\frac{1}{2}$
$\frac{1}{2}$	$+\frac{1}{2}$	$\frac{1}{2}$	$-\frac{1}{2}$
$\frac{1}{2}$	$-\frac{1}{2}$	$\frac{1}{2}$	$+\frac{1}{2}$
$\frac{1}{2}$	$-\frac{1}{2}$	$\frac{1}{2}$	$-\frac{1}{2}$

For the coupled basis states, the total J_{12} can be 0 or 1:

J_{12}	M_{12}
0	0
1	-1
1	0
1	-1

So we see explicitly that both the coupled and uncoupled bases have the same dimensions. You can try other examples.

Because the coupled and uncoupled bases have the same dimensions, there is a unitary transformation between them. (We assume the states are orthonormalized already). To find this unitary transformation, we simply use the completeness relation.

$$|J_1, M_1, J_2 M_2\rangle = \sum_{J_{12}} |J_{12}, M_{12}\rangle\langle J_{12}, M_{12}|J_1, M_1; J_2, M_2\rangle.. \tag{15.16}$$

As always the matrix element of a unitary transformation is just the inner product between two basis states, $\langle J_{12}, M_{12}|J_1, M_1; J_2, M_2\rangle..$ As it happens (though I will not prove it) these matrix elements are real, so we can take the transpose without harm. The matrix elements

$$(J_1, M_1, J_2, M_2|J_{12} M_{12}) \tag{15.17}$$

are the *Clebsch-Gordan coefficient*, sometimes also called the *vector-coupling coefficients*. Sometimes one writes $(J_1 M_1, J_2 M_2|(J_1, J_2) J_{12} M_1 2)$ to emphasize in pedagogy that the coupled basis is constucted from J_1 and J_2. There are alternate notations, but (15.17) is the most common; it also helps to remind us that the Clebsch-Gordan coefficients are not so very esoteric but simply the matrix elements of the unitary transformation from the uncoupled basis to the coupled basis, or vice-versa. (You may also notice that we wrote states with angle brackets $\rangle$ but the Clebsch-Gordan coefficients, despite their origin from and interpretation in terms of states, use round brackets. This is convention; convention is not always consistent.)

Indeed, now we can combine angular momenta to get a state of definite total angular momentum:

$$|(J_1, J_2) J_{12}, M_{12}\rangle = \sum_{J_{12}} |J_1, M_1; J_2, M_2\rangle\langle J_1, M_1; J_2, M_2|J_{12} M_{12}\rangle. \tag{15.18}$$

This is immensely important for many applications in many-body physics, for it tells us how to construct states with good total angular momentum.

15.3.1 Example: $\frac{1}{2} \otimes \frac{1}{2}$

Here is a table of Clebsch-Gordan coefficients for $j_1 = j_2 = 1/2$; blank spots indicate zeroes due to selection rules.

				J_{12}:	0	1	1	1
				M_{12}	0	0	1	-1
j_1	m_1	j_2	m_2					
$\frac{1}{2}$	$+\frac{1}{2}$	$\frac{1}{2}$	$-\frac{1}{2}$		$\frac{1}{\sqrt{2}}$	$\frac{1}{\sqrt{2}}$		
$\frac{1}{2}$	$-\frac{1}{2}$	$\frac{1}{2}$	$+\frac{1}{2}$		$-\frac{1}{\sqrt{2}}$	$\frac{1}{\sqrt{2}}$		
$\frac{1}{2}$	$+\frac{1}{2}$	$\frac{1}{2}$	$+\frac{1}{2}$				1	
$\frac{1}{2}$	$-\frac{1}{2}$	$\frac{1}{2}$	$-\frac{1}{2}$					1

Notice the block-diagonal structure, which arises from the selection rule on the M values.

If we interpret these as spin-1/2 states, with $m == +1/2$ as spin up or $|\uparrow\rangle$ and $m = -1/2$ as spin down or $|\downarrow\rangle$, then coupling two spin-1/2 states into a state of total spin S, we have

$$\begin{aligned} |S=0, M_S=0\rangle &= \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right), \\ |S=1, M_S=0\rangle &= \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\right), \\ |S=1, M_S=+1\rangle &= |\uparrow\uparrow\rangle, \\ |S=1, M_S=-1\rangle &= |\downarrow\downarrow\rangle . \end{aligned} \tag{15.19}$$

15.3.2 Properties of Clebsch-Gordan coefficients

Clebsch-Gordan coefficients have many useful properties, only a few of which I summarize here. Refer to your favorite book on angular momentum algebra for more details and examples.

Real-valued. Although formally Clebsch-Gordan coefficients are the matrix elements of a unitary transformation, we choose them to be real-valued,

$$(j_1 m_1, j_2 m_2 | JM) = (JM | j_1 m_1, j_2 m_2), \tag{15.20}$$

which means that the transformation is an *orthogonal* transformation

Orthonormality. Because the Clebsch-Gordan coefficients represent an orthogonal, that is, unitary and real-valued, transformation between the coupled and uncoupled bases, they have orthonormality relations. First, by summing over the uncoupled basis:

$$\sum_{m_1 m_2} (j_1\, m_1, j_2\, m_2 | j\, m)(j_1\, m_1, j_2\, m_2 | j'\, m') = \delta_{jj'}\delta_{mm'}. \tag{15.21}$$

Although Clebsch-Gordan orthonormality relations look straightforward, you have to apply them carefully. In particular you must pay attention to selection rules and any external constraints. Because $m = m' = m_1 + m_2$, if m is externally constrained.

$$\sum_{m_1}(j_1\, m_1, j_2\, m - m_1|j\, m)(j_1\, m_1, j_2\, m - m_1|j'\, m) = \delta_{jj'}. \tag{15.22}$$

Alternately, one can sum over the coupled basis:

$$\sum_{jm}(j_1\, m_1, j_2\, m_2|j\, m)(j_1\, m_1', j_2\, m_2'|j\, m) = \delta_{m_1 m_1'}\delta_{m_2 m_2'} \tag{15.23}$$

or, again, because $m_1 + m_2 = m_1' + m_2' = m$, if m itself is fixed, then

$$\sum_{j}(j_1\, m_1, j_2\, m - m_1|j\, m)(j_1\, m_1', j_2\, m - m_1'|j\, m) = \delta_{m_1 m_1'}. \tag{15.24}$$

In many applications one has to apply symmetry relations (below) to bring the Clebsch-Gordan coefficients into proper form.

Symmetries. The Clebsch-Gordan coefficients have a number of symmetry relations useful for manipulation. A useful symmetry relation is

$$\begin{aligned}(j_a m_a, j_b m_b|j_c m_c) &= (-1)^{j_a - m_a}\frac{[j_c]}{[j_b]}(j_c\, m_c, j_a\, -m_a|j_b\, m_b); &(15.25)\\ &= (-1)^{j_b + m_b}\frac{[j_c]}{[j_a]}(j_b\, m_b, j_a\, -m_a|j_b\, m_b). &(15.26)\end{aligned}$$

Another one is

$$\begin{aligned}(j_a\, m_a, j_b\, m_b|j_c\, m_c) &= (-1)^{j_a + j_b - j_c}(j_b\, m_b, j_a\, m_a|j_c\, m_c) &(15.27)\\ &= (-1)^{j_a + j_b - j_c}(j_a\, -m_a, j_b\, -m_b|j_c\, -m_c) &(15.28)\end{aligned}$$

15.3.3 Wigner 3-j symbols

A widely used alternate to Clebsch-Gordan coefficients are the *Wigner* 3-j *symbols*:

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = \frac{(-1)^{j_1 - j_2 - m_3}}{[j_3]}(j_1\, m_1, j_2\, m_2|j_3\, -m_3). \tag{15.29}$$

While the Clebsch-Gordan coefficients have a direct meaning as matrix elements of an orthogonal transformation, in other circumstances the 3-j symbols are more convenient. For example, the 3-j symbols have simpler symmetry relations. Even permutations of the columns do not change the value

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = \begin{pmatrix} j_3 & j_1 & j_2 \\ m_3 & m_1 & m_2 \end{pmatrix} = \begin{pmatrix} j_2 & j_3 & j_1 \\ m_2 & m_3 & m_1 \end{pmatrix}, \tag{15.30}$$

while odd permutations pick up a phase:

$$= (-1)^{j_1+j_2+j_3} \begin{pmatrix} j_2 & j_1 & j_3 \\ m_2 & m_1 & m_3 \end{pmatrix}, \tag{15.31}$$

etc., as does flipping the signs on the m's:

$$= (-1)^{j_1+j_2+j_3} \begin{pmatrix} j_1 & j_2 & j_3 \\ -m_1 & -m_2 & -m_3 \end{pmatrix}. \tag{15.32}$$

As both Clebsch-Gordan coefficients and 3-j symbols are used one should be familiar with both.

15.4 Worked example: Normalization of two-body states in a single-j shell

Suppose we have two particles, both with the same j; this is called a single j-shell. To create two particles coupled up to good angular momentum J with z-component M, we simply use Clebsch-Gordan coefficients:

$$\left[\hat{a}^\dagger_j \otimes \hat{a}^\dagger_j\right]_{J\,M} = \sum_{\mu_1,\mu_2} (j\,\mu_1, j\,\mu_2|J\,M)\hat{a}^\dagger_{j\,\mu_1}\hat{a}^\dagger_{j\,\mu_2}. \tag{15.33}$$

The two-particle state itself is

$$|(j)^2; J\,M\rangle = \frac{1}{\sqrt{2}}\left[\hat{a}^\dagger_j \otimes \hat{a}^\dagger_j\right]_{J\,M}|0\rangle, \tag{15.34}$$

Our task now is to confirm this normalization:

$$\left\langle (j)^2; J\,M|(j)^2; J\,M\right\rangle = \tag{15.35}$$
$$\frac{1}{2}\sum_{m_1,m_2,\mu_1,\mu_2} (j\,m_1, j\,m_2|J\,M)(j\,\mu_1, j\,\mu_2|J\,M) \quad \left\langle 0|\hat{a}_{j\,m_2}\hat{a}_{j\,m_1}\,\hat{a}^\dagger_{j\,\mu_1}\hat{a}^\dagger_{j\,\mu_2}|0\right\rangle$$

(remember when you take the adjoint of a fermion state, you have to put the operators in reverse order as well as taking the Hermitian conjugate of each one, that is, if $|ab\rangle = \hat{a}^\dagger\hat{b}^\dagger|0\rangle$, then $\langle ab| = \langle 0|\hat{b}\hat{a})$. If you have practiced your fermion algebra, you should be able to reproduce

$$\left\langle 0|\hat{a}_{j\,m_2}\hat{a}_{j\,m_1}\,\hat{a}^\dagger_{j\,\mu_1}\hat{a}^\dagger_{j\,\mu_2}|0\right\rangle = \delta_{m_1,\mu_1}\delta_{m_2,\mu_2} - \delta_{m_1,\mu_2}\delta_{m_2,\mu_1}.$$

Then continuing (15.35),

$$= \frac{1}{2}\sum_{m_1,m_2} (j\,m_1, j\,m_2|J\,M)\left[(j\,m_1, j\,m_2|J\,M) - (j\,m_2, j\,m_1|J\,M)\right]. \tag{15.36}$$

But by the symmetry (15.27) $(j\,m_2, j\,m_1|J\,M) = (-1)^{2j-J}(j\,m_1, j\,m_2|J\,M)$; because these are fermions, j is a half-integer and $2j$ is an odd integer. Thus we have

$$= \frac{1+(-1)^J}{2} \sum_{m_1,m_2} (j\,m_1, j\,m_2|J\,M)(j\,m_1, j\,m_2|J\,M) = \frac{(1+(-1)^J}{2} \quad (15.37)$$

where I've used the orthogonality relation (15.21). Thus the two-body state (15.34) is correctly normalized; furthermore, it only exists for even total J.

15.5 Rotations and spherical tensors

Before going futher, we have to look at some technical properties of various operators. In particular we have to introduce the idea of *spherical tensors*. This is a deep and rich topic and I will only skim just enough to get us what we need.

Often in physics we invoke the idea of invariants. For example, the speed of light c is invariant for all observers, an empirical fact, as is the rest mass. The technical term for such invariant terms are *scalars*. Of course, some things are not invariant, such as position and linear and angular momentum. Such quantities depend upon the observers inertial frame and orientation, among other things. It is important to notes, however, that these dependencies are not arbitrary but defined through rigorous *transformations*. Quantities that transform in a particular way we called *tensors*.

(A comment on notation. General tensors are indexed, that is, we write them as $T_{abc\ldots}$, and when we call an object we mean that its representation in different frames are related by specific transformations, e.g., $T'_{abc\ldots} = U_{ar}U_{bs}U_{ct}\ldots T_{rst\ldots}$ with sums over repeated indices implied, and $\mathbf{U}$ is a specific transformation. Now: we often refer to a tensor with a single index, i.e., V_a, as a *vector*. In general in quantum mechanics when we use the word 'vector' we mean 'an element of a vector space', but in this context 'vector' means an object with specific transformation property. The two usages are not mutually exclusive, of course. For the topic here the standard usage is to refer to spherical tensors, even for objects with one index, but for other groups one might talk about Lorentz vectors, tensors, and scalars, a *scalar* having no indices and being invariant under change of frame.)

For this chapter we will look exclusively at rotations. Even though we live in a three-dimensional space, we define rotations about one-dimensional axes. The most general rotation can described by a sequence of three rotations through the *Euler angles*: a rotation by α radians about the z-axis, followed by a rotation by β about the y-axis, followed by a final rotation of γ about the z-axis again.

Here we must appeal to group theory, which is the foundational branch of mathematics for quantum mechanics, and in particular to the theory of continuous groups; in particular these are called *Lie* groups, if you wish to read in more depth elsewhere. The group of rotations are such an example, and the

SU(2) operators $\hat{J}_x, \hat{J}_y, \hat{J}_z$ are the *generators* of this group. For example,

$$\exp\left(i\alpha\hat{J}_z\right)$$

generates rotations by an angle α about the z axis. The rotations defined by the Euler angles, thus, are given by the rotation operator

$$\hat{R}(\alpha,\beta,\gamma) = \exp\left(i\gamma\hat{J}_z\right)\exp\left(i\beta\hat{J}_y\right)\exp\left(i\alpha\hat{J}_z\right). \tag{15.38}$$

Sometimes we replace α, β, γ by the single symbol Ω which, in this context, implies the Euler angles. As the generators are Hermitian operators, we can see that $\hat{R}$ is a manifestly unitary operator, so that the inverse

$$\hat{R}^{-1}(\alpha,\beta,\gamma) = \hat{R}^\dagger(\alpha,\beta,\gamma) = \hat{R}(-\gamma,-\beta,-\alpha).$$

For an object (here, a wavefunction) with good angular momentum j, rotation about the Euler angles will not change the magnitude of angular momentum, but it can and will change the orientation. The mixing of orientations is given by the *Wigner D-matrices*:

$$\hat{R}(\alpha,\beta,\gamma)|j\,m\rangle = \sum_{m'} \mathcal{D}^{(j)}_{m'\,m}(\alpha,\beta,\gamma)|j\,m'\rangle. \tag{15.39}$$

Alternately, we can define the Wigner D-matrices as the matrix elements of the rotation operator:

$$\mathcal{D}^{(j)}_{m'\,m}(\alpha,\beta,\gamma) \equiv \langle j\,m'|\hat{R}(\alpha,\beta,\gamma)|j\,m\rangle. \tag{15.40}$$

For properties of the the Wigner D-matrices see your favorite text on angular momentum such as Edmonds. (I will probably expand this later).

Eqn. (15.39) tells us how a wavefunction, that is, an element of a vector space, transforms under rotation. A *spherical tensor* is an operator whose transformations are also given by Wigner D-matrices, specifically,

$$\hat{R}(\Omega)\hat{\mathcal{O}}_{j\,m}\hat{R}^{-1}(\Omega) = \sum_{m'} \hat{\mathcal{O}}_{j\,m'}\mathcal{D}^{(j)}_{m'\,m}(\Omega). \tag{15.41}$$

Any object we call a spherical tensor must adhere to the transformation law (15.41). Alternately, one can show the following commutators of the generators of rotation for a spherical tensor:

$$\left[\hat{J}_z, \hat{\mathcal{O}}_{j\,m}\right] = \hbar m\hat{\mathcal{O}}_{j\,m} \tag{15.42}$$

$$\left[\hat{J}_\pm, \hat{\mathcal{O}}_{j\,m}\right] = \hbar\sqrt{(j\mp 1)(j\pm m+1)}\hat{\mathcal{O}}_{j\,m\pm 1}$$

15.5.1 Hermitian adjoints of operators and coupling of operators

The idea of spherical tensors is important because we will be constructing many-body states (wavefunctions or vectors) and operators, and in order to handle angular momentum correctly we need to be working with spherical tensors. In particular an important question is how a spherical tensor behaves under the Hermitian adjoint. It turns out that the adjoint of a spherical tensor is *not* a spherical tensor. Rather (see Edmonds section 5.5 for a discussion),but for a spherical tensor $\hat{F}_{KM}$, one expects either

$$\left(\hat{F}_{KM}\right)^\dagger = (-1)^M \hat{F}_{K,-M}, \tag{15.43}$$

or $\left(\hat{F}_{KM}\right)^\dagger = (-1)^{K+M}\hat{F}_{K,-M}$. We will see that for more physical operators we consider, such as spin, momentum, multipole moments, etc., all of which have integer rank K, eqn. (15.43) applies.

Half-integer operators are different. In particular, consider fermion operators, such as $c^\dagger_{jm}$ which creates a particle in a state of good angular momentum j, m, we have to choose the second option. While $\hat{c}^\dagger_{jm}$ is a spherical tensor, $\hat{c}_{jm}$ is not; rather the time-reverse

$$\tilde{c}_{j,\,m} \equiv (-1)^{j+m} c_{j,-m} \tag{15.44}$$

is a spherical tensor. This allows one to construct one-body operators which properly transform as spherical tensors,

$$\begin{aligned}\left[c^\dagger_a \otimes \tilde{c}_b\right]_{KM} &= \sum_{m_a m_b} (j_a m_a, j_b m_b | KM) c^\dagger_{j_a m_a} \tilde{c}_{j_b m_b} \\ &= \sum_{m_a m_b} (j_a m_a, j_b m_b | KM)(-1)^{j_b+m_b} c^\dagger_{j_a m_a} c_{j_b -m_b}\end{aligned} \tag{15.45}$$

To see that this is sensible, consider

$$\begin{aligned}\left[c^\dagger \otimes \tilde{c}\right]_{00} &= \sum_m (jm, j-m|00) c^\dagger_{jm} \tilde{c}_{j,-m} \\ &= \sum_m (-1)^{j-m} \frac{1}{[j]} c^\dagger_{jm} (-1)^{j-m} c_{jm} \\ &= \frac{1}{[j]} \sum_m c^\dagger_{jm} c_{jm} = \frac{1}{[j]} \hat{n}_j\end{aligned} \tag{15.46}$$

where I used

$$(jm, j-m|00) = \frac{(-1)^{j-m}}{[j]}, \tag{15.47}$$

so that the number operator $\hat{n}$ is proportional to $\left[c^\dagger \otimes \tilde{c}\right]_{00}$ as it should be.

Not only is this sensible, it is mandatory: **in order to construct meaningful operators with good angular momentum**, one must use $\tilde{c}$. This will become important in the next chapter.

15.5.2 Scalar products

While vectors, and more broadly tensors, have orientations and thus depend in detail upon rotations and other transformations, we think of dot products between vectors, $\vec{v} \cdot \vec{w}$, also called scalar products or inner products, as being invariant and independent of the representation. Indeed the reason they are called scalar products is that *scalars* are objects invariant under rotation or other transformations.

While the broad definition of a scalar product is obvious (coupling to angular momentum zero) there is some ambiguity in phase and amplitude. Edmonds (5.2.4) defines the scalar product of two tensor operators of rank k as

$$\left(\vec{T}_k \cdot \vec{U}_k\right) = \sum_m (-1)^m T_{km} U_{k,-m} = (-1)^k [k] \left[T_k \otimes U_k\right]_{00} . \tag{15.48}$$

To see if this is reasonable, try

$$r_1 r_2 (Y_1(1) \cdot Y_1(2)) \tag{15.49}$$

by using Table 1 in Edmonds, you will find this $= \frac{3}{4\pi} \vec{r}_1 \cdot \vec{r}_2 = \frac{3}{4\pi}(x_1 x_2 + y_1 y_2 + z_1 z_2)$ which, except for the overall constant, is reasonable.

15.5.3 Two-body operators and spherical tensors

Before we can talk about Hamiltonians, we need to talk about generic two-body operators and some important subtleties.

First we define the pair creation operator

$$\hat{A}^\dagger_{JM}(ab) \equiv \left[c^\dagger_a \times c^\dagger_b\right]_{JM} = \sum_{m_a, m_b} (j_a m_a, j_b m_b | JM) \hat{c}^\dagger_{j_a m_a} \hat{c}^\dagger_{j_b m_b}. \tag{15.50}$$

If we include isospin we have

$$\hat{A}^\dagger_{JM,TM_T}(ab) \equiv \left[c^\dagger_a \times c^\dagger_b\right]_{JM,TM_T} = \tag{15.51}$$
$$\sum_{m_a, m_b} (j_a m_a, j_b m_b | JM) \sum_{\mu_a, \mu_b} \left(\frac{1}{2}\mu_a, \frac{1}{2}\mu_b | T M_T\right) \hat{c}^\dagger_{j_a m_a, \frac{1}{2}\mu_a} \hat{c}^\dagger_{j_b m_b, \frac{1}{2}\mu_b}.$$

For atomic situations one can replace J by L or J and T by L and S.

A properly antisymmeterized and normalized two-body state is (using operators)

$$|ab; JM\rangle \equiv \frac{1}{\sqrt{1+\delta_{ab}}} \hat{A}^\dagger_{JM}(ab)|0\rangle. \tag{15.52}$$

Because of symmetries of the Clebsch-Gordon coefficients,

$$|ba; JM\rangle = -(-1)^{j_a + j_b - J} |ab; JM\rangle \tag{15.53}$$

or, with isospin,

$$|ba; JM, TM_T\rangle = -(-1)^{j_a + j_b - J} (-1)^{1-T} |ab; J\,M, T\,M_T\rangle. \tag{15.54}$$

As with one-body operators, for the adjoints we have to deal with true spherical tensors, in other words, we must use

$$[\tilde{c}_a \times \tilde{c}_b]_{J\,M} \tag{15.55}$$

$$= (-1)^{J+M} [c_a \times c_b]_{J\,-M} = -(-1)^{J-M} \left(\left[c_a^\dagger \times c_b^\dagger \right]_{J\,-M} \right)^\dagger . \tag{15.56}$$

I leave it as an exercise for the reader to show (15.55) can be rewritten as (15.56).

Therefore a scalar constructed from annihilation and creation of fermion pairs must be proportional to

$$\begin{aligned} \left[\left[c_a^\dagger \times c_b^\dagger \right]_J \otimes [\tilde{c}_a \times \tilde{c}_b]_J \right]_{00} = \\ \sum_M (J\,M, J\,-M|0\,0) \left[c_a^\dagger \times c_b^\dagger \right]_{JM} [\tilde{c}_a \times \tilde{c}_b]_{J\,-M} = \\ -\frac{1}{\sqrt{2J+1}} \sum_M \hat{A}^\dagger_{JM}(ab) \hat{A}_{JM}(cd), \end{aligned} \tag{15.57}$$

where I've made the obvious definition

$$\hat{A}_{JM}(ab) \equiv -\left[c_a \times c_b \right]_{JM} = \left(\hat{A}^\dagger_{JM}(ab) \right)^\dagger \tag{15.58}$$

It is crucial to note, however, that despite the notation, the object $\hat{A}_{JM}(ab)$ transforms under rotations like an object with angular momentum $J, -M$.

We'll use (15.57), up to some constants, when we construct Hamiltonians in Chapter (17). We may also need non-scalar operators, which we now know how to define:

$$\left[\left[c_a^\dagger \times c_b^\dagger \right]_{J'} \otimes [\tilde{c}_c \times \tilde{c}_d]_J \right]_{KM} \tag{15.59}$$

$$= -\sum_{m'm} (-1)^{J+m} (J'\,m', J\,-m|KM) \hat{A}^\dagger_{J'\,m'}(ab) \hat{A}_{J\,m}(cd).$$

15.6 The Wigner-Eckart Theorem and reduced matrix elements

One of the most important results to come from the quantum theory of angular momentum is the Wigner-Eckart theorem. Suppose we take the matrix element of an operator between two states, all of which have definite angular momentum,

$$\langle J_f M_f | \hat{O}_{KM} | J_i M_i \rangle.$$

Now this matrix element will be zero unless (a) $M_f = M_i + M$ and (b) the triangle rule is satisfied, namely $|J_i - J_f| \leq K \leq J_i + J_f$. But beyond this, one can intuit the result should be in some sense independent of overall orientation;

if one rotates the coordinate frame the matrix element should change in a well-defined manner. This is of course an application of the Wigner matrices, and the final answer [may or may not do the derivation] is the Wigner-Eckart theorem, which says that the matrix element is proportional to a Clebsch-Gordan coefficient. Specifically, adopting the convention followed by Wigner, Racah, and also Edmonds,

$$\begin{aligned}\langle J_f M_f|\hat{O}_{KM}|J_i M_i\rangle &= [J_f]^{-1}(J_i M_i, KM|J_f M_f)(J_f||\hat{O}_K||J_i) \\ &= (-1)^{J_f - M_f}\begin{pmatrix} J_f & K & J_i \\ -M_f & M_K & M_i\end{pmatrix}(J_f||\hat{O}_K||J_i)\end{aligned} \tag{15.60}$$

where $(J_f||\hat{O}_K||J_i)$ is the *reduced matrix element*, which encapuslates the fundamental matrix element independent of orientation, and which we'll see below in 15.6.2 is related to a sum over *all* orientations. Eq. (15.60) can also be thought of as the definition of the reduced matrix element (and the Wigner-Eckart theorem a statement that this definition is consistent using any set of Ms). Note that it is possible to have a variant definition with different pre-factors, that is, the phase and factors like $\sqrt{2J_f+1}$ are conventions. Only the Clebsch-Gordan coefficients are dictated by the theorem. The choices of (15.60) are the most widely used one.

The Wigner-Eckart theorem applies not just to angular momentum but any SU(2) algebra; hence one can reduce in isospin as well, and a *doubly*-reduced matrix element follows naturally:

$$\begin{aligned}\langle J_f M_f; T_f M_{Tf}|\hat{O}_{KM;TM_T}|J_i M_i; T_i M_{Ti}\rangle = \\ \frac{(J_i M_i, KM|J_f M_f)}{[J_f]}\frac{(T_i M_{Ti}, TM_T|T_f M_{Tf})}{[T_f]}(J_f, T_F||\hat{O}_{K,T}||J_i, T_i).\end{aligned} \tag{15.61}$$

15.6.1 Worked example: density matrix in a single j-shell

To demonstrate in detail how to use angular momentum algebra, as well as fermion operator algebra, I will derive in detail the reduced density matrix between one-particle states in a single j-shell, that is,

$$\langle j||[\hat{a}_j^\dagger \times \tilde{a}_j]_K||j\rangle. \tag{15.62}$$

First we must unpack each piece of this expression. This is a reduced matrix element, defined by the Wigner-Eckart theorem (15.60):

$$\langle j||[\hat{a}_j^\dagger \times \tilde{a}_j]_K||j\rangle = \frac{[j]}{(j\,m_i, K\,M|j\,m_f)}\left\langle j\,m_f\left|[\hat{a}_j^\dagger \times \tilde{a}_j]_{K\,M}\right|j\,m_i\right\rangle, \tag{15.63}$$

where we must have $M = m_f - m_i$ to make sense of this. Furthermore, the single-particle states are just $|jm_i\rangle = \hat{a}^\dagger_{j\,m_i}|0\rangle$ and the same for $|jm_f\rangle$, while

$$[\hat{a}_j^\dagger \times \tilde{a}_j]_{K\,M} = \sum_{\mu_1\mu_2}(j\,\mu_1, j\,\mu_2|KM)\hat{a}^\dagger_{j\,\mu_1}\tilde{a}_{j\,\mu_2}. \tag{15.64}$$

In the next Chapter we will introduce and justify the notation

$$\tilde{a}_{j\,\mu_2} = (-1)^{j+\mu_2}\hat{a}_{j\,-\mu_2},$$

so that altogether we have

$$\sum_{\mu_1\mu_2} \frac{(-1)^{j+\mu_2}[j](j\,\mu_1, j\,\mu_2|KM)}{(j\,m_i, K\,M|j\,m_f)} \left\langle 0 \left| \hat{a}_{j\,m_i}\hat{a}^\dagger_{j\,\mu_1}\hat{a}_{j\,-\mu_2}\hat{a}^\dagger_{j\,m_i} \right| 0 \right\rangle. \tag{15.65}$$

The fermion algebra is straightforward, and one can show

$$\left\langle 0 \left| \hat{a}_{j\,m_i}\hat{a}^\dagger_{j\,\mu_1}\hat{a}_{j\,-\mu_2}\hat{a}^\dagger_{j\,m_i} \right| 0 \right\rangle = \delta_{m_i,\mu_1}\delta_{m_f,-\mu_2}$$

leaving us with

$$\frac{(-1)^{j-m_i}[j](j\,m_f, j\,-m_i|KM)}{(j\,m_i, K\,M|j\,m_f)}.$$

Finally we apply a symmetry relation (15.25) to

$$(j\,m_i, K\,M|j\,m_f) = (-1)^{j-m_i}\frac{[j]}{[K]}(j\,m_f, j\,-m_i|K\,M).$$

Often in these kind of derivations one has to pick a particular value of m_i, m_f in order to evaluation the Clebsch-Gordan coefficients, but for this simple case when we combine our terms they cancel, leaving us our final result:

$$\langle j||[\hat{a}^\dagger_j \times \tilde{a}_j]_K||j\rangle = \sqrt{2K+1} \tag{15.66}$$

15.6.2 Application: Strength functions

To see the utility of the Wigner-Eckart theorem, consider the strength function. Given some transition operator $\hat{O}_K$ carrying definite angular momentum K, the strength function between an initial and final state is just the square of the matrix element:

$$\left|\langle J_f M_f|\hat{O}_{KM}|J_i M_i\rangle\right|^2.$$

But in most experimental situations we cannot pick out specific values of $M_{i,f}$ (unless we are doing an experiment with polarization). The final result must then *average* over initial states and *sum* over final states, that is,

$$\frac{1}{2J_i+1}\sum_{M_i}\sum_{M_f}\left|\langle J_f M_f|\hat{O}_{KM}|J_i M_i\rangle\right|^2. \tag{15.67}$$

In most cases there is also implicitly a sum over M. (If not, the final result will be different.) Now we can use the Wigner-Eckhart theorem t to rewrite the average/sum as:

$$\frac{1}{2J_i+1}\sum_{M_f}\sum_{M_i}\sum_{M}|(J_i M_i, KM|J_f M_f)|^2\left|(J_f||\hat{O}_K||J_i)\right|^2. \tag{15.68}$$

Now we can use the the selection rule $M_f = M_i + M_f$ to eliminate the sum over M_f and the orthogonality of the Clebsch-Gordan coefficients to sum over M_i and M

$$\sum_{M_i} \sum_{M} |(J_i M_i, KM | J_f M_i + M_f)|^2 = 1 \tag{15.69}$$

Thus we get the result in terms of reduced matrix elements,

$$\begin{aligned} \frac{1}{(2J_i+1)} \sum_{M_i} \sum_{M_f} \sum_{M} \left| (J_f M_f | \hat{\mathcal{O}}_{KM} | J_i M_i) \right|^2 \\ = \frac{1}{(2J_i+1)} \left| (J_f || \hat{\mathcal{O}}_K || J_i) \right|^2, \end{aligned} \tag{15.70}$$

As one often calls

$$\frac{1}{2J_i+1} \left| (J_f || \hat{\mathcal{O}}_K || J_i) \right|^2, \tag{15.71}$$

the *reduced* or B-value, written $B(\mathcal{O})$ (for example, $B(GT)$ for Gamow-Teller, $B(E2)$ for electric quadrupole, etc.), this says the strength for an operator is $B(\mathcal{O})$. If we calculate directly not the reduced matrix element but a matrix element with specific values of $M_{i,f}$, the result is still straightforward:

$$\begin{aligned} \frac{1}{(2J_i+1)} \sum_{M_i} \sum_{M_f} \sum_{M} \left| (J_f M_f | \hat{\mathcal{O}}_{KM} | J_i M_i) \right|^2 = \\ \frac{2J_f+1}{(2J_i+1)} \left| \frac{\langle J_f M_f | \hat{\mathcal{O}}_{K M_f - M_i} | J_i M_i \rangle}{(J_i M_i, K M_f - M_i | J_f M_f)} \right|^2. \end{aligned} \tag{15.72}$$

Consider a special case that can arise when doing configuration-interaction calculations in the fixed M-scheme: let $J_i = 0$, then $J_f = K$ and $M_f = M$ (and usually $M = 0$); furthermore the Clebsch-Gordan $(00, KM|KM) = 1$. In that case the total strength is just

$$(2K+1) |\langle K0 | \hat{\mathcal{O}}_{K0} | 00 \rangle|^2$$

15.7 Recoupling angular momentum: 3-j symbols

What about combining more than two angular momenta? That is, combine three angular momenta J_1, J_2, J_3 into some total J_{123}? The most obvious way would be to first combine $J_1, J2$ into J_{12} and then add J_3 to get J_{123}. But why not instead combine J_2, J_3 into J_{23} instead? One could, and it turns out that these different choices are not orthogonal to each other; instead they give rise to the 'six-j symbols' defined as:

$$\left\{ \begin{array}{ccc} j_1 & j_2 & j_{12} \\ j_3 & J & j_{23} \end{array} \right\} = (-1)^{j_1+j_2+j_3+J} [j_{12}][j_{23}] \, \langle (j_1 j_2) j_{12}, j_3 : J | j_1 (j_2 j_3) j_{12} : J \rangle \tag{15.73}$$

The 6-j symbol has many household uses; an example is rearranging Clebsch-Gordan coefficients, for example:

$$\begin{aligned}(j_1\,m_1, j_2\,m_2|JM)\,(j_3\,m_3, j_4\,m_4|JM) = \\ \sum_K (-1)^{J+M}(-1)^{j_2-j_4+\mu}(2J+1)\left\{\begin{array}{ccc} j_1 & j_2 & J \\ j_4 & j_3 & K \end{array}\right\} \\ (j_1\,m_1, j_3\,-m_3|K\,\mu)\,(j_2\,m_2, j_4\,-m_4|K\,-\mu)\end{aligned} \tag{15.74}$$

By judicious application of symmetry relations, one can find similar rearrangement theorems, for example the related but subtly different

$$\begin{aligned}(j_1\,m_1, j_2\,m_2|J\,M)\,(j_3\,m_3, j_4\,m_4|J\,-M) = \\ \sum_K (-1)^{M}(-1)^{j_2+j_3+\mu}(2J+1)\left\{\begin{array}{ccc} j_1 & j_2 & J \\ j_4 & j_3 & K \end{array}\right\} \\ (j_1\,m_1, j_3\,m_3|K\,\mu)\,(j_2\,m_2, j_4\,m_4|K\,-\mu)\,.\end{aligned} \tag{15.75}$$

The 6-j symbols also have symmetry relations which are simpler than those of the 3-j symbols. They are invariant under *any* permutation of the columns:

$$\left\{\begin{array}{ccc} j_1 & j_2 & j_{12} \\ j_3 & J & j_{23} \end{array}\right\} = \left\{\begin{array}{ccc} j_1 & j_{12} & j_2 \\ j_3 & j_{23} & J \end{array}\right\} = \left\{\begin{array}{ccc} j_2 & j_{12} & j_1 \\ J & j_{23} & j_3 \end{array}\right\},$$

etc., and also one can "flip" any two columns:

$$= \left\{\begin{array}{ccc} j_3 & J & j_{12} \\ j_1 & j_2 & j_{23} \end{array}\right\} = \left\{\begin{array}{ccc} j_3 & j_2 & j_{23} \\ j_1 & J & j_{12} \end{array}\right\} = \left\{\begin{array}{ccc} j_1 & J & j_{23} \\ j_3 & j_2 & j_{12} \end{array}\right\}.$$

15.7.1 Example: density matrix in a single j-shell

We have developed enough of the machinery to work out a detailed illustration of its application. Consider the density matrix elements for two-body states in the same single-j space,

$$\langle (j)^2; J_f || [\hat{a}_j^\dagger \times \tilde{a}_j]_K || (j)^2; J_i \rangle. \tag{15.76}$$

Again we must unpack each piece of this expression. By the Wigner-Eckart theorem, this equals

$$\frac{[J_f]}{(J_i\,M_i, K\,M_K|J_f M_f)} \left\langle (j)^2; J_f\,M_f \left| [\hat{a}_j^\dagger \times \tilde{a}_j]_{K\,M_K} \right| (j)^2; J_i\,M_i \right\rangle.$$

An important, and not-so-obvious step, is to realize that the the action of the operator of rank K on the initial state of rank J_i is to create a new state of rank J', that is $J_i \otimes K = J'$, or

$$[\hat{a}_j^\dagger \times \tilde{a}_j]_{K\,M_K} \left|(j)^2; J_i\,M_i\right\rangle \to C \left|(j)^2; J'\,M'\right\rangle \tag{15.77}$$

which must follow the angular momentum selection rules, that is, $M' = M_i + M_K$ and $|J_i - K| \leq J' \leq J_i + K$. Of course the point of the exercise is to find the value of C. Towards this end, let's expand

$$[\hat{a}_j^\dagger \times \tilde{a}_j]_{K\,M_K} \left|(j)^2; J_i\, M)i\right\rangle = \tag{15.78}$$
$$\sum_{\mu\,\mu'} (j\,\mu, j\,\mu'|K\,M_K)\hat{a}_{j\,\mu}^\dagger (-1)^{j+\mu'}\hat{a}_{j\,-\mu'} \times$$
$$\frac{1}{\sqrt{2}}\sum_{m'\,m} (j\,m', j\,m|J_i\,M_i)\hat{a}_{j\,m'}^\dagger \hat{a}_{j\,m}^\dagger|0\rangle.$$

You'll see why I chose the ordering of μ, μ' and m, m' in a moment. The next step is to evaluate

$$\hat{a}_{j\,\mu}^\dagger \hat{a}_{j\,-\mu'}\hat{a}_{j\,m'}^\dagger \hat{a}_{j\,m}^\dagger|0\rangle$$
$$= \delta_{-\mu',m'}\hat{a}_{j\,\mu}^\dagger \hat{a}_{j\,m}^\dagger|0\rangle - \delta_{-\mu',m}\hat{a}_{j\,\mu}^\dagger \hat{a}_{j\,m'}^\dagger|0\rangle \tag{15.79}$$

which ought to be routine for you at this point. Applying the first term of (15.79) to (15.78) we get

$$\sum_{mm'\mu} (-1)^{j-m'}(j\,\mu, j\,-m'|KM_K)(j\,m', j\,m|J_i\,M_i)\frac{1}{\sqrt{2}}\hat{a}_{j\,\mu}^\dagger \hat{a}_{j\,m}^\dagger|0\rangle. \tag{15.80}$$

The second term gives something almost the same:

$$-\sum_{mm'\mu} (-1)^{j-m}(j\,\mu, j\,-m|KM_K)(j\,m', j\,m|J_i\,M_i)\frac{1}{\sqrt{2}}\hat{a}_{j\,\mu}^\dagger \hat{a}_{j\,m'}^\dagger|0\rangle.$$

Because they are dummy variables, we can swap $m \leftrightarrow m'$ and use $(j\,m, j\,m'|J_i\,M_i)$ $= (-1)^{j+j-J_i}(j\,m', j\,m|J_i\,M_i)$; because $2j$ is an odd integer and, as we found in Eq. (15.4), J_i must be even, we end up with *exactly* the same expression. Hence we have

$$2\sum_{mm'\mu} (-1)^{j-m'}(j\,\mu, j\,-m'|KM_K)(j\,m', j\,m|J_i\,M_i)\frac{1}{\sqrt{2}}\hat{a}_{j\,\mu}^\dagger \hat{a}_{j\,m}^\dagger|0\rangle.$$

Next we want to rearrange the Clebsch-Gordan coefficients as in (15.75), so that the fermion operators are coupled up to good angular momentum. (Don't fret if it is not immediately obvious to you which formula to use. Even skilled practioners can take two or three tries to get a derivation right, especially as the phases and factors of $\sqrt{2j+1}$ can be tricky.) As I stated above, we expect to create a state of angular momentum $J' = J_i \otimes K$ but also we must have $J' = j \otimes j$. This give us the hint for exactly how to rearrange the angular momentum coupling. To do so, we first apply symmetry relations to our Clebsch-Gordan coefficients so as to line up with Eq. (15.75):

$$(j\,\mu, j\,-m'|KM_K)(j\,m', j\,m|J_i\,M_i) =$$
$$(-1)^{m-\mu+K}\frac{[J_i][K]}{2j+1}(j\,-\mu, K\,M_K|j\,-m')(j\,-m, J_i\,M_i|jm').$$

Now we can apply the reordering formula (15.75):

$$2[J_i][K][J_f](-1)^K \left\{ \begin{array}{ccc} j & K & j \\ J_i & j & J_f \end{array} \right\}. \tag{15.81}$$

15.7.2 More recoupling: 9-j symbols

Another recoupling is through the 9-j symbol. Suppose you have four angular momenta, j_a, j_b, j_c, j_d, with j_a and j_b coupled up to J_{ab} and j_c, j_d coupled up to J_{cd}, and finally J_{ab} and J_{cd} coupled up to some total J. (Exercise: write this out in Clebsch-Gordan coefficients; you will have to assume some $m_a, \ldots$.) We can rearrange the couplings using the 9-j symbol:

$$|(j_a, j_b)J_{ab}, (j_c, j_d)J_{cd} : J\rangle = \sum_{J_{ac}, J_{bd}} [J_{ab}][J_{cd}][J_{ac}][J_{bd}] \left\{ \begin{array}{ccc} j_a & j_c & J_{ac} \\ j_b & j_d & J_{bd} \\ J_{ab} & J_{cd} & J \end{array} \right\} \tag{15.82}$$

(Remember the convention $[x] = \sqrt{2x+1}$.) The 9-j symbol is real-valued and invariant without phases under permutation of rows or columns, as well as under transposition. A particularly simple but useful simplification is when $J = 0$

$$\left\{ \begin{array}{ccc} j_a & j_c & K \\ j_b & j_d & K \\ K' & K' & 0 \end{array} \right\} = \frac{(-1)^{j_c + j_b + K + K'}}{[K][K']} \left\{ \begin{array}{ccc} j_a & j_c & K \\ j_d & j_b & K' \end{array} \right\} \tag{15.83}$$

Recoupling is an important topic, but nowadays finding the n-body generalization of Clebsch-Gordan coefficients–which historically are called *coefficients of fractional parentage* or CFPs–are not. The reason is, for most practical purposes, the CFPs can only be computed numerically, either explicitly or implicitly.

15.7.3 Worked example: going from jj-coupled to LS coupled and vice versa

The 9-j symbol from section 15.7.2 can be useful in rewriting commonly encountered matrix elements. Let's consider scalar two-body matrix elements of single-particle states $\langle a, b : J|\hat{H}c, d : J\rangle$. What this means is we have two single-particle states a, b coupled up to total angular momentum J, and states c, d also coupled up to the same total J, as by scalar we mean an operator carrying no angular momentum so J (and also M) cannot change. I will take these up in more detail in Chapter 17, where we'll see these are independent of M. Furthermore, let the single-particle states all have orbital angular momentum l, which may differ from state to state, and intrinsic spin $s = 1/2$ which is fixed, and total angular momentum j which also may differ from state to state. To express this in detail, we write this as

$$\langle (l_a, 1/2)j_a, (l_b, 1/2)j_b : J|\, \hat{H}\, |(l_c, 1/2)j_b, (l_d, 1/2)j_d : J\rangle\,.$$

There should be some indices telling us about the radial wave functions for the single particle states a, b, c, d, but I am suppressing those for now.

Applying (15.82) to both sides:

$$\begin{aligned}\langle (l_a, 1/2)j_a, (l_b, 1/2)j_b : J| \hat{H} |(l_c, 1/2)j_b, (l_d, 1/2)j_d : J\rangle = \\ \sum_{L_{ab}, S_{ab}, L_{cd}, S_{cd}} [j_a][j_b][L_{ab}][S_{ab}] \left\{ \begin{array}{ccc} l_a & 1/2 & j_a \\ l_b & 1/2 & j_b \\ L_{ab} & S_{ab} & J \end{array} \right\} \\ [j_c]\,[j_d][L_{cd}][S_{cd}] \left\{ \begin{array}{ccc} l_c & 1/2 & j_c \\ l_d & 1/2 & j_d \\ L_{cd} & S_{cd} & J \end{array} \right\} \\ \langle (l_a, l_b)L_{ab}, (1/2, 1/2)S_{ab} : J| \hat{H} |(l_c, l_d)L_{cd}, (1/2, 1/2)S_{cd} : J\rangle \end{aligned} \tag{15.84}$$

15.8 Tensor products and composite states and operators

Frequently we work with tensor composition of two (or more) objects. What do I mean by this? Consider a single-particle state with good angular momentum j which is composed from orbit angular momentum l and spin s. Another example is a two-particle state, each state having good angular momentum and then combined into some total angular momentum. We write these symbolically as $l \otimes s = j$ and $j_1 \otimes j_2 = J_{12}$ respectively, with the $\otimes$ signalling tensor composition using Clebsch-Gordan coefficients.

Operators, too, can be tensor composites, not only with fundamental creation and annihilation operators, but on what part of the wavefunction the components of an operator act on. For example, Pauli matrices $\vec{\sigma}$ only act on the spin part of a single-particle wavefunction, while a gradient $\vec{\nabla}$ would act only on the coordinate-space part; or one might have an composite operator $\hat{\mathcal{O}}_1 \otimes \hat{\mathcal{O}}_2$, where $\hat{\mathcal{O}}_1$ acts only on coordinates of particle 1 and $\hat{\mathcal{O}}_2$ acts only on the coordinates of particle 2.

In this section I will briefly give the expressions needed for handling such composite systems. I will not derive them. For derivations and more detailed discussion, see Edmonds Chapter 7.

We consider generic two-component states we write as $|j_1\, j_2; J)$, where we have coupled $j_1 \otimes j_2 = J$. We suppress M as we will either use reduced matrix elements or, in the case of matrix elements of scalar operators (those that do not change angular momentum), we will have results independent of M. For single-particle states j_1 and j_2 may represent l and s; for two-particle states they may be the js for each state, although as seen above one could recouple to L and S of the two-particle state. There are likely other quantum numbers we are ignoring for now.

Let $\hat{T}_{k_1}(1)$ be an operator of angular momentum rank k_1, operating only on component 1 of the states, and $\hat{U}_{k_2}(2)$ act only on component 2. If they are coupled up to some total angular momentum K, then the reduced matrix

element is

$$\left\langle j_1' \, j_2'; J' \left|\left| \left[\hat{T}_{k_1}(1) \otimes \hat{U}_{k_2}(2)\right]_K \right|\right| j_1 \, j_2; J \right\rangle \tag{15.85}$$
$$= [J'][K][J] \left\{ \begin{array}{ccc} j_1' & j_1 & k_1 \\ j_2' & j_2 & k_2 \\ J' & J & K \end{array} \right\} \langle j_1' || \hat{T}_{k_1} || j_1 \rangle \langle j_2' || \hat{U}_{k_2} || j_2 \rangle$$

This simplies the work of finding the composite matrix element to finding the individual matrix elements of the components.

This can be simplified by setting one of the operator angular momenta (K, k_1, or k_2) to zero, which by (15.94) given at the end of this chapter, reduces the 9-j to a 6-j.

If we take $K = 0$ (which requires $k_1 = k_2 = k$ and $J' = J$

$$\left\langle j_1' \, j_2'; J \left|\left| \left[\hat{T}_k(1) \otimes \hat{U}_k(2)\right]_0 \right|\right| j_1 \, j_2; J \right\rangle \tag{15.86}$$
$$= (-1)^{j_2'+j_1+J+K} \frac{[J]}{[k]} \left\{ \begin{array}{ccc} j_1' & j_2' & J \\ j_2 & j_1 & K \end{array} \right\} \langle j_1' || \hat{T}_k || j_1 \rangle \langle j_2' || \hat{U}_k || j_2 \rangle.$$

But we can reinterpret $K = 0$ as a dot product between the two operators

If either $\hat{T}$ or $\hat{U}$ is the identity, we only need the matrix element for the first or second components, respectively:

$$\left\langle j_1' \, j_2'; J' \left|\left| \hat{T}_k(1) \right|\right| j_1 \, j_2; J \right\rangle = \tag{15.87}$$
$$\delta_{j_2' j_2} (-1)^{j_1'+j_2+J+k} [J'][J] \left\{ \begin{array}{ccc} j_1' & J' & j_2 \\ J & j_1 & k \end{array} \right\} \langle j_1' || \hat{T}_k || j_1 \rangle$$

and

$$\left\langle j_1' \, j_2'; J' \left|\left| \hat{U}_k(2) \right|\right| j_1 \, j_2; J \right\rangle = \tag{15.88}$$
$$\delta_{j_1' j_1} (-1)^{j_1+j_2+J'+k} [J'][J] \left\{ \begin{array}{ccc} j_2' & J' & j_1 \\ J & j_2 & k \end{array} \right\} \langle j_2' || \hat{U}_k || j_2 \rangle$$

15.8.1 Worked example: matrix elements in spin-orbit coupled states

15.8.2 Worked example: two-body matrix elements of S^2

Here I will work out in detail another example, calculation of the two-body matrix elements of total spin S^2 between jj-coupled states:

$$\left\langle (l_1', 1/2) \, j_1', (l_2', 1/2) \, j_2'; J' | \vec{S}_1 \cdot \vec{S}_2 | \, (l_1, 1/2) \, j_1, (l_2, 1/2) \, j_2; J \right\rangle \tag{15.89}$$

15.9 Frequently used expressions

Calculations require numbers. There exist of course routines and libraries for computing the values of Clebsch-Gordan coefficients and 3-j, 6-j, and 9-j symbols, as well as old-fashioned printed-on-paper tables of values, it is convenient

to have some values right at hand. In this section I give some simple expressions for the most commonly used values. You can find expanded tables in Edmonds and Varshalovich et al. These can be expanded by using symmetry relations.

Clebsch-Gordan coefficients. By selection rules, $m + 0 = m$ and $j + 0 = j$, hence one gets trivially

$$(j\,m, 0\,0|j\,m) = 1. \tag{15.90}$$

By applying symmetry relations, it is easy to show

$$(j\,m, j\;-m|0\,0) = \frac{(-1)^{j-m}}{[j]}. \tag{15.91}$$

3-j symbols.

$$\begin{pmatrix} j & j & k \\ j & -j & 0 \end{pmatrix} = \frac{(2j)!}{\sqrt{(2j+k+1)(2j+k)!(2j-k)!}}. \tag{15.92}$$

6-j symbols.

$$\begin{Bmatrix} j_1 & j_2 & J \\ j_2 & j_1 & 0 \end{Bmatrix} = \frac{(-1)^{j_1+j_2+J}}{[j_1][j_2]}. \tag{15.93}$$

9-j symbols.

$$\begin{Bmatrix} j_a & j_b & J \\ j_c & j_d & J \\ K & K & 0 \end{Bmatrix} = \frac{(-1)^{j_b+j_c+J+K}}{[J][K]} \begin{Bmatrix} j_a & j_b & J \\ j_d & j_c & K \end{Bmatrix} \tag{15.94}$$

15.10 Summary

What you should get from this chapter:

• A review of the basic rules for representing and adding angular momenta in quantum systems.

• The introduction, via the Wigner-Eckart theorem, of *reduced matrix elements*, which are "orientation-independent" and thus fundamental to most physics calculations. (Note: one can extend the Wigner-Eckart theorem to other groups, but that is beyond our scope.)

• Some examples of carrying out calculations with quantum angular momenta.

15.11 Exercises

(16.1) Consider two angular momenta, $J_1 = 1$ and $J_2 = 5/2$. Write out explicitly all the possible uncoupled and coupled basis states, and demonstrate they have the same dimension.

(16.2) Expand the uncoupled basis state $|J_1 M_1, J_2 M_2\rangle = \left|2\ 1, \frac{5}{2}\ \frac{1}{2}\right\rangle$ in terms of the coupled basis; just write the Clebsch-Gordans as symbols, not worrying about the values.

(16.3) Expand the coupled basis state $|(J_1 J_2) J_{12} M_{12}\rangle = |(2,3)4-2\rangle$ in the uncoupled basis. Do not worry about the numerical values of the Clebsch-Gordan coefficients.

(16.4) If j has a half-integer value, use symmetry relations to prove that the Clebsch-Gordan coefficient $(jm, jm|J\,2m)$ is nonzero only for J even. Can you say anything if j has integer value?

(16.5) Generalizing the results of section 15.4, show that

$$|ab; JM\rangle = \frac{1}{\sqrt{1+\delta_{ab}}} \left[\hat{a}_a^\dagger \otimes \hat{a}_b^\dagger\right]_{J\,M} |0\rangle$$

is properly normalized.

(16.6) Show that

$$\left(\left[\hat{a}_a^\dagger \times \tilde{a}_b\right]_{K\,M}\right)^\dagger = (-1)^{M+j_a-j_b} \left[\hat{a}_b^\dagger \times \tilde{a}_a\right]_{K\,-M}.$$

(16.7) Show that

$$\langle J_f || \left[\hat{a}_a^\dagger \times \tilde{a}_b\right]_K || J_i\rangle = (-1)^{J_f - J_i + j_a - j_b} \left\langle J_i \left|\left| \left[\hat{a}_b^\dagger \times \tilde{a}_a\right]_K \right|\right| J_f \right\rangle^*.$$

(16.8) In analogy to (15.19), write the isospin singlet ($T = 0$) and triplet ($T = 1$) states in terms of proton-neutron basis states, that is, $|pp\rangle, |pn\rangle, |np\rangle$, and $|nn\rangle$.

(16.9) Show that under certain circumstances the Clebsch-Gordan coefficient $(l_1\,0, l_2\,0|L\,0) = 0$ even if the triangle rule is satisfied. This is called an 'accidental' zero (because it is unrelated to angular momentum selection rules).

Chapter 16

Matrix elements of one-body operators

> The art of doing mathematics consists in finding that special case which contains all the germs of generality.–*David Hilbert*

Physicists are not interested in just eigenstates. A clue why is the fact that eigenstates are sometimes called stationary states. But much of physics is devoted to *change*, and indeed in Chapter 1 we saw how one can built a generally evolving (changing) wavefunction out of 'stationary' eigenstates.

One of the most fundamental 'changes' are discrete transitions between eigenstates, for example through emission or absorption of a photon. In advanced quantum mechanics courses one computes the transition rate assuming a weak, oscillatory external field and using time-dependent perturbation theory: the result is the famous Fermi's Golden Rule (originally derived by Dirac):

$$T_{i\to f} = \frac{2\pi}{\hbar}\left|\left\langle \Psi_f \left| \hat{\mathcal{O}}_{\rm trans} \right| \Psi_i \right\rangle\right|^2 \frac{dN}{dE}. \tag{16.1}$$

Here dN/dE is the density of final states, also called the phase-space factor, but as plenty of books discuss this in detail I won't consider it further here.

The piece that concerns us is the matrix element $\left\langle \Psi_f \left| \hat{\mathcal{O}}_{\rm trans} \right| \Psi_i \right\rangle$, where $\hat{\mathcal{O}}_{\rm trans}$ is the external perturbing field that drives the transition, for example an electric dipole or quadrupole field. In most cases it is a one-body operator, in which case we can represent it using creation and annihilation operators:

$$\hat{\mathcal{O}} = \sum_{ab} \langle a|\hat{\mathcal{O}}|b\rangle \hat{a}_a^\dagger \hat{a}_b \tag{16.2}$$

where lowercase Latin letters *a,b* represent single-particle orbits. In order to compute the transition rate, we then insert this:

$$\left\langle \Psi_f \left| \hat{\mathcal{O}} \right| \Psi_i \right\rangle = \sum_{ab} \langle a|\hat{\mathcal{O}}|b\rangle \left\langle \Psi_f \left| \hat{a}_a^\dagger \hat{a}_b \right| \Psi_i \right\rangle, \tag{16.3}$$

where we call $\left\langle f \left| \hat{a}_a^\dagger \hat{a}_b \right| i \right\rangle$ the one-body *density matrix*. Note that the density matrix is independent of the transition operator but depends on the initial and final eigenstates.

In we consider angular momentum algebra (see Appendix 1), we can go further. As argued there, we often find convenient reduced matrix elements which are independent of orientation. Therefore it is also convenient to introduce coupled density matrix elements,

$$\rho_K^{(fi)}(a,b) \equiv \left\langle \Psi_f \left| \left| \left[\hat{a}_a^\dagger \times \tilde{a}_b \right]_K \right| \right| \Psi_i \right\rangle \frac{1}{\sqrt{2K+1}} \tag{16.4}$$

which have the convenient property that

$$\left\langle \Psi_f \left| \left| \hat{\mathcal{O}}_K \right| \right| \Psi_i \right\rangle = \sum_{ab} \rho_K^{(fi)}(a,b) \langle a||\hat{\mathcal{O}}||b\rangle. \tag{16.5}$$

In practice, the matrix elements $\langle a||\hat{\mathcal{O}}||b\rangle$ are straightforward to calculate, and in Appendix C I'll discuss how. The density matrix elements generally must come from a many-body code. Be sure to pay attention to exactly how the density matrices are defined, however, as conventions frequently differ. With the above definition, a useful symmetry relation is

$$\rho_K^{if}(b,a) = (-1)^{j_a - j_b + J_i - J_f} \rho_K^{fi}(a,b). \tag{16.6}$$

A good exercise is to prove this.

In Chapter 15 I introduced briefly the quantum theory of angular momentum, which was then applied to general one- and two-body operators in Chapter 17. This Chapter is devoted to computing matrix elements of specific one- and two-body operators. The use of angular momentum algebra in computing matrix elements is a skill best learned by following detailed examples while thumbing though a well-worn reference; my favorite is Edmond's *Angular momentum in quantum mechanics*.

As we get into specifics, we have to of course define our states. If there is no spin involved, then a single-particle state is of the form

$$\phi_{nlm} = R_{nl}(r) Y_{lm}(\theta, \phi) \tag{16.7}$$

while with spin, as one usually has with nuclear matrix elements, we couple

$$\phi_{n(l)jm} = R_{n(l)j}(r) \left[Y_l(\theta,\phi) \otimes \chi_{1/2} \right]_{jm} \tag{16.8}$$

where χ is a *spinor* with spin $\frac{1}{2}$ and

$$\left[Y_l(\theta,\phi) \otimes \chi_{1/2} \right]_{jm} = \sum_{m_l m_s} \left(l m_l, \tfrac{1}{2} m_s | jm \right) Y_{lm}(\theta,\phi) \chi_{1/2,m_s}. \tag{16.9}$$

Actually, the ordering of the coupling between orbital angular momentum and spin is important, and I assume $j = l \otimes 1/2$ rather than $1/2 \otimes l$. (One can check this by computing quadrupole transitions: in realistic nuclear systems, there is usually a strong low-lying E2 transition.) In the above, n labels different wavefunctions for the same value of l (and j), and often either counts the number of nodes in the radial wavefunction or is the principal quantum number. The radial wavefunctions often depend not only upon the orbital angular momentum l but also upon the total angular momentum j.

For some cases I will assume harmonic oscillator wavefunctions, but I will also give more expressions for more general radial wavefunctions which can be integrated numerically.

Because we will always be dealing with either angular momentum scalars (operators invariant under rotation) or spherical tensors (operators that transform as a spherical tensor; scalars are spherical tensors of rank 0), we compute matrix elements not between specific single-particle *states*, which are labeled by both j and m, but between single-particle *orbits*, labeled only by j (so that a single-particle state is a specific instance of a single-particle orbit, and an orbit is a set of $2j + 1$ states with $m = -j, -j + 1, \ldots, +j$). In the case of general operators, this means computing a reduced matrix element, as defined by the Wigner-Eckart theorem, from which all dependence upon m has been eliminated. Matrix elements of scalar operators, such as Hamiltonians, already have no dependence upon m.

I remind the reader I use the box convention

$$[x] = \sqrt{2x + 1}. \tag{16.10}$$

Some authors use $[x] = 2x + 1$, which other eschew it altogether.

16.1 Examples of one-body matrix elements

Consider a one-body operator that is a spherical tensor of rank K:

$$\hat{F}_{KM} = \sum_{ab} F_{ab} [K]^{-1} [\hat{c}^\dagger_a \otimes \hat{\tilde{c}}_b]_{KM}. \tag{16.11}$$

Here the time-reversed annihilation operator is $\tilde{c}_{j,m} = (-1)^{j+m} c_{j,-m}$, and F_{ab} is the reduced matrix element, $\langle a||F||b\rangle$, from the Wigner-Eckart theorem. If we have isospin, then we have

$$\hat{F}_{KM,TM_T} = \sum_{ab} F_{ab} [K]^{-1} [T]^{-1} [\hat{c}^\dagger_a \otimes \hat{\tilde{c}}_b]_{KM,TM_T}, \tag{16.12}$$

where now $F_{ab} = \langle a|||F|||b\rangle$ is *doubly-reduced*, i.e., with the Wigner-Eckart theorem applied twice.

It is straightforward to show

$$\left(\left[c^\dagger_a \otimes \tilde{c}_b \right]_{KM} \right)^\dagger = (-1)^{j_a - j_b + M} [c^\dagger_b \otimes \tilde{c}_a]_{K,-M}. \tag{16.13}$$

Including isospin,

$$\left(\left[c_a^\dagger \otimes \tilde{c}_b\right]_{KM,TM_T}\right)^\dagger = (-1)^{j_a-j_b+M+M_T}[c_b^\dagger \otimes \tilde{c}_a]_{K,-M,T-M_T}. \tag{16.14}$$

From this we can deduce the symmeteries the reduced matrix elements of these 'one-body' operators must have. Combining (15.43) and (16.13) ,

$$F_{ab} = (-1)^{j_a-j_b}F_{ba}^*. \tag{16.15}$$

Below we will see this holds in specific calculations.

16.1.1 Angular momentum

The operator $\vec{J}$, which has $K = 1$ (because it has three components) is not generally a transition operator, but it allows us to practice deriving matrix elements, in this case $\langle a||\vec{J}||b\rangle$. Because we almost always work with single-particle states which are eigenstates of J^2, the matrix elements must be diagonal with $a = b$. We apply the Wigner-Eckart theorem and choose $m_a = m_b = j_a$, sometimes called the *stretched state*, because we know trivially that $\langle j_a, m_a = j_a|\hat{J}_z|j_a, j_a\rangle = j_a$. Then (cf. Edmonds 5.4.1)

$$\langle a||\vec{J}||b\rangle = \delta_{ab}(-1)^{j_a-j_a}\begin{pmatrix} j_a & 1 & j_a \\ -j_a & 0 & j_a \end{pmatrix}^{-1}\langle j_a, m_a = j_a|\hat{J}_z|j_a, j_a\rangle. \tag{16.16}$$

Looking up the $3j$ symbol (for example, footnote 12 on page 77 of Edmonds),

$$\begin{pmatrix} j & 1 & j \\ -j & 0 & j \end{pmatrix} = \sqrt{\frac{j}{(j+1)(2j+1)}}, \tag{16.17}$$

we combine to get

$$\langle a||\vec{J}||b\rangle = \delta_{ab}\sqrt{j(j+1)(2j+1)}. \tag{16.18}$$

We'll have occasion to use this in the next chapter.

16.1.2 Spin

Next simplest is the spin operator. This is simple enough we can directly calculate the results of the Wigner-Eckart theorem. The spin operator for a single particle is $\vec{S} = \frac{1}{2}\vec{\sigma}$, where $\vec{\sigma}$ is the vector of Pauli matrices. In order to apply the Wigner-Eckhart theorem, we only need one explicit matrix element, traditionally one that is easy to compute. In this case the matrix element might look like

$$\left\langle \tfrac{1}{2}, m_s + M\left|S_{KM}\right|\tfrac{1}{2}, m_s\right\rangle, \tag{16.19}$$

which is the matrix element of the spin operator between two spinors. A spinor is a two-component vector, and we call $|\chi_\uparrow\rangle = |\frac{1}{2}, +\frac{1}{2}\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ a *spin-up* spinor and $|\chi_\downarrow\rangle = |\frac{1}{2}, -\frac{1}{2}\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ a *spin-down* spinor.

Before going further it is worth elucidating more on the operator $\vec{S}$; in particular, while we know it in Cartesian coordinates, S_x, S_y, S_z, we actually need it in spherical coordinates, $S_M, M = -1, 0, +1$. The simplest way to figure out the relationship is by example by the simplest rank-one spherical tensor: the spherical harmonic $Y_{1m}(\theta, \phi)$, or, more usefully, rY_{1m}. In fact this is easy to work out:

$$\begin{aligned} rY_{1,+1}(\theta,\phi) &= -\sqrt{\frac{3}{8\pi}}\sin\theta e^{+i\phi} = -\sqrt{\frac{3}{8\pi}}(x+iy), \\ rY_{1,0}(\theta,\phi) &= -\sqrt{\frac{3}{4\pi}}\cos\theta = \sqrt{\frac{3}{4\pi}}z, \\ rY_{1,-1}(\theta,\phi) &= \sqrt{\frac{3}{8\pi}}\sin\theta e^{-i\phi} = \sqrt{\frac{3}{8\pi}}(x-iy), \end{aligned} \tag{16.20}$$

Working by analogy, and discarding most of the prefactors, we obtain

$$\begin{aligned} S_{1,+1} = \frac{1}{2}\sigma_{1,+1} = -\frac{1}{\sqrt{2}}(\sigma_x + i\sigma_y) &= \frac{1}{2\sqrt{2}}\begin{pmatrix} 0 & -1 \\ 0 & 0 \end{pmatrix}, \\ S_{1,0} = \frac{1}{2}\sigma_z &= \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \\ S_{1,-1} = \frac{1}{2}\sigma_{1,-1}\frac{1}{2\sqrt{2}}(\sigma_x - i\sigma_y) &= \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}. \end{aligned} \tag{16.21}$$

We sometimes call

$$\sigma_+ = \begin{pmatrix} 0 & -1 \\ 0 & 0 \end{pmatrix}$$

the *spin-raising* operator, because $\sigma_+|\chi_\downarrow\rangle = -|\chi_\uparrow\rangle$ and

$$\sigma_- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

the *spin-lowering* operator. Notice the subtle but important difference between $S_{1,\pm1}$, $\sigma_{1,\pm1}$ and $\sigma_\pm = 2^{-1/2}\sigma_{1,\pm1}$.

While the sign on σ_+ may appear superfluous or even wrong, if one flips a down spin up and then down again, that is, $\sigma_-\sigma_+|\chi_\downarrow\rangle = -|\chi_\downarrow\rangle$; this arises because rotation of any fermion with half-integer spin through 2π induces an overall phase of -1. This also occurs with the time-reverse operation: $\tilde{c}_{jm} = (-1)^{j+m}c_{j,-m}$ but $\tilde{c}_{j,-m} = (-1)^{j-m}c_{j,m}$ so that $\tilde{\tilde{c}}_{jm} = -c_{jm}$.

Even the factors of $1/2\sqrt{2}$ are important. For example, the Gamow-Teller operator for β-decay is actually written in terms of the isospin raising/lowering operator, that is, $\vec{\sigma}\tau_\pm$ (where $\vec{\tau}$ is the vector of Pauli matrices, but in isospin space), but one usually computes it in terms of the spherical tensor, $\vec{\sigma}\tau_{1,\pm}$; the relation ship is clearly

$$\tau_\pm = \frac{1}{\sqrt{2}}\tau_{1,\pm1}. \tag{16.22}$$

Such details are important in getting β-decay and other matrix elements correct!

With that digression over, we can now compute the matrix element we need. In deriving a reduced matrix element from first principles, one usually opts for the easiest calculation: in this case we compute

$$\langle\chi_\uparrow|S_z|\chi_\uparrow\rangle = (1,0)\frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{1}{2}. \tag{16.23}$$

To get the reduced matrix element, we take

$$\left\langle \tfrac{1}{2}||S||\tfrac{1}{2}\right\rangle = \left\langle \tfrac{1}{2},+\tfrac{1}{2}\right| S_{1,0} \left|\tfrac{1}{2},+\tfrac{1}{2}\right\rangle \frac{(-1)^{\frac{1}{2}-\frac{1}{2}}[1]}{\left(\frac{1}{2}\,\frac{1}{2},\,\frac{1}{2}\,-\,\frac{1}{2}|10\right)} \tag{16.24}$$

and looking up the Clebsch-Gordan coefficient, $\left(\frac{1}{2}\,\frac{1}{2},\,\frac{1}{2}\,-\,\frac{1}{2}|10\right) = 1/\sqrt{2}$, we arrive at the final result

$$\left\langle \tfrac{1}{2}||S||\tfrac{1}{2}\right\rangle = \sqrt{\frac{3}{2}}. \tag{16.25}$$

(Note: actually, the spin operator $\vec{S}$ carries with it an $\hbar$ to provide to units, but I have left that off.)

Almost as useful–and as necessary–is the lack of an operator:

$$\left\langle \tfrac{1}{2}||1||\tfrac{1}{2}\right\rangle = \sqrt{2}. \tag{16.26}$$

For other basic reduced matrix elements, I will just provide the results and leave the derivation to the reader as an exercise. Some follow automatically; for example, $\langle\frac{1}{2}||\sigma||\frac{1}{2}\rangle = \sqrt{6}$.

Now let me take the case $F_{KM} = \vec{\sigma} = 2\vec{S}$, which has rank $K = 1$. This acts only on the spin part, not the space part, so we used Edmonds (7.1.8) and, for the spin matrix element, Edmonds (5.4.4), so the reduced matrix element between two nucleon states is

$$\langle n'(l',1/2)j'||\sigma||n(l,1/2)j\rangle = \\ \delta_{n,n'}\delta_{l,l'}(-1)^{l+1/2+j'+1}[j][j']\sqrt{6}\begin{Bmatrix} 1/2 & j' & l \\ j & 1/2 & 1 \end{Bmatrix} \tag{16.27}$$

Because we must have $l = l'$, under exchange $j \leftrightarrow j'$, we get the time reversed relations

$$\langle n'(l',1/2)j'||\sigma||n(l,1/2)j\rangle = (-1)^{j-j'}\,\langle n(l,1/2)j||\sigma||n'(l',1/2)j'\rangle \tag{16.28}$$

the same as for many other operators. Here the notation $(l,\frac{1}{2})j$ means $[l\otimes\frac{1}{2}] = j$.

Some sample matrix elements Here, as throughout, I use spectroscopic notation, so that $s \to l = 0$, $p \to l = 1$, etc.; and, for example, $p_{1/2}$ means $[Y_1 \times \chi_{1/2}]_{j=1/2}$:

$$\langle s_{1/2}||\sigma||s_{1/2}\rangle = \sqrt{6}; \quad \langle p_{1/2}||\sigma||p_{1/2}\rangle = -\sqrt{\frac{2}{3}};$$
$$\langle p_{1/2}||\sigma||p_{3/2}\rangle = \frac{4}{\sqrt{3}}; \quad \langle p_{3/2}||\sigma||p_{1/2}\rangle = -\frac{4}{\sqrt{3}}.$$

The results independent of the radial quantum number n; furthermore n for both intial and final states must be the same.

16.1.3 Isospin

Isospin is even easier, although one has to pay attention to whether one wants the isospin operator $\vec{T}$, the Pauli isospin operator $\tau_{1,m}$, or the isospin raising/lowering operator $\tau_\pm$. Because $\langle \frac{1}{2}||\tau||\frac{1}{2}\rangle = \sqrt{6}$, the double-reduced marix element is

$$\langle n'(l',1/2)j'|||\sigma\tau|||n(l,1/2)j\rangle = \\ \delta_{n,n'}\delta_{l,l'}(-1)^{l+1/2+j'+1}[j][j']6 \left\{ \begin{array}{ccc} 1/2 & j' & l \\ j & 1/2 & 1 \end{array} \right\} \tag{16.29}$$

with example matrix elements

$$\langle s_{1/2}|||\sigma\tau|||s_{1/2}\rangle = 6; \quad \langle p_{1/2}|||\sigma\tau|||p_{1/2}\rangle = -2; \\ \langle p_{1/2}|||\sigma\tau|||p_{3/2}\rangle = 4\sqrt{2}; \quad \langle p_{3/2}|||\sigma\tau|||p_{1/2}\rangle = -4\sqrt{2}.$$

Once again, however, if one is applying the actual Gamow-Teller operator, with isospin lowering / raising, or charge-changing operator, then this must be, as discussed above, divided by an addition factor of $\sqrt{2}$.

$$\langle s_{1/2}|||\sigma\tau_\pm|||s_{1/2}\rangle = \sqrt{\frac{3}{2}}; \quad \langle p_{1/2}|||\sigma\tau_\pm|||p_{1/2}\rangle = -\sqrt{2}; \\ \langle p_{1/2}|||\sigma\tau_\pm|||p_{3/2}\rangle = 4; \quad \langle p_{3/2}|||\sigma\tau_\pm|||p_{1/2}\rangle = -4.$$

It's always good to have alternate ways to confirm calculations; in the case of $\sigma\tau_\pm$, the Ikeda sum rule is extremely useful.

If one has a doubly-reduced matrix element, and there is no isospin operator, then keep in mind that $\langle \frac{1}{2}||1||\frac{1}{2}\rangle = \sqrt{2}$, which is necessary to keep all factors correct. For example, the doubly-reduced matrix element $\langle s_{1/2}|||\sigma||s_{1/2}\rangle = 2\sqrt{3}$. As other examples, the doubly-reduced matrix element of $\vec{J}$ is $(a|||\vec{J}|||a) = \sqrt{2j_a(j_a+1)(2j_a+1)}$, while the doubly-reduced matrix element of $\vec{T}$ is $(a|||\vec{T}|||a) = \sqrt{\frac{3}{2}(2j_a+1)}$

16.1.4 Multipole

Multipole operators are operators of the form $F_{KM}(\vec{r}) = f_K(r)Y_{KM}(\theta,\phi)$, though often one wants specifically $r^K Y_{KM}(\theta,\phi)$. We can actually get two equivalent expressions.

First expression: Because this operator acts only on the space part and not the spin part of the wavefunction, we use Edmonds (7.1.7) to get

$$\langle n'(l',1/2)j'||f_K(r)Y_K||n(l,1/2)j\rangle = \\ (-1)^{l'+1/2+j+K}[j][j'] \left\{ \begin{array}{ccc} l' & j' & 1/2 \\ j & l & K \end{array} \right\} \langle n'l'||f_K(r)Y_K||nl\rangle \,. \tag{16.30}$$

The radial and angular integral factorize, and using Edmonds (5.4.5) the matrix element is then

$$= (-1)^{1/2+j+K} \frac{[j][j'][l'][l][K]}{\sqrt{4\pi}} \tag{16.31}$$
$$\left\{ \begin{array}{ccc} l' & j' & 1/2 \\ j & l & K \end{array} \right\} \left(\begin{array}{ccc} l' & K & l \\ 0 & 0 & 0 \end{array} \right) \langle n'l'|f_K(r)|nl\rangle \,.$$

Because of the symmetry property Edmonds (3.7.6) of the Wigner 3-j symbol, this is zero unless $l + l' + K$ is even.

I leave the particulars of the radial integral

$$\langle n'l'|f_K(r)|nl\rangle = \int r^2 dr\, f_K(r) R_{n'l'}(r) R_{nl}(r) \tag{16.32}$$

to the reader. For the common case where $f_K(r) \propto r^K$ and for harmonic oscillator radial wavefunctions $R_{nl}(r)$, there exist closed (but complicated) expressions in, for example, Lawson. Some formulas for radial integrals between harmonic oscillator states and r^K can be found in Subsection 16.1.5.

Now we can look at the time-reversed matrix element. This corresponds to exchanging $j \leftrightarrow j'$ and $l \leftrightarrow l'$. By symmetry property Edmonds (3.7.5) and the already-established fact that $l + l' + K$ is even, the Wigner 3-j is invariant under this exchange; and by symmetry property Edmonds (6.2.4) the 6-j is also invariant. The radial matrix element, if it is real, is easily invariant. Thus we conclude that

$$\langle n'(l',1/2)j'||f_K(r)Y_K||n(l,1/2)j\rangle =$$
$$(-1)^{j-j'} \langle n(l,1/2)j||f_K(r)Y_K||n'(l',1/2)j'\rangle \tag{16.33}$$

There is another, equivalent expression... (later) [Expression from Lawson]

We can compute example cases for the harmonic oscillator, in terms of the oscillator parameter b, using matrix elements given below in Subsection 16.1.5:
• *Electric dipole.* Here the $E1$ operator is $e\vec{r}$, where e is the charge, often an "effective charge." The $m = 0$ or z-component is $er\cos\theta$ but $Y_{1,0}(\theta,\phi) = \sqrt{3/4\pi}\cos\theta$ so that here the function $f_K(r) = e\sqrt{4\pi/3}r$. We need the fundamental radial matrix elements,

$$\langle 0p|r|0s\rangle = b\sqrt{3/2}, \quad \langle 0p|r|1s\rangle = -b,$$

Then

$$\langle 0p_{1/2}||E1||0s_{1/2}\rangle = -e\,b; \quad \langle 0p_{3/2}||E1||0s_{1/2}\rangle = +\sqrt{2}e\,b;$$
$$\langle 0p_{1/2}||E1||1s_{1/2}\rangle = +\sqrt{\frac{2}{3}}e\,b; \quad \langle 0p_{3/2}||E1||1s_{1/2}\rangle = -\frac{2}{\sqrt{3}}e\,b.$$

If we include isospin, so that we have the isoscalar ($T = 0$, $E1 = rY_{1m}$) or isovector ($T = 1$, $E1 = rY_{1m}\tau$) dipole operator, then the doubly -reduced matrix elements are

$$\langle 0p_{1/2}|||E1_T|||0s_{1/2}\rangle = -\sqrt{2(2T+1)}e\,b; \quad \langle 0p_{3/2}|||E1_T|||0s_{1/2}\rangle = +2\sqrt{(2T+1)}e\,b;$$

$$\langle 0p_{1/2}|||E1_T|||1s_{1/2}\rangle = 2\sqrt{\frac{(2T+1)}{3}}e\,b;\quad \langle 0p_{3/2}|||E1_T|||1s_{1/2}\rangle = -2\sqrt{\frac{(2T+1)}{3}}e\,b$$

• *Electric quadrupole.* Here the function $f_K(r) = \sqrt{16\pi/5}e\,r^2$. We take the fundamental matrix elements

$$\langle 0d|r^2|0s\rangle = b^2\sqrt{15/4},\ \ \langle 0d|r^2|1s\rangle = -b^2\sqrt{10},\ \ \langle 0p|r^2|0p\rangle = \tfrac{5}{2}b^2,$$

and from this construct the reduced matrix elements

$$\langle 0d_{3/2}||E2||0s_{1/2}\rangle = -\sqrt{12}\,e\,b^2;\ \ \langle 0d_{5/2}||E2||0s_{1/2}\rangle = \sqrt{18}\,e\,b^2;$$

$$\langle 0d_{3/2}||E2||1s_{1/2}\rangle = \sqrt{32}\,e\,b^2;\ \ \langle 0d_{5/2}||E2||1s_{1/2}\rangle = -4\sqrt{3}\,e\,b^2;$$

$$\langle 0p_{3/2}||E2||0p_{1/2}\rangle = -\sqrt{20}\,e\,b^2;\ \ \langle 0p_{3/2}||E2||0p_{3/2}\rangle = -\sqrt{20}\,e\,b^2.$$

If we add in isospin operators $1, \tau$, as usual to get the doubly-reduced matrix elements we multiple by $\sqrt{2(2T+1)}$.

16.1.5 Useful integrals

. Here are some useful integrals, with harmonic oscillator wavefunctions, with $b = \sqrt{\hbar/m\omega}$ being the harmonic oscillator length. Below n denotes the *radial nodal* quantum number, starting with $n = 0$; the principal quantum number $N = 2n + l$.

Radial integrals were computed using the formula out of Lawson (11.1a), which actually originates from Nilsson (1955).

$$\langle n, l+1|r|n, l\rangle = b\sqrt{n+l+3/2} \tag{16.34}$$

$$\langle n-1, l+1|r|n, l\rangle = -b\sqrt{n} \tag{16.35}$$

With a fair amount of work, I can compute the needed harmonic oscillator matrix elements needed to get the gradient matrix elements:

$$\left\langle n, l+1\left|\frac{\partial}{\partial r} - \frac{l}{r}\right|n, l\right\rangle = -\frac{1}{b}\sqrt{n+l+3/2} \tag{16.36}$$

$$\left\langle n-1, l+1\left|\frac{\partial}{\partial r} - \frac{l}{r}\right|n, l\right\rangle = -\frac{1}{b}\sqrt{n}. \tag{16.37}$$

I can also compute matrix elements of (scalar) r^2; from this and using the fact that these are eigenstates of the harmonic oscillator Hamiltonian, we can directly deduce matrix elements of p^2:

$$\langle n, l|r^2|nl\rangle = b^2(2n+l+3/2); \tag{16.38}$$

$$\langle n-1, l+2|r^2|nl\rangle = -b^2\sqrt{2n(2n+2l+3)}; \tag{16.39}$$

$$\langle n, l+2|r^2|nl\rangle = b^2\sqrt{(n+l+3/2)(n+l+5/2)}; \tag{16.40}$$

$$\langle n+1,l|r^2|nl\rangle = -b^2\sqrt{(n+1)(n+l+3/2)}; \tag{16.41}$$

$$\langle n,l|p^2|n,l\rangle = \frac{\hbar^2}{b^2}(2n+l+3/2); \tag{16.42}$$

$$\langle n-1,l+2|p^2|n,l\rangle = +\frac{\hbar^2}{b^2}\sqrt{2n(2n+2l+3)}; \tag{16.43}$$

$$\langle n,l+2|p^2|n,l\rangle = -\frac{\hbar^2}{b^2}\sqrt{(n+l+3/2)(n+l+5/2)}; \tag{16.44}$$

$$\langle n+1,l|p^2|n,l\rangle = +\frac{\hbar^2}{b^2}\sqrt{(n+1)(n+l+3/2)} \tag{16.45}$$

16.1.6 Matrix elements of $\vec{r}$

Let compute the matrix elements of $\vec{r}$ in a harmonic oscillator basis. Ignoring spin at first, we note

$$\langle n'l'||\vec{r}||nl\rangle = \sqrt{\frac{4\pi}{3}}\langle l'||Y_1||l\rangle\langle n'l'|r|nl\rangle, \tag{16.46}$$

where

$$\langle n'l'|r|nl\rangle = \int_0^\infty R_{n'l'}(r)rR_{nl}(r)r^2\,dr \tag{16.47}$$

is jus a radial integral. Then by Edmonds (5.4.3)

$$\sqrt{\frac{4\pi}{3}}\langle l'||Y_1||l\rangle = (-1)^{l'}[l'][l]\begin{pmatrix} l' & 1 & l \\ 0 & 0 & 0 \end{pmatrix}. \tag{16.48}$$

From Table 2 in Edmonds one can deduce that

$$\begin{pmatrix} l' & 1 & l \\ 0 & 0 & 0 \end{pmatrix} = (-1)^{l_>}\frac{[l_>]}{[l][l']}, \tag{16.49}$$

where $l_>$ is the larger of l, l'. This then simplifies

$$\sqrt{\frac{4\pi}{3}}\langle l'||Y_1||l\rangle = (-1)^{l+l_>}[l_>]. \tag{16.50}$$

Putting all the cases together, I get:

$$\langle n,l+1||\vec{r}||nl\rangle = b\sqrt{(2l+3)(n+l+3/2)}, \tag{16.51}$$

$$\langle n-1,l+1||\vec{r}||nl\rangle = -b\sqrt{(2l+3)n}, \tag{16.52}$$

$$\langle n,l-1||\vec{r}||nl\rangle = -b\sqrt{(2l+1)(n+l+1/2)}, \tag{16.53}$$

$$\langle n+1,l+1||\vec{r}||nl\rangle = b\sqrt{(2l+3)(n+1)}. \tag{16.54}$$

16.1.7 Momentum

A useful matrix element is $\hat{F} = \vec{p} = \frac{\hbar}{i}\vec{\nabla}$. Again, this operates only on the space part so we apply Edmonds (7.1.7). After that, however, we need the reduced matrix element of the gradient operator $\vec{\nabla}$. This is found in most convenient form in the useful book by Varshalovich, Moskalev, and Khersonskii (VMK, also highly recommened to would-be practitioners). Not surprisingly, $\vec{\nabla}$ acts as an orbital angular momentum raising/lowering operator, meaning that $l' = l \pm 1$. In VMK p. 486, eqn (22) and (23),

$$\left\langle n'l'||\vec{\nabla}||nl \right\rangle = \delta_{l',l+1}\sqrt{l'}A_{n'l'nl} - \delta_{l',l-1}\sqrt{l}B_{n'l'nl} \tag{16.55}$$

where

$$A_{n'l'nl} = \int_0^\infty r^2 dr\, R_{n',l'}(r)\left(\frac{\partial}{\partial r} - \frac{l}{r}\right)R_{nl}(r), \tag{16.56}$$

$$B_{n'l'nl} = \int_0^\infty r^2 dr\, R_{n',l'}(r)\left(\frac{\partial}{\partial r} + \frac{l+1}{r}\right)R_{nl}(r). \tag{16.57}$$

This can actually be simplified a bit, I think. First, note that for A one always has $l' = l + 1$ while for B $l' = l - 1$. Integrating by parts one gets

$$\left\langle n'l'||\vec{\nabla}||nl \right\rangle = \delta_{l',l+1}\sqrt{l'}\left\langle n'l'\left|\frac{\partial}{\partial r} - \frac{l}{r}\right|nl\right\rangle + \delta_{l',l-1}\sqrt{l}\left\langle nl\left|\frac{\partial}{\partial r} - \frac{l'}{r}\right|n'l'\right\rangle^* \tag{16.58}$$

This makes sense, because the time-reversed matrix elements ought to be related by a simple phase factor. In the appendix I compute these matrix elements for harmonic oscillator wavefunctions.

$$\left\langle n, l+1\left|\frac{d}{dr} - \frac{l}{r}\right|n, l\right\rangle = -\sqrt{n+l+3/2}, \tag{16.59}$$

$$\left\langle n-1, l+1\left|\frac{d}{dr} - \frac{l}{r}\right|n, l\right\rangle = -\sqrt{n} \tag{16.60}$$

16.2 Sum rules

For Hermitian operators,

$$\sum_f (E_f - E_i)\left|\langle f|\hat{\mathcal{O}}|i\rangle\right|^2 = \frac{1}{2}\left\langle i\left|\left[\hat{\mathcal{O}}, \left[\hat{H}, \hat{\mathcal{O}}\right]\right]\right|i\right\rangle. \tag{16.61}$$

16.2.1 Example: the Ikeda sum rule

The Ikeda sum rule is a non-energy-weight sum rule for Gamow-Teller transitions in nuclear physics. It involves a non-Hermitian operator.

16.2.2 Example: the Thomas-Reiche-Kuhn sum rule

The Thomas-Reiche-Kuhn (TRK) sum rule is an example of an energy-weighted sum rule. We consider the specific case for atoms with N electrons. The operator is the dipole operator,

$$\sum_{a=1}^{N} e\vec{r}_a, \tag{16.62}$$

and the nonrelativistic Hamiltonian is

$$\hat{H} = \sum_{a=1}^{N} \frac{\vec{p}_a^2}{2m_e} - \frac{Ze^2}{r_a} + \sum_{a<b} \frac{e^2}{|\vec{r}_a - \vec{r}_b|}. \tag{16.63}$$

The key step is computing the double-commutator (16.61). In doing so, we note that the dipole operator commutes with the potential terms; therefore we only have to consider the kinetic energy. (This is not the case for nuclear physics, where the interactions have a strong momentum dependence and hence do not simply commute with $\vec{r}$; this can modify the TRK sum rule by a large fraction. There are also relativistic corrections for atoms, but this is small.)

The double commutator is

$$\left[\vec{r}_a \cdot, \left[p_b^2, \vec{r}_c\right]\right] = 6\hbar^2 \delta_{bc}\delta_{ab}; \tag{16.64}$$

the details are left as an exercise, but one picks up a factor of 3 from summing over the three components x, y, z (here indicated by the dot product $\cdot$) ; the addition factor of 2 comes from the innermost commutator of p^2 with r. Putting in the rest of the terms, one gets the TRK sum rule

$$\frac{3}{2}\frac{e^2\hbar^2}{m_e}N. \tag{16.65}$$

Often in atomic physics one talks about the dimensionless (dipole) *oscillator strength*

$$f_{if} = \frac{2}{3}\frac{m_e}{e^2\hbar^2}(E_f - E_i)\sum_{m_f} \left|\langle f m_f | e\vec{r} | i\rangle\right|^2, \tag{16.66}$$

where the sum is over all degenerate m values for the final states. Then the TRK sum rule can be written simply as

$$\sum_f f_{if} = N. \tag{16.67}$$

There is a corresponding TRK sum rule for nuclear physics, which has slightly different form; one has to account for (a) the fact that neutrons have no charge and (b) the dipole is relative to the center of mass (in atoms the massive nucleus effectively nails the center of mass in space). The result is

$$\frac{NZe^2\hbar^2}{Am_N} \tag{16.68}$$

which generally falls short by as much as 40% due to the momentum dependence of the nuclear force.

16.3 Summary

What you should get out of this chapter:
• Basic ideas about how we represent one-body operators, representing transitions and moments;
• Examples of how to compute matrix elements of one-body operators, with attention paid to angular momentum algebra.

16.4 Exercises

Show that (16.4) leads to (16.5).

(17.x) Derive (16.64).

Chapter 17

Representation of Hamiltonians and other operators

> An expert is someone who knows some of the worst mistakes that can be made in his subject, and how to avoid them. – *Werner Heisenberg*

In this chapter I discuss the general formalism of representing Hamiltonian and transition operators in terms of creation and annihilation operators. How to compute specific matrix elements is given in chapter 16.

We must perforce pay attention to angular momentum coupling, of which a brief introduction is given in chapter 15. In nuclei, one must couple up to good total angular momentum J, and often isospin T. The total angular momentum J may be decomposed into total orbital angular momentum L and total spin S. In atoms, L and S are almost good quantum numbers by themselves, with only a weak coupling through relativistic terms. Much of this discussion also applies to cold atomic gases in a spherically symmetric trap. I will focus on the nuclear case, with some discussion of atomic physics.

17.1 The Hamiltonian

I restrict myself to one- and two-body Hamiltonians for A-body systems, that is the Hamiltonian has terms for only one and two particles at a tie. An example is

$$\hat{H} = \sum_{i=1}^{A} -\frac{\hbar^2}{2M}\nabla_i^2 + U(\vec{r}_i) + \sum_{i<j} V(\vec{r}\_\vec{r}_j). \tag{17.1}$$

(As a small aside, this is called a *local* Hamiltonian. One can also consider *nonlocal* interactions. For a single particle, the action of a nonlocal interaction on a wavefunction looks like

$$\int V(\vec{r},\vec{r}')\psi(\vec{r}')\,d^3r'. \tag{17.2}$$

These are also called momentum-dependent forces, because one can expand the nonlocality in terms of derivatives and hence momentum operators. I will not go into detail here.)

The one-body Hamiltonian, $\hat{H}_1$, consists of the kinetic energy and any external potential; the latter may come from interactions with an inert, frozen 'core' or from a truly external potential such as the Coulomb potential from the atomic nucleus in the case or a trapping potential.

I assume the one-body part is an angular momentum scalar (although a non-scalar potential, for example in an external magnetic or electric field, is possible). Often for simplicity one assumes the one-body part is diagonal, that is, written as

$$\hat{H}_1 = \sum_a \epsilon_a \hat{n}_a \tag{17.3}$$

where $\hat{n}_a$ is the number operator for orbit a. This simplicity of course depends upon the definition of the single-particle wavefunctions. Later I will show how one can always embed a general one-body Hamiltonian as a number-dependent two-body interaction.

The two-body Hamiltonian is characterized by matrix elements between antisymmeterized two-body states. Any general many-body code reads in these two-body matrix elements, as well as single-particle energies or single-particle Hamiltonian matrix elements.

To look at the two-body part, first define the pair creation operator The pair creation operator are defined as

$$\hat{A}^\dagger_{JM}(ab) \equiv \left[c^\dagger_a \times c^\dagger_b\right]_{JM} \tag{17.4}$$

where the coupling is accomplished through Clebsch-Gordon coefficients, that is,

$$\left[c^\dagger_a \times c^\dagger_b\right]_{JM} = \sum_{m_a,m_b} (j_a m_a, j_b m_b | JM) \hat{c}^\dagger_{j_a m_a} \hat{c}^\dagger_{j_b m_b}. \tag{17.5}$$

If we include isospin we have

$$\hat{A}^\dagger_{JM,TM_T}(ab) \equiv \left[c^\dagger_a \times c^\dagger_b\right]_{JM,TM_T}, \tag{17.6}$$

with

$$\left[c^\dagger_a \times c^\dagger_b\right]_{JM,TM_T} = \sum_{m_a,m_b} (j_a m_a, j_b m_b | JM)$$
$$\sum_{\mu_a,\mu_b} ((1/2)\mu_a, (1/2)\mu_b | TM_T)) \hat{c}^\dagger_{j_a m_a,(1/2)\mu_a} \hat{c}^\dagger_{j_b m_b,(1/2)\mu_b}. \tag{17.7}$$

For atomic situations one can replace J by L or J and T by L and S.

A properly antisymmeterized and normalized two-body state is (using operators)

$$|ab;JM\rangle \equiv \frac{1}{\sqrt{1+\delta_{ab}}}\hat{A}^\dagger_{JM}(ab)|0\rangle. \tag{17.8}$$

or, including isospin,

$$\hat{A}^\dagger_{JM,TM_T}(ab) \equiv \left[c^\dagger_a \times c^\dagger_b\right]_{JM,TM_T} \tag{17.9}$$

Because of symmetries of the Clebsch-Gordon coefficients,

$$|ba;JM\rangle = -(-1)^{j_a+j_b-J}|ab;JM\rangle \tag{17.10}$$

or, with isospin,

$$|ba;JM,TM_T\rangle = -(-1)^{j_a+j_b-J}(-1)^{1-T}|ab;JM,TM_T\rangle. \tag{17.11}$$

Because the Hamiltonian is presumably an angular momentum scalar as well as an isoscalar, the matrix elements do not depend on M, M_T, which can thus be supressed: the matrix elements are

$$V_J(ab,cd) = \langle ab;JM|\hat{H}_2|cd;JM\rangle, \tag{17.12}$$

independent of M, or with isospin,

$$V_{JT}(ab,cd) = \langle ab;JM,TM_T|\hat{H}_2|cd;JM,TM_T\rangle, \tag{17.13}$$

independent of M and M_T. We have the symmetry relations

$$\begin{aligned} V_J(ab,cd) &= -(-1)^{j_a+j_b-J}V_J(ba,cd) \\ &= -(-1)^{j_c+j_d-J}V_J(ab,dc) = (-1)^{j_a+j_b+j_c+jd}V_J(ba,dc) \end{aligned} \tag{17.14}$$

or with isospin

$$\begin{aligned} V_{JT}(ab,cd) &= -(-1)^{j_a+j_b+1-J-T}V_{JT}(ba,cd) \\ &= -(-1)^{j_c+j_d+1-J-T}V_{JT}(ab,dc) = (-1)^{j_a+j_b+j_c+jd}V_{JT}(ba,dc) \end{aligned} \tag{17.15}$$

The two-body part of the Hamiltonian is

$$\begin{aligned} \hat{H}_2 = \frac{1}{4}\sum_{abcd}\sqrt{(1+\delta_{ab})(1+\delta_{cd})} \\ \sum_{JT}V_{JT}(ab,cd)\sum_{M,M_T}\hat{A}^\dagger_{JM,TM_T}(ab)\hat{A}_{JM,TM_T}(cd). \end{aligned} \tag{17.16}$$

This Hamiltonian is appropriate for many-body systems; the choice of convention for the V_{JT} is derived from the matrix elements of the two-body system. That is, the V_J are the *matrix elements for the two-body system*, and the states

$|ab;J\rangle$ are properly normalized two-body basis states. With this convention in hand, the definition for the two-body part of the Hamiltonian becomes automatic.

(Note: one way to see this is to sum only over unique two-body states, by insisting $a \le b$ and $c \le d$. The restricted sum can be rewritten

$$\sum_{a\le b} = \frac{1+\delta_{ab}}{2}\sum_{ab}. \tag{17.17}$$

Thus we can rewrite the two-body Hamiltonian

$$\hat{H}_2 = \sum_{a\le b, c\le d}\sum_{JT} V_{JT}(ab,cd) \tag{17.18}$$
$$\sum_{M,M_T} \frac{1}{\sqrt{1+\delta_{ab}}}\hat{A}^\dagger_{JM,TM_T}(ab)\frac{1}{\sqrt{1+\delta_{cd}}}\hat{A}_{JM,TM_T}(cd).$$

so that it is now expressed in terms of manifestly normalized two-body operators.) To simply notation we sometimes use

$$\zeta_{ab} = \sqrt{1+\delta_{ab}}, \tag{17.19}$$

so that we can write

$$\hat{H}_2 = \frac{1}{4}\sum_{abcd}\zeta_{ab}\zeta_{cd}\sum_{JT}V_{JT}(ab,cd)\sum_{M,M_T}\hat{A}^\dagger_{JM,TM_T}(ab)\hat{A}_{JM,TM_T}(cd)$$
$$= \sum_{a\le b,c\le d}\sum_{JT}V_{JT}(ab,cd)\sum_{M,M_T}\zeta^{-1}_{ab}\hat{A}^\dagger_{JM,TM_T}(ab)\zeta^{-1}_{cd}\hat{A}_{JM,TM_T}(cd).$$

The one-body part of the Hamiltonian is

$$\hat{H}_1 = \sum_{\alpha\beta}\epsilon_{\alpha\beta}[j_\alpha]\left[c^\dagger_\alpha \times \tilde{c}_\beta\right]_{J=0} \tag{17.20}$$

Here $\tilde{c}_{jm} = (-1)^{j+m}c_{j-m}$ is the time-reversed operator. If the ϵ_{ab} are diagonal, as is usually assumed to be the case, then

$$\hat{H}_1 = \sum_a \epsilon_a \hat{n}_a, \tag{17.21}$$

where $\hat{n}_a$ is the number operator for the orbit a.

Sometimes it is necessary to work in coordinate space. A single-particle wavefunction is

$$\phi^a_{jm}(\vec{r}) = R_a(r)\left[Y_\ell \times \chi\right]_{jm}. \tag{17.22}$$

The normalized, antisymmetrized coordinate-space wfn is

$$\psi^{(ab)}_{JM}(\vec{r},\vec{r}') = \tag{17.23}$$
$$\frac{1}{\sqrt{2}}\zeta^{-1}_{ab}\left(\left[\phi_a(\vec{r})\times\phi_b(\vec{r}')\right]_{JM} - (-1)^{j_a+j_b+J}\left[\phi_b(\vec{r})\times\phi_a(\vec{r}')\right]_{JM}\right)$$

In order to get the antisymmeterized matrix element $V_J(ab,cd)$ we first construct the the non-antisymmetrized matrix element $\tilde{V}_J^N(ab,cd) =$

$$\int\int [\phi_a^*(\vec{r}) \times \phi_b^*(\vec{r}')]_{JM} \, V(\vec{r},\vec{r}') \, [\phi_c(\vec{r}) \times \phi_d(\vec{r}')]_{JM} \; d^3r \, d^3r', \tag{17.24}$$

and then

$$V_J(ab,cd) = \zeta_{ab}^{-1}\zeta_{cd}^{-1} \left(\tilde{V}_J^N(ab,cd) - (-1)^{J+j_c+j_d} \tilde{V}_J^N(ab,dc) \right). \tag{17.25}$$

For isospin (see appendix for some more details)

$$V_{J,T=1}(ab,cd) = \zeta_{ab}^{-1}\zeta_{cd}^{-1} \left(\tilde{V}_J^N(\alpha_\pi\beta_\pi,\gamma_\pi\delta_\pi) - (-1)^{J+j_c+j_d} \tilde{V}_J^N(\alpha_\pi\beta_\pi,\delta_\pi\gamma_\pi) \right), \tag{17.26}$$

$$V_{J,T=0}(ab,cd) = \zeta_{ab}^{-1}\zeta_{cd}^{-1} \left(\tilde{V}_J^N(\alpha_\pi\beta_\nu,\gamma_\pi\delta_\nu) + (-1)^{J+j_c+j_d} \tilde{V}_J^N(\alpha_\pi\beta_\nu,\delta_\pi\gamma_\nu) \right)$$

There are multiple ways to compute two-body matrix elements. I will detail three.

In addition to chapter 15, a good reference on angular momentum algebra is Edmond's slim little book. As noted in chapter 17, because the Hamiltonian is an angular momentum scalar, the matrix element

$$(ab;JM|\hat{H}|cd;JM)$$

is independent of M, and so thus are the two-body matrix elements $V_J(ab,cd)$ needed for any computation. We therefore should note the simple, but important, relation between the two-body matrix elements and the *reduced* matrix elements introduced via the Wigner-Eckart theorem:

$$(ab;JM|\hat{H}|cd;JM) = \frac{1}{[J]}(ab;J||\hat{H}||cd;J). \tag{17.27}$$

If one has isospin,

$$(ab;JM,TM_T|\hat{H}|cd;JM,TM_T) = \frac{1}{[J][T]}(ab;JT|||\hat{H}|||cd;JT). \tag{17.28}$$

The analogy if one has orbital angular momentum L and optionally spin S is straightforward.

17.2 Separable interactions

The most common and straightforward approach is separable or quasi-separable interactions. A separable interaction is of the form $V(r_1,r_2) = u(r_1)u(r_2)$. Separable interactions are easy to use in mean-field and RPA calculations (if one ignores the exchange term!) but more generally, one can extend the formalism to a sum of separable interactions, or tensor separable interactions, interactions

of the form $\vec{F}^\dagger \cdot \vec{F}$. The complex conjugation † is important to guarantee Hermiticity. Even if one does not use the separability, such a form is useful in interpreting the interaction, as $\vec{F}$ may be a well-known operator such as dipole, quadrupole, spin, and so on.

The interaction is

$$\vec{F}^\dagger \cdot \vec{F} = \sum_M \left(F_{KM}\right)^\dagger F_{KM} = \sum_M (-1)^M F_{K-M} F_{KM}, \tag{17.29}$$

where I've used (15.43). I will compute both the one- and two-body parts.

After a page or two of algebra (I rely heavily upon equation (6.2.6) in Edmonds) I obtain for the two-body part of $\vec{F}^\dagger \cdot \vec{F}$

$$\sum_{abcd} F^*_{ca} F_{bd} \sum_J (-1)^{j_a+j_b-J} \left\{ \begin{array}{ccc} j_a & j_c & K \\ j_d & j_b & J \end{array} \right\} \times \sum_\mu A^\dagger_{J\mu}(ab) A_{J\mu}(cd). \tag{17.30}$$

We need to extract the antisymmetrized V_{JT}. I leave this for the next two subsections, where I deal with the isospin structure.

The one-body part is

$$\sum_{ab} [c^\dagger_a \otimes \tilde{c}_b]_{00} \sum_c (-1)^{j_a-j_c} [j_a]^{-1} F_{ac} F_{cb} = \sum_{ab} [c^\dagger_a \otimes \tilde{c}_b]_{00} \sum_c [j_a]^{-1} F^*_{ca} F_{cb}, \tag{17.31}$$

that is,

$$\epsilon_{ab} = \frac{1}{(2j_a+1)} \sum_c F^*_{ca} F_{cb}. \tag{17.32}$$

Note that $j_a = j_b$. For the frequent diagonal case($a = b$), the induced single particle energy is

$$\epsilon_a = \frac{1}{(2j_a+1)} \sum_c |F_{ac}|^2. \tag{17.33}$$

17.2.1 Example of applied angular momentum algebra

Here I derive in detail Eq. (17.30). Starting from (16.11), (17.29), and the results of Exercise 16.6,

$$\sum_M \left(\hat{F}_{KM}\right)^\dagger \hat{F}_{KM} = \sum_{abcd} \frac{F^*_{ab} F_{cd}}{2K+1} \sum_M (-1)^{j_a-j_b+M} \left(\hat{c}^\dagger_b \times \tilde{c}_a\right)_{K,\,-M} \left(\hat{c}^\dagger_c \times \tilde{c}_d\right)_{K,\,M} \tag{17.34}$$

$$= \sum_{abcd} \frac{F^*_{ab} F_{cd}}{2K+1} \sum_M (-1)^{j_a-j_b+M}$$

$$\sum_{m's}(j_b m_b, j_a m_a|K,\,-M)(j_c m_c, j_d m_d|K,\,M)\hat{c}_b^\dagger \tilde{c}_a \hat{c}_c^\dagger \tilde{c}_d. \tag{17.35}$$

Putting the operators into antinormal form,

$$\hat{c}_b^\dagger \tilde{c}_a \hat{c}_c^\dagger \tilde{c}_d = -\hat{c}_b^\dagger \hat{c}_c^\dagger \tilde{c}_a \tilde{c}_d + (-1)^{j_a+m_a}\delta_{ac}\delta_{m_a,\,-m_c}\hat{c}_b^\dagger \tilde{c}_d, \tag{17.36}$$

where the phase in the second term arises, of course, from the definition of a time-reversed operator, (15.44). Now we have to apply recoupling theorems as in section 15.7. By applying (15.75) we get

$$(j_b m_b, j_a m_a|K,\,-M)(j_c m_c, j_d m_d|K,\,M) = \sum_J (-1)^{M+\mu+j_a+j_c}\times$$
$$(2K+1)\begin{Bmatrix} j_b & j_a & K \\ j_d & j_c & J \end{Bmatrix}(j_b m_b, j_c m_c|J\mu)(j_a m_a, j_d m_d|J\,-\mu), \tag{17.37}$$

which, inserting into (17.35) and the two-body part of (17.36) yield

$$\sum_{abcd} F_{ab}^* F_{cd} \sum_J \begin{Bmatrix} j_b & j_a & K \\ j_d & j_c & J \end{Bmatrix} \sum_\mu (-1)^{j_b+j_c+\mu}\hat{A}^\dagger_{J\mu}(bc)\tilde{A}_{J\,-\mu}(ad) \tag{17.38}$$

where, by using

$$\tilde{A}_{J\,-\mu}(ad) = [\tilde{c}_a \times \tilde{c}_d]_{J,mu} = (-1)^{J+\mu}\hat{A}_{J\mu}(ad) \tag{17.39}$$

obtain

$$\sum_{abcd} F_{ab}^* F_{cd} \sum_J \begin{Bmatrix} j_b & j_a & K \\ j_d & j_c & J \end{Bmatrix} \sum_\mu (-1)^{j_b+j_c+J}\hat{A}^\dagger_{J\mu}(bc)\hat{A}_{J\,\mu}(ad) \tag{17.40}$$

Rearranging the labels we regain (17.30).

17.2.2 Isospin structure

First consider the case where F is also an isospin tensor of rank I ($I = 0, 1$ only), that is,

$$\hat{F}_{KM,IM_I} = \sum_{ab} F_{ab}[K]^{-1}[I]^{-1}\left[c_a^\dagger \otimes \tilde{c}_b\right]_{KM,IM_I} \tag{17.41}$$

where now F_{ab} is the doubly-reduced matrix element $(a|||F_{KI}|||b)$. Then following the development above we write the two-body part of $\vec{F}^\dagger \cdot \vec{F}$

$$\sum_{abcd}\sum_{JT}(-1)^{j_b+j_c-J}\begin{Bmatrix} j_a & j_c & K \\ j_d & j_b & J \end{Bmatrix}$$
$$\times(-1)^{1-T}\begin{Bmatrix} \frac{1}{2} & \frac{1}{2} & I \\ \frac{1}{2} & \frac{1}{2} & T \end{Bmatrix} F_{ca}^* F_{bd} \sum_{\mu\mu_T} A^\dagger_{J\mu,T\mu_T}(ab)A_{J\mu,T\mu_T}(cd) \tag{17.42}$$

I need the following 6-j symbols:

$$\left\{ \begin{array}{ccc} \frac{1}{2} & \frac{1}{2} & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 \end{array} \right\} = -\frac{1}{2}, \quad \left\{ \begin{array}{ccc} \frac{1}{2} & \frac{1}{2} & 0 \\ \frac{1}{2} & \frac{1}{2} & 1 \end{array} \right\} = \frac{1}{2}, \tag{17.43}$$

$$\left\{ \begin{array}{ccc} \frac{1}{2} & \frac{1}{2} & 1 \\ \frac{1}{2} & \frac{1}{2} & 0 \end{array} \right\} = \frac{1}{2}, \quad \left\{ \begin{array}{ccc} \frac{1}{2} & \frac{1}{2} & 1 \\ \frac{1}{2} & \frac{1}{2} & 1 \end{array} \right\} = \frac{1}{6} \tag{17.44}$$

Then for isoscalar interactions ($I = 0$)

$$V_{JT}(ab, cd) = \zeta_{ab}^{-1}\zeta_{cd}^{-1}(-1)^{j_b+j_c-J} \times \tag{17.45}$$
$$\left[\left\{ \begin{array}{ccc} j_a & j_b & J \\ j_d & j_c & K \end{array} \right\} F_{ac}^{(0)}F_{bd}^{(0)} - (-1)^{J+T} \left\{ \begin{array}{ccc} j_a & j_b & J \\ j_c & j_d & K \end{array} \right\} F_{ad}^{(0)}F_{bc}^{(0)} \right]$$

Here I have used $\zeta_{ab} = \sqrt{1+\delta_{ab}}$. From isovector interactions ($I = 1$) the result is very similar:

$$V_{JT}(ab, cd) = \zeta_{ab}^{-1}\zeta_{cd}^{-1} \frac{(-1)^{j_b+j_c-J+1-T}}{2T+1} \times \tag{17.46}$$
$$\left[\left\{ \begin{array}{ccc} j_a & j_b & J \\ j_d & j_c & K \end{array} \right\} F_{ac}^{(1)}F_{bd}^{(1)} - (-1)^{J+T} \left\{ \begin{array}{ccc} j_a & j_b & J \\ j_c & j_d & K \end{array} \right\} F_{ad}^{(1)}F_{bc}^{(1)} \right]$$

For the one-body part, independent of I,

$$\epsilon_{ab} = \frac{1}{2}\frac{1}{(2j_a+1)}\sum_x F_{ax}F_{bx}^*, \tag{17.47}$$

or, for common diagonal single-particle energies

$$\epsilon_a = \frac{1}{2}\frac{1}{(2j_a+1)}\sum_x |F_{ax}|^2. \tag{17.48}$$

17.2.3 Examples: Matrix elements of J^2 and T^2

As a test of these equations, let's consider the matrix elements of the operators J^2 and T^2. Because the one-body states are eigenstates of those operators, and the two-body states are constructed as eigenstates of these operators, the matrix elements are diagonal; furthermore we trivially the values of those matrix elements. The one-body matrix elements, akin to "single-particle energies," are, for the single particle state a, $j_a(j_a+1)$ for J^2 and just $3/4$ for T^2.

The two-body matrix elements are similarly easy to find. Because

$$\langle ab; JT|\hat{J}^2|ab; JT\rangle = J(J+1), \tag{17.49}$$

the two-body matrix element is just $J(J+1)$ minus the one-body contributions:

$$V_{JT}(ab, ab) = J(J+1) - j_a(j_a+1) - j_b(j_b+1). \tag{17.50}$$

The same holds for T^2.

We have calculated from (16.18) and the isospin-reduced factor $\langle a|||\vec{J}|||b\rangle = \delta_{ab}\sqrt{2j_a(j_a+1)(2j_a+1)}$. Then the single particle energies are, from (17.48), $j_a(j_a+1)$ as expected.

To compute the two-body matrix elements for J^2 (which has $K=1, I=0$) we need the 6-j symbol (see Table 5 in Edmonds):

$$\left\{ \begin{array}{ccc} J & j_a & j_b \\ 1 & j_b & j_a \end{array} \right\} \tag{17.51}$$
$$= (-1)^{J+j_a+j_b} \frac{J(J+1) - j_a(j_a+1) - j_b(j_b+1)}{2\sqrt{j_a(j_a+1)(2j_a+1)j_b(j_b+1)(2j_b+1)}}.$$

Combining into (17.46), we get exactly (17.50). We can do the same with the matrix elements $(a|||\vec{T}|||a) = \sqrt{\frac{3}{2}(2j+1)}$, which has $K=0, I=1$.

17.3 More general interactions

In this section I discuss how to compute general matrix elements for a translationally invariant potential $V(|\vec{r}-\vec{r}'|)$.

To do this we use the Slater decomposition (cf., for example, Lawson):

$$V(|\vec{r}-\vec{r}'|) = \sum_\ell F_\ell(r,r')P_\ell(\cos\theta) = \sum_\ell F_\ell(r,r')\frac{4\pi}{\sqrt{2\ell+1}}(-1)^\ell \left[Y_\ell(\Omega)\times Y_\ell(\Omega')\right]_{00}, \tag{17.52}$$

where $\cos\theta = \vec{r}\cdot\vec{r}'/rr'$, and $P_\ell(x)$ are Legendre polynomials. The functions $F_\ell(r,r')$ are computed

$$F_\ell(r,r') = \frac{2\ell+1}{2}\int_0^\pi V(|\vec{r}-\vec{r}'|)P_\ell(\cos\theta)\sin\theta d\theta. \tag{17.53}$$

Now we can compute the non-antisymmetrized matrix elements

$$\tilde{V}^N_J(ab,cd) = [J][j_a][j_b][j_c][j_d](-1)^{J+j_a+j_c}\times \tag{17.54}$$
$$\sum_\ell \left(\begin{array}{ccc} j_a & \ell & j_c \\ -\frac{1}{2} & 0 & \frac{1}{2} \end{array} \right) \left(\begin{array}{ccc} j_b & \ell & j_d \\ -\frac{1}{2} & 0 & \frac{1}{2} \end{array} \right) \left\{ \begin{array}{ccc} j_a & j_c & \ell \\ j_d & j_b & J \end{array} \right\} I_\ell(ab,cd),$$

with the radial integrals

$$I_\ell(ab,cd) = \int r^2 dr \int r'^2 dr'\, R^*_a(r)R^*_b(r')F_\ell(r,r')R_c(r)R_d(r'). \tag{17.55}$$

17.3.1 Slater functions

For Coulomb interaction $V = |\vec{r}-\vec{r}'|$,

$$F_\ell(r,r') = \frac{r^\ell_<}{r^{\ell+1}_>}. \tag{17.56}$$

For a Gaussian potential, $V = \exp(-\beta^2(\vec{r}-\vec{r}')^2)$,

$$F_\ell(r,r') = (2\ell+1)\exp(-\beta^2 r^2)\exp(-\beta^2 r'^2) i^\ell j_\ell(-2i\beta^2 rr'). \tag{17.57}$$

17.4 Center-of-mass

Let

$$\vec{R}_{\rm cm} = \frac{1}{A}\sum_i \vec{r}_i, \;\; \vec{P}_{\rm cm} = \frac{\hbar}{i}\sum_i \vec{\nabla}_i. \tag{17.58}$$

These have the correct commutation relation, that is, $[\vec{R}_{\rm cm}, \vec{P}_{\rm cm}] = i\hbar$, so that $\vec{P}_{\rm cm}$ is the conjugate momentum to $\vec{R}_{\rm cm}$. Then

$$\hat{H}_{\rm cm} = \frac{P_{\rm cm}^2}{2AM} + \frac{1}{2}AM\Omega^2 R_{\rm cm}^2. \tag{17.59}$$

It is useful to separate this out into one- and two-body parts:

$$\hat{H}_{\rm cm} = \frac{1}{2AM}\sum_i p_i^2 + \frac{1}{2A}M\Omega^2\sum_i r_i^2 + \frac{1}{2AM}\sum_{i\neq j}\vec{p}_i\cdot\vec{p}_j + \frac{1}{2A}M\Omega^2\sum_{i\neq j}\vec{r}_i\cdot\vec{r}_j \tag{17.60}$$

The one-body matrix elements can only change the radial quantum number:

$$\langle n'\,(\ell)\,j|\,\hat{H}_{\rm cm}\,|n'\,(\ell)\,j\rangle = \frac{1}{2AM}\,\langle n'\,(\ell)\,j|\,p^2\,|n'\,(\ell)\,j\rangle + \frac{1}{2A}M\Omega^2\,\langle n'\,(\ell\;)\,j|\,r^2\,|n'\,(\ell)\,j\rangle\,, \tag{17.61}$$

By Edmonds (7.1.7), and also Eq. (17.27) above,

$$\langle n'(\ell,1/2)jm|\mathcal{O}|n(\ell,1/2)jm\rangle = \frac{1}{[j]}\,\langle n'(\ell,1/2)j||\mathcal{O}||n(\ell,1/2)j\rangle = \frac{1}{[\ell]}(n'\ell||\mathcal{O}||n\ell) = (n'\ell|\mathcal{O}|n\ell) \tag{17.62}$$

Using the results for the appendix for matrix elements of r^2 and p^2, and using $b^2 = \hbar/M\Omega$, for the one-body term only $n' = n$ survives and

$$\langle n'\,(\ell,1/2)\,j|\,\hat{H}_{\rm cm}\,|n'\,(\ell,1/2)\,j\rangle = \frac{1}{A}(2n+\ell+3/2)\hbar\Omega \tag{17.63}$$

(note A^{-1} dependence). This gives the correct c.m. energy for 1-4 particles in the $0s$ shell, as a test.

For the two-body matrix elements, the non-antisymmeterized matrix elements are

$$(ab;J|H_{\rm cm}|cd;J) = \hbar\Omega\frac{1}{A}(-1)^{J+j_b+j_d+\ell_a+\ell_b}[j_a][j_b][j_c][j_d]\times \tag{17.64}$$

$$\left\{\begin{array}{ccc} j_a & j_c & 1 \\ j_d & j_b & J \end{array}\right\}\left\{\begin{array}{ccc} \ell_a & j_a & 1/2 \\ j_c & \ell_c & 1 \end{array}\right\}\left\{\begin{array}{ccc} \ell_b & j_b & 1/2 \\ j_d & \ell_d & 1 \end{array}\right\}$$

$$\times(\Delta N = 0)(n_a\ell_a||\vec{r}/b||n_c\ell_c)(n_b\ell_b||\vec{r}/b||n_d\ell_d) \tag{17.65}$$

Here the notation ($\Delta N = 0$) means that one cannot change the total principle quantum number, that is, $2(n_a + n_b) + \ell_a + \ell_b = 2(n_c + n_d) + \ell_c + \ell_d$. (When $\Delta N = 0$ the contributions from $\vec{p}\cdot\vec{p}$ equal that from $\vec{r}\cdot\vec{r}$; otherwise they cancel exactly.)

One can compute the needed one-body matrix elements:

$$(n_a\ell_a||\vec{r}/b||n_c\ell_c) = (-1)^{\ell_a}[\ell_a][\ell_c] \begin{pmatrix} \ell_a & 1 & \ell_c \\ 0 & 0 & 0 \end{pmatrix} (n_a\ell_a|r|n_c\ell_c)$$
$$= (-1)^{\ell_a+\ell_>}\sqrt{\ell_>}(n_a\ell_a|r|n_c\ell_c) \qquad (17.66)$$

whre $\ell_>$ is the greater of ℓ_a, ℓ_c, and where the last matrix element is just a radial integral, given below in the appendices. There are only four possible reduced one-body matrix elements, those with $\Delta N = +1$:

$$(n, \ell+1||\vec{r}/b||n,\ell) = \sqrt{(\ell+1)(n+\ell+3/2)}, \qquad (17.67)$$
$$(n+1, \ell-1||\vec{r}/b||n\ell) = \sqrt{\ell(n+1)}, \qquad (17.68)$$

and the conjugate $\Delta N = -1$ matrix elements,

$$(n, \ell-1||\vec{r}/b||n\ell) = -\sqrt{\ell(n+\ell+1/2)}, \qquad (17.69)$$
$$(n-1, \ell+1||\vec{r}/b||n,\ell) = -\sqrt{(\ell+1)n}. \qquad (17.70)$$

Note: In order to get agreement with other calculations, I need to multiply the two-body matrix elements above by a factor of 2. I haven't yet tracked it down.

17.5 Isospin versus proton-neutron formalisms

Because the nuclear interaction conserves isospin to about 1%, one often writes the nuclear Hamiltonian in a manifestly isospin-conserving formalism, as done above. Nonetheless, even in those cases, for actual calculations one may find an explicit proton-neutron decomposition useful.

Using

$$|T=0, M_T=0\rangle = \frac{1}{\sqrt{2}}\left(|\pi\nu\rangle - |\nu\pi\rangle\right)$$
$$|T=1, M_T=0\rangle = \frac{1}{\sqrt{2}}\left(|\pi\nu\rangle + |\nu\pi\rangle\right)$$
$$|T=1, M_T=1\rangle = |\pi\pi\rangle, \quad |T=1, M_T=-1\rangle = |\nu\nu\rangle, \qquad (17.71)$$

one finds that $\hat{H}_2 = \hat{H}_{pp} + \hat{H}_{nn} + \hat{H}_{pn}$ with

$$\hat{H}_{pp} = \frac{1}{4}\sum_{abcd}\sqrt{(1+\delta_{ab})(1+\delta_{cd})} \times \sum_J V_{J,T=1}(ab,cd)$$
$$\times \sum_M \hat{A}^\dagger_{JM}(a_\pi b_\pi)\hat{A}_{JM}(c_\pi d_\pi) \qquad (17.72)$$

with $\hat{H}_{nn}$ of identical structure, and

$$\hat{H}_{pn} = \frac{1}{2}\sum_{abcd}\sqrt{(1+\delta_{ab})(1+\delta_{cd})}\sum_{J}\left[V_{J,T=0}(ab,cd)+V_{J,T=1}(ab,cd)\right] \times\sum_{M}\hat{A}^{\dagger}_{JM}(a_\pi b_\nu)\hat{A}_{JM}(c_\pi d_\nu) \quad (17.73)$$

In all of these, a, b, c, d refer to all the quantum numbers *except* isospin.

The equation (17.73) is useful for some applications, such as mean-field calculations. For other applications, however, it is useful to relabel the orbits and treat all particles as identical particles. In this case we have

$$\hat{H}_2 = \frac{1}{4}\sum_{\alpha\beta\gamma\delta}\sqrt{(1+\delta_{\alpha\beta})(1+\delta_{\gamma\delta})}\sum_{J}V_J(\alpha\beta,\gamma\delta)\sum_{M}\hat{A}^{\dagger}_{JM}(\alpha\beta)\hat{A}_{JM}(\gamma\delta) \quad (17.74)$$

but with

$$V^{pp}_{J}(\alpha_\pi\beta_\pi,\gamma_\pi\delta_\pi) = V_{J,T=1}(ab,cd) \quad (17.75)$$

with the same for V^{nn}, and

$$V_J(\alpha_\pi\beta_\nu,\gamma_\pi\delta_\nu) = \frac{\sqrt{(1+\delta_{ab})(1+\delta_{cd})}}{2}\left[V_{J,T=0}(ab,cd)+V_{J,T=1}(ab,cd)\right] \quad (17.76)$$

Here, $\alpha, \beta, \gamma, \delta$ refer to the new orbits, where protons and neutrons are considered distinct orbits, while a, b, c, d are the old labels, with protons and neutrons in the same orbits.

To make things very clear, we write

$$\hat{H}^{pp} = \frac{1}{4}\sum_{abcd}\sqrt{(1+\delta_{ab})(1+\delta_{cd})}\sum_{J}V^{(pp)}_{J}(ab,cd) \times\sum_{M}\hat{A}^{(pp),\,\dagger}_{JM}(a_\pi b_\pi)\hat{A}^{(pp)}_{JM}(c_\pi d_\pi), \quad (17.77)$$

and

$$\hat{H}^{pn} = \sum_{abcd}\sum_{J}V^{(pn)}_{J}(ab,cd)\sum_{M}\hat{A}^{(pn),\,\dagger}_{JM}(a_\pi b_\nu)\hat{A}^{(pn)}_{JM}(c_\pi d_\nu). \quad (17.78)$$

What we if we want to go in the reverse direction? That is, from an interaction in proton-neutron formalism, which make break isospin, to an approximate but isospin-conserving interaction?

This issue is complicated by the choice of single-particle wavefunctions; if the proton and neutron wavefunctions are the same (i.e., harmonic oscillators) or may differ (i.e., from a mean-field or other calculation). In the following I assume the latter. Some of the details are in the next section (17.5.1).

$$V_{J,T=0}(ab,cd) = \frac{1}{2\sqrt{(1+\delta_{ab})(1+\delta_{cd})}} \tag{17.79}$$
$$\times \Big[V_J^{(pn)}(a_\pi b_\nu, c_\pi d_\nu) + (-1)^{j_a+j_b+j_c+j_d} V_J^{(pn)}(b_\pi a_\nu, d_\pi c_\nu)$$
$$-(-1)^{j_a+j_b+J} V_J^{(pn)}(b_\pi a_\nu, c_\pi d_\nu) - (-1)^{j_c+j_d+J} V_J^{(pn)}(a_\pi b_\nu, d_\pi c_\nu) \Big] ;$$
$$V_{J,T=1}(ab,cd) = \frac{1}{3} \Big\{ V_J^{(pp)}(ab,cd) + V_J^{(nn)}(ab,cd) \tag{17.80}$$
$$+\frac{1}{2\sqrt{(1+\delta_{ab})(1+\delta_{cd})}} \Big[V_J^{(pn)}(a_\pi b_\nu, c_\pi d_\nu)$$
$$+(-1)^{j_a+j_b+j_c+j_d} V_J^{(pn)}(b_\pi a_\nu, d_\pi c_\nu)$$
$$+(-1)^{j_a+j_b+J} V_J^{(pn)}(b_\pi a_\nu, c_\pi d_\nu) + (-1)^{j_c+j_d+J} V_J^{(pn)}(a_\pi b_\nu, d_\pi c_\nu) \Big] \Big\} . \tag{17.81}$$

In the above the proton-neutron states are normalized. Note that some configuration-interaction codes, such as `NuShell/NuShellX` use unnormalized matrix elements. In those cases

$$V_J^{upn}(ab,cd) = \frac{2}{\sqrt{(1+\delta_{ab})(1+\delta_{cd})}} V_J^{pn}(ab,cd), \tag{17.82}$$

where the superscript *upn* denotes the 'unnormalized' *pn* matrix elements and *pn* denotes the normalized *pn* matrix elements above.

17.5.1 Isospin breaking

In general, I prefer the explicit proton-neutron formalism, but using an isospin formalism has two uses: first, it allows us to unambiguously extract the isospin-conserving part of an interaction, and second, if we are interested in the part of the interaction which can change isospin by 1 or 2 units.

If we insist upon pairs of orbits (a,b) with $a \leq b$, there are six kinds of matrix elements in the proton-neutron formalism: $V_J^{(pp)}(ab,cd), V_J^{(nn)}(ab,cd)$, $V_J^{(pn)}(a_\pi b_\nu, c_\pi d_\nu)$ (where I make explicit whether an orbit contains a proton or a neutron) and $V_J^{(pn)}(b_\pi a_\nu, c_\pi d_\nu), V_J^{(pn)}(a_\pi b_\nu, d_\pi c_\nu)$, and $V_J^{(pn)}(b_\pi a_\nu, d_\pi c_\nu)$. While this might seem overmuch, let's consider coupling of isospins. Each pair creation operator $\hat{A}^\dagger_{JM}(ab)$ can have isospin $T = 0$ or 1, and the same for the pair annihilation operator $\hat{A}_{JM}(cd)$. Coupling together we can get an operator with total isospin $\Delta T = 0, 1$, or 2, which we call *isoscalar, isovector*, and *isotensor*, respectively. There are actually three isovector constructs, which I detail below.

As discussed previously, however, in section (15.5) and in particular (15.5.3), while $\hat{A}^\dagger_{JM}(ab)$ is a spherical tensor, $\hat{A}_{JM}(cd)$ is not. This means some subtlety in coupling their angular momentum is required, as discussed back in sections 15.5-15.5.3.

Ignoring angular momentum and focusing entirely on isospin, and using Eq. (15.59)

$$\left[\left[c_a^\dagger \times c_b^\dagger\right]_{T_c} \otimes [\tilde{c}_c \times \tilde{c}_d]_{T_a}\right]_{\Delta T,0}$$
$$= -\sum_{M_T} (-1)^{T_a+M_T} (T_c\, M_T, T_a\, -M_T|\Delta T 0) \hat{A}^\dagger_{T_c,M_T}(ab) \hat{A}_{T_a\, M_T}(cd), \quad (17.83)$$

where T_a is the isospin of the pair annihilation operator, T_c is the isospin of the pair creation operator, and ΔT is the isospin of the coupled operator. Here I consider only charge-conserving interactions, although the generalization is straightforward.

One can use the orthogonality of Clebsch-Gordan coefficients (15.24) to invert (17.83):

$$\hat{A}^\dagger_{T_c,M_T}(ab) \hat{A}_{T_a\, M_T}(cd) = -(-1)^{T_a+M_T} \sum_{\Delta T} (T_c\, M_T, T_a\, -M_T|\Delta T 0)$$
$$\times \left[\left[c_a^\dagger \times c_b^\dagger\right]_{T_c} \otimes [\tilde{c}_c \times \tilde{c}_d]_{T_a}\right]_{\Delta T,0} \quad (17.84)$$

With this in mind, we can enumerate the six matrix elements in isospin formalism, writing $V^{\Delta T}_{T_c,T_a}(ab,cd)$ (again suppressing angular momentum J):

Isoscalar: $V^0_{0,0}(ab,cd)$ and $V^0_{1,1}(ab,cd)$ (these correspond to $V_{J,T=0}(ab,cd)$ and $V_{J,T=1}(ab,cd)$ in our isospin-conserving formalism, respectively);

Isovector: $V^1_{0,1}(ab,cd)$, $V^1_{1,0}(ab,cd)$, and $V^1_{1,1}(ab,cd)$; and

Isotensor: $V^2_{1,1}(ab,cd)$.

There are manifestly six matrix elements, just as in the proton-neutron formalism. It is crucial to note that here isoscalar, isovector, and isotensor refer to the isospin rank of the *operator*, not of the two-body states. Sometimes people refer to the isospin-conserving matrix elements $V^0_{0,0}$ as *isoscalar* and $V^0_{1,1}$ as *isovector* matrix elements; the reader has to judge the appropriate meaning from the context.

To do the expansion, we need the Clebsch-Gordan coefficients, which are the same whether we are considering angular momentum or isospin (and, indeed, this is part of the motivation for isospin: once we've gone to the trouble of master the underlying algebra of angular momentum, we can apply it directly to isospin), given here:

T_c	T_a	M_T	ΔT	$(T_c\, M_T, T_c - M_T \vert \Delta T\, 0)$		
0	0	0	0	1	isoscalar	pn
1	1	0	0	$-1/\sqrt{3}$	isoscalar	pn
1	1	1	0	$1/\sqrt{3}$	isoscalar	pp
1	1	-1	0	$1/\sqrt{3}$	isoscalar	nn
1	0	0	1	1	isovector	pn
0	1	0	1	1	isovector	pn
1	1	0	1	0	isovector	pn
1	1	1	1	$1/\sqrt{2}$	isovector	pp
1	1	-1	1	$1/\sqrt{2}$	isovector	nn
1	1	0	2	$\sqrt{2/3}$	isotensor	pn
1	1	1	2	$1/\sqrt{6}$	isotensor	pp
1	1	-1	2	$1/\sqrt{6}$	isotensor	nn

With these coupling coefficients in hand, we can rewrite operators, which in turn will allow us to rewrite matrix elements. We first note that (still suppressing the J, M indices)

$$\begin{aligned}
\hat{A}^\dagger(a_\pi, b_\pi) &= \hat{A}^\dagger_{T=1,M_T=1}(a,b), \\
\hat{A}^\dagger(a_\nu b_\nu) &= \hat{A}^\dagger_{T=1,M_T=-1}(a,b), \\
\hat{A}^\dagger(a_\pi, b_\nu) &= \frac{1}{\sqrt{2}}\left(\hat{A}^\dagger_{T=0,M_T=0}(a,b) + \hat{A}^\dagger_{T=1,M_T=0}(a,b)\right),
\end{aligned} \tag{17.85}$$

where the subscripts π and ν denote proton and neutron orbitals, respectively. Thus we get

$$\begin{aligned}
\hat{A}^\dagger(a_\pi, b_\pi)\hat{A}(c_\pi, d_\pi) &= \hat{A}^\dagger_{T=1,M_T=1}(a,b)\hat{A}_{T=1,M_T=1}(c,d) \\
\hat{A}^\dagger(a_\nu, b_\nu)\hat{A}(c_\nu, d_\nu) &= \hat{A}^\dagger_{T=1,M_T=-1}(a,b)\hat{A}_{T=1,M_T=-1}(c,d) \\
\hat{A}^\dagger(a_\pi, b_\nu)\hat{A}(c_\pi, d_\nu) &= \frac{1}{2}\Big\{\hat{A}^\dagger_{T=0,M_T=0}(a,b)\hat{A}_{T=0,M_T=0}(c,d) \\
&+ \hat{A}^\dagger_{T=1,M_T=0}(a,b)\hat{A}_{T=0,M_T=0} + \hat{A}^\dagger_{T=0,M_T=0}(a,b)\hat{A}_{T=1,M_T=0} \\
&+ \hat{A}^\dagger_{T=1,M_T=0}(a,b)\hat{A}_{T=1,M_T=0}\Big\}
\end{aligned} \tag{17.86}$$

Finally, combining all these:

$$\begin{aligned}
\hat{A}^\dagger(a_\pi, b_\pi)\hat{A}(c_\pi, d_\pi) &= -\frac{1}{\sqrt{3}}\left[\left[c^\dagger_a \times c^\dagger_b\right]_1 \otimes [\tilde{c}_c \times \tilde{c}_d]_1\right]_{0,0} \\
&- \frac{1}{\sqrt{2}}\left[\left[c^\dagger_a \times c^\dagger_b\right]_1 \otimes [\tilde{c}_c \times \tilde{c}_d]_1\right]_{1,0} \\
&- \frac{1}{\sqrt{6}}\left[\left[c^\dagger_a \times c^\dagger_b\right]_1 \otimes [\tilde{c}_c \times \tilde{c}_d]_1\right]_{2,0},
\end{aligned} \tag{17.87}$$

$$\hat{A}^\dagger(a_\nu, b_\nu)\hat{A}(c_\nu, d_\nu) = -\frac{1}{\sqrt{3}}\left[\left[c^\dagger_a \times c^\dagger_b\right]_1 \otimes [\tilde{c}_c \times \tilde{c}_d]_1\right]_{0,0}$$

$$+ \quad \frac{1}{\sqrt{2}}\left[\left[c_a^\dagger \times c_b^\dagger\right]_1 \otimes [\tilde{c}_c \times \tilde{c}_d]_1\right]_{1,0} \tag{17.88}$$
$$- \quad \frac{1}{\sqrt{6}}\left[\left[c_a^\dagger \times c_b^\dagger\right]_1 \otimes [\tilde{c}_c \times \tilde{c}_d]_1\right]_{2,0},$$

and

$$\begin{aligned}
\hat{A}^\dagger(a_\pi, b_\nu)\hat{A}(c_\pi, d_\nu) &= -\frac{1}{2}\left[\left[c_a^\dagger \times c_b^\dagger\right]_0 \otimes [\tilde{c}_c \times \tilde{c}_d]_0\right]_{0,0} \\
+\frac{1}{2}\left[\left[c_a^\dagger \times c_b^\dagger\right]_1 \otimes [\tilde{c}_c \times \tilde{c}_d]_0\right]_{1,0} &+ \frac{1}{2}\left[\left[c_a^\dagger \times c_b^\dagger\right]_0 \otimes [\tilde{c}_c \times \tilde{c}_d]_1\right]_{1,0} \\
-\frac{1}{\sqrt{12}}\left[\left[c_a^\dagger \times c_b^\dagger\right]_1 \otimes [\tilde{c}_c \times \tilde{c}_d]_1\right]_{0,0} &+ \sqrt{\frac{2}{3}}\left[\left[c_a^\dagger \times c_b^\dagger\right]_1 \otimes [\tilde{c}_c \times \tilde{c}_d]_1\right]_{2,0}
\end{aligned} \tag{17.89}$$

In order to connect the six isospin components, we have to use all four permutations of the proton-neutron operators, i.e., $a_\pi b_\nu, c_\pi d_\nu$, $b_\pi a_\nu, c_\pi d_\nu$, $a_\pi b_\nu, d_\pi c_\nu$, and $b_\pi a_\nu, d_\pi c_\nu$. By using symmetries of the Clebsch-Gordan coefficients (and not forgetting the fundamental antisymmetry of fermions), which leads to

$$[c_a^\dagger \times c_b^\dagger]_{J,T} = -(-1)^{J+T-j_a-j_b-1}[c_b^\dagger \times c_a^\dagger]_{J,T}.$$

Using this, one can for example find

$$\begin{aligned}
(-1)^{J-j_a-j_b}\hat{A}^\dagger(b_\pi, a_\nu)\hat{A}(c_\pi, d_\nu) &= -\frac{1}{2}\left[\left[c_a^\dagger \times c_b^\dagger\right]_0 \otimes [\tilde{c}_c \times \tilde{c}_d]_0\right]_{0,0} \\
-\frac{1}{2}\left[\left[c_a^\dagger \times c_b^\dagger\right]_1 \otimes [\tilde{c}_c \times \tilde{c}_d]_0\right]_{1,0} &+ \frac{1}{2}\left[\left[c_a^\dagger \times c_b^\dagger\right]_0 \otimes [\tilde{c}_c \times \tilde{c}_d]_1\right]_{1,0} \\
+\frac{1}{\sqrt{12}}\left[\left[c_a^\dagger \times c_b^\dagger\right]_1 \otimes [\tilde{c}_c \times \tilde{c}_d]_1\right]_{0,0} &- \sqrt{\frac{2}{3}}\left[\left[c_a^\dagger \times c_b^\dagger\right]_1 \otimes [\tilde{c}_c \times \tilde{c}_d]_1\right]_{2,0}.
\end{aligned} \tag{17.90}$$

I leave it to the reader to find the other two permutations. Then one can invert the relationships, for example,

$$\begin{aligned}
&\left[\left[c_a^\dagger \times c_b^\dagger\right]_0 \otimes [\tilde{c}_c \times \tilde{c}_d]_0\right]_{0,0} = \\
&-\frac{1}{2}\Big\{\hat{A}^\dagger(a_\pi, b_\nu)\hat{A}(c_\pi, d_\nu) + (-1)^{j_a+j_b+j_c+j_d}\hat{A}^\dagger(b_\pi, a_\nu)\hat{A}(d_\pi, c_\nu) \\
&+(-1)^{J-j_a-j_b}\hat{A}^\dagger(b_\pi, a_\nu)\hat{A}(c_\pi, d_\nu) + (-1)^{J-j_c-j_d}\hat{A}^\dagger(a_\pi, b_\nu)\hat{A}(d_\pi, c_\nu)\Big\},
\end{aligned} \tag{17.91}$$

$$\begin{aligned}
&\left[\left[c_a^\dagger \times c_b^\dagger\right]_0 \otimes [\tilde{c}_c \times \tilde{c}_d]_1\right]_{1,0} = \\
&\frac{1}{2}\Big\{\hat{A}^\dagger(a_\pi, b_\nu)\hat{A}(c_\pi, d_\nu) - (-1)^{j_a+j_b+j_c+j_d}\hat{A}^\dagger(b_\pi, a_\nu)\hat{A}(d_\pi, c_\nu) \\
&+(-1)^{J-j_a-j_b}\hat{A}^\dagger(b_\pi, a_\nu)\hat{A}(c_\pi, d_\nu) - (-1)^{J-j_c-j_d}\hat{A}^\dagger(a_\pi, b_\nu)\hat{A}(d_\pi, c_\nu)\Big\},
\end{aligned} \tag{17.92}$$

$$\left[\left[c_a^\dagger \times c_b^\dagger\right]_1 \otimes [\tilde{c}_c \times \tilde{c}_d]_0\right]_{1,0} = \tag{17.93}$$
$$\frac{1}{2}\left\{\hat{A}^\dagger(a_\pi, b_\nu)\hat{A}(c_\pi, d_\nu) - (-1)^{j_a+j_b+j_c+j_d}\hat{A}^\dagger(b_\pi, a_\nu)\hat{A}(d_\pi, c_\nu)\right.$$
$$\left.-(-1)^{J-j_a-j_b}\hat{A}^\dagger(b_\pi, a_\nu)\hat{A}(c_\pi, d_\nu) + (-1)^{J-j_c-j_d}\hat{A}^\dagger(a_\pi, b_\nu)\hat{A}(d_\pi, c_\nu)\right\},$$

$$\left[\left[c_a^\dagger \times c_b^\dagger\right]_1 \otimes [\tilde{c}_c \times \tilde{c}_d]_1\right]_{1,0} = \tag{17.94}$$
$$\frac{1}{\sqrt{2}}\left\{\hat{A}^\dagger(a_\nu, b_\nu)\hat{A}(c_\nu, d_\nu) - \hat{A}^\dagger(a_\pi, b_\pi)\hat{A}(c_\pi, d_\pi)\right\}$$

17.6 One-body potentials as two-body interactions

Suppose I want to convert a single-particle energy to a two-body operator. This can be done, but at the price of a *number-dependent* coefficient.

I first consider the simple case of a diagonal energy,

$$\hat{U}_x^{(1)} = \epsilon_x \hat{N}_x = \epsilon_x \sum_m a_{x,m}^\dagger a_{x,m}$$

. One can easily show that

$$(\hat{N}-1)\hat{U}_x^{(1)} = \epsilon_x \sum_b \sum_m \sum_\mu a_{x,m}^\dagger a_{b,\mu}^\dagger a_{b,\mu} a_{x,m}. \tag{17.95}$$

For fixed particle number N, and coupling up to good angular momentum, the equivalent (but N-dependent) operator

$$\hat{U}_x^{(2)} = \frac{1}{N-1}\epsilon_x \sum_b \sum_{JM,TM_T} \hat{A}^\dagger(xb)_{JM,TM_T}\hat{A}(xb)_{JM,TM_T}. \tag{17.96}$$

Fully antisymmeterizing and putting into canonical form, one finds

$$V_{JT}(ab,cd) = \frac{1}{N-1}\frac{\epsilon_a+\epsilon_b}{1+\delta_{ab}}\left[\delta_{ac}\delta_{bd} + (-1)^{j_a+j_b+J+T}\delta_{ad}\delta_{bc}\right]. \tag{17.97}$$

This contribution to the interaction has to be recomputed for different numbers of particles.

We can simplify this to the most usual application:

$$V_{JT}(ab,ab) = \frac{1}{N-1}\left(\epsilon_a+\epsilon_b\right). \tag{17.98}$$

Suppose ϵ_{ab} is *not* diagonal, that is, we want a general one-body (scalar) potential. Let $U_{ab} = \langle a|\hat{U}|b\rangle$. As above, one can show

$$\hat{U}(\hat{N}-1) = \sum_{rs} U_{rs} \sum_t \sum JM \hat{A}^\dagger_{JM}(rt)\hat{A}_{JM}(st). \tag{17.99}$$

The generalization to include isospin is straightforward and obvious.

From this one derives

$$V^{(1)}_J(ab,cd) = \langle ab;JM|\hat{U}(\hat{N}-1)|cd;JM\rangle \tag{17.100}$$
$$= \frac{1}{\sqrt{(1+\delta_{ab})(1+\delta_{cd})}} \left(U_{ac}\delta_{bd} + \Phi_{cd}U_{ad}\delta_{bc} + \Phi_{ab}U_{bc}\delta_{ad} + U_{bd}\delta_{ac}\right)$$

where $\Phi_{ab} = -(-1)^{j_a+j_b+J+1+T}$ is the phase introduced by swapping a and b. We can simplify this: when $b = d$, as forced by δ_{bd}, then $j_b = j_d$ and, because both are half-integers, $2j_b$ must be an odd integer; and, because one has identical orbits, $J + T$ must be odd, so $j_b + j_d + J + T$ is therefore even, meaning that $\Phi_{bd} = +1$. This holds even in LS coupling, that is when j_a etc are actually integers, because in that case $L + S$ must be even. Then

$$V^{(1)}_J(ab,cb) = \langle ab;JM|\hat{U}(\hat{N}-1)|cb;JM\rangle \tag{17.101}$$
$$= \frac{1}{\sqrt{(1+\delta_{ab})(1+\delta_{cb})}} \left(U_{ac}(1+\delta_{bc}+\delta_{ab}) + U_{bb}\delta_{ac}\right),$$

which, if $U_{ab} = \epsilon_a\delta_{ab}$ is diagonal, reduces to the above. Another special case, easy for comparison, is

$$V^{(1)}_J(ab,ab) = U(a,a) + U(b,b). \tag{17.102}$$

17.7 Center-of-mass

In nuclear physics especially, one worries about the center of mass and going between the lab frame and the relative or center-of-mass frame. This is less important in the electronic structure of atoms and molecules as the nuclei dominate the center of mass, providing a fixed lab frame.

For A particles of the same mass M, with lab frame coordinates $\vec{r}_i, i = 1 \ldots A$, the general Hamiltonian for a system of A particles with the same mass M interacting by a relative potential $V(\vec{r}_i - \vec{r}_j)$ is:

$$\sum_{i=1}^{A} \frac{p_i^2}{2M} + \sum_{i<j} V(\vec{r}_i - \vec{r}_j). \tag{17.103}$$

The restricted sum $i < j$ prevents double counting interactions; because the potential is symmetric, one can replace $\sum_{i<j}$ by $\frac{1}{2}\sum_{i\neq j}$. We define the lab frame kinetic energy as

$$\mathrm{KE}_{\mathrm{lab}} = \sum_{i=1}^{A} \frac{p_i^2}{2M}. \tag{17.104}$$

But because physics should be independent of center-of-mass motion, we should try to factor that out. To do that, we first consider the center-of-mass coordinate,

$$\vec{R}_{\rm c.m.} = \frac{1}{A}\sum_{i=1}^{A}\vec{r}_i. \tag{17.105}$$

Then we can define the conjugate center-of-mass momentum to be

$$\vec{P}_{\rm c.m.} = \sum_{i=1}^{A}\vec{p}_i = \sum_i \frac{\hbar}{i}\nabla_i, \tag{17.106}$$

so that for each direction x, y, z we still satisfy the fundamental commutation relation

$$[R_{\rm c.m.,x}, P_{c.m.,x}] = i\hbar, \tag{17.107}$$

etc..

The center-of-mass kinetic energy is

$$\mathrm{KE}_{\rm c.m.} = \frac{P^2_{\rm c.m.}}{2AM} \tag{17.108}$$

because the whole system has, ignoring binding energy, mass AM. We rewrite explicitly

$$\mathrm{KE}_{\rm c.m.} = \frac{1}{2AM}\sum_{i=1}^{A} p_i^2 + \frac{1}{2AM}\sum_{i\neq j}\vec{p}_i\cdot\vec{p}_j \tag{17.109}$$

In the lab frame, the first term is explicitly a one-body operator, because it is a sum of terms depending upon only one coordinate, while the second term is explicitly two-body because each term requires the coordinates of two different particles.

Straightforward algebra shows that

$$\mathrm{KE}_{\rm lab} = \mathrm{KE}_{\rm c.m.} + \mathrm{KE}_{\rm rel}, \tag{17.110}$$

where

$$\mathrm{KE}_{\rm rel} = \sum_{i<j}\frac{1}{2AM}\left(\vec{p}_i - \vec{p}_j\right)^2. \tag{17.111}$$

To make this clear, expand this last out, starting by replacing $\sum_{i<j}$ with $\frac{1}{2}\sum_{i\neq j}$:

$$\mathrm{KE}_{\rm rel} = \frac{1}{2}\sum_{i\neq j}\frac{1}{2AM}\left(\vec{p}_i - \vec{p}_j\right)^2 \tag{17.112}$$

$$= \frac{1}{4AM}\sum_{i\neq j}\left(p_i^2 + p_j^2 - 2\vec{p}_i\cdot\vec{p}_j\right)^2. \tag{17.113}$$

The sum $\sum_{i\neq j} p_i^2 + p_j^2$ must be counted carefully:

$$\sum_{i\neq j} p_i^2 + p_j^2 = \sum_{i,j}(p_i^2 + p_j^2) - \sum_i (p_i^2 + p_i^2) = 2(A-1)\sum_i p_i^2$$

leaving us with

$$\mathrm{KE}_{\mathrm{rel}} = \frac{(A-1)}{2AM}\sum_{i=1}^{A} p_i^2 - \frac{1}{2AM}\sum_{i\neq j}\vec{p}_i\cdot\vec{p}_j, \tag{17.114}$$

which satisfies (17.110).

How do we interpret $\mathrm{KE}_{\mathrm{rel}}$? One approach to illuminate the issue is to add in a confining potential,

$$\mathrm{PE}_{\mathrm{lab}} = \frac{1}{2}M\Omega^2 R_{\mathrm{lab}}^2 = \sum_{i=1}^{A}\frac{1}{2}M\Omega^2 r_i^2. \tag{17.115}$$

We then introduce the center-of-mass potential energy,

$$\mathrm{PE}_{\mathrm{cm}} = \frac{1}{2}AM\Omega^2 R_{\mathrm{c.m.}}^2 = \frac{1}{2A}M\Omega^2\left(\sum_{i=1}^{A} r_+^2 \sum_{i\neq j}\vec{r}_i\cdot\vec{r}_j\right) \tag{17.116}$$

and then as before

$$\mathrm{PE}_{\mathrm{lab}} = \mathrm{PE}_{\mathrm{c.m.}} + \mathrm{PE}_{\mathrm{rel}}, \tag{17.117}$$

with

$$\mathrm{PE}_{\mathrm{rel}} = \sum_{i<j}\frac{1}{2A}M\Omega^2\left(\vec{r}_i - \vec{r}_j\right)^2. \tag{17.118}$$

Combining these, we get the relative harmonic oscillator Hamiltonian

$$H_{\mathrm{rel}}^{h.o.} = \sum_{i<j}\frac{1}{2AM}\left(\vec{p}_i - \vec{p}_j\right)^2 + \frac{1}{2A}M\Omega^2\left(\vec{r}_i - \vec{r}_j\right)^2 \tag{17.119}$$

In the relative two-body frame, $\vec{p}_{ij} = (\vec{p}_i - \vec{p}_j)/2$ is the conjugate momentum to the relative coordinate $\vec{r}_{ij} = (\vec{r}_i - \vec{r}_j)$ (again the factor of $1/2$ arises to preserved the canonical commutation relation). We then rewrite this so it looks like the standard harmonic oscillator:

$$\sum_{i<j}\frac{1}{2(AM/4)}p_{ij}^2 + \frac{1}{2}\left(\frac{AM}{4}\right)\frac{4\Omega^2}{A^2}r_{ij}^2 \tag{17.120}$$

that is, with an effective mass of $AM/4$ and an effective frequency of $2\Omega/A$. While this looks strange, we find that the harmonic oscillator wavefunctions always have oscillator length

$$b = \sqrt{\frac{\hbar}{m_{\mathrm{eff}}\omega_{\mathrm{eff}}}} = \sqrt{\frac{2\hbar}{M\Omega}}, \tag{17.121}$$

that is, independent of A, but with the standard reduced mass for two particles of $M/2$. The energies, however, scale as $1/A$.

One can consider the "relative" rms radius using the operator

$$R^2_{\rm el} = \frac{1}{A}\sum_{i<j}\left(\vec{r}_i - \vec{r}_j\right)^2 . \tag{17.122}$$

If we expand it out,

$$R^2_{\rm rel} = \frac{1}{A}\left[(A-1)\sum_i r_i^2 - \sum_{i\neq j}\vec{r}_i\cdot\vec{r}_j\right] . \tag{17.123}$$

The second term is manifestly a two-body operator, because i cannot be the same as j so i and j must label two different particles. But the first term looks like a sum of one-body operators r_i.

Notice, however, the factor of $A-1$ in front, so that if there is only one particle, $A=1$, then both terms vanish as we expect. In fact we can convert this first term into a manifestly two-body operator by the old trick of multiplying by $(\hat{N}-1)/(A-1)$ which is 1 for any $A>1$, and we then have

$$R^2_{\rm rel} = \frac{1}{A}\left[\sum_i r_i^2(\hat{N}-1) - \sum_{i\neq j}\vec{r}_i\cdot\vec{r}_j\right] . \tag{17.124}$$

which is a purely two-body operator whose terms do not depend upon A. Below we will derive the lab-frame matrix elements of this operator two different ways.

Before doing that, let's arrive at this operator a second way. We can define the coordinate of the ith particle relative to the center of mass by

$$\vec{r}_i^{\,\rm rel} = \vec{r}_i - \vec{R}_{\rm c.m.}. \tag{17.125}$$

Note that $\sum_i \vec{r}_i^{\,\rm rel} = 0$ as it should. A "natural" measure of the size of a many-body system, independent of the position of the center of mass, would be

$$\sum_{i=1}^{A}\left(\vec{r}_i^{\,\rm rel}\right)^2 \tag{17.126}$$

which we can expand to get

$$R^2_{\rm rel} = \left(1-\frac{1}{A}\right)\sum_{i=1}^{A} r_i^2 - \frac{1}{A}\sum_{i\neq j}\vec{r}_i\cdot\vec{r}_j \tag{17.127}$$

the same as before.

17.7.1 Calculation of the matrix elements in the lab frame

We want to compute

$$\begin{aligned}\langle n_a l_a, n_b l_b; LS|R^2_{\rm rel}|n_c l_c, n_d l_d; LS\rangle = \\ = \frac{1}{A}\langle n_a l_a, n_b l_b; LS|r^2(\hat{N}-1)|n_c l_c, n_d l_d; LS\rangle \\ -\frac{1}{A}\langle n_a l_a, n_b l_b; LS|\vec{r}_1\cdot\vec{r}_2|n_c l_c, n_d l_d; LS\rangle\end{aligned} \tag{17.128}$$

The one body piece is easy, computing the one-body potential

$$\langle n_a l_a|r^2|n_b l_b\rangle\delta_{l_a,l_b} \tag{17.129}$$

and embedding it in a two-body matrix element as described above.

We start with the two-body matrix element,

$$-\langle n_a l_a, n_b l_b; LS|\vec{r}_1\cdot\vec{r}_2|n_c l_c, n_d l_d; LS\rangle \tag{17.130}$$

which is independent of S. Using Edmonds (7.1.6),

$$= -(-1)^{l_c+l_b+L}\left\{\begin{array}{ccc} L & l_b & l_a \\ 1 & l_c & l_d\end{array}\right\}\langle n_a l_a||\vec{r}||n_c l_c\rangle\langle n_b l_b||\vec{r}||n_d l_d\rangle. \tag{17.131}$$

Using

$$\vec{r}_m = r\sqrt{\frac{4\pi}{3}}Y_{1m},$$

we get

$$\begin{aligned}\langle n_a l_a||\vec{r}||n_c l_c\rangle = (n_a l_a|r|n_c l_c)\sqrt{\frac{4\pi}{3}}\langle Y_{l_a}||Y_1||Y_{l_c}\rangle \\ = (-1)^{l_a}\sqrt{(2l_a+1)(2l_c+1)}\left(\begin{array}{ccc} l_a & 1 & l_c \\ 0 & 0 & 0\end{array}\right)(n_a l_a|r|n_c l_c)\end{aligned} \tag{17.132}$$

which we got using (Edmonds 5.4.5)

$$\langle Y_{l_a}||Y_k||Y_{l_c}\rangle = (-1)^{l_a}\sqrt{\frac{(2l_a+1)(2l_c+1)(2k+1)}{4\pi}}\left(\begin{array}{ccc} l_a & k & l_c \\ 0 & 0 & 0\end{array}\right) \tag{17.133}$$

The necessary matrix elements are found elsewhere.

Then the final matrix element is

$$\begin{aligned}-(-1)^{l_a+l_c+L}\sqrt{(2l_a+1)(2l_b+1)(2l_c+1)(2l_d+1)}\left\{\begin{array}{ccc} L & l_b & l_a \\ 1 & l_c & l_d\end{array}\right\} \\ \times\left(\begin{array}{ccc} l_a & 1 & l_c \\ 0 & 0 & 0\end{array}\right)\left(\begin{array}{ccc} l_b & 1 & l_d \\ 0 & 0 & 0\end{array}\right)\langle n_a l_a|r|n_c l_c\rangle\langle n_b l_b|r|n_d l_d\rangle\end{aligned} \tag{17.134}$$

which must still be antisymmeterized, and where $\langle n_a l_a|r|n_c l_c\rangle$ is a purely radial integral.

17.7.2 Calculation of the matrix elements in the relative frame: Talmi-Brody-Moshinsky brackets

The harmonic oscillator basis is useful for many reasons. One of these is that it is easy to go between the center-of-mass or relative frame and the lab frame.

Although one can compute few-body systems in relative or Jacobi coordinates, beyond 4 particles this becomes increasingly difficult; the hindrance is antisymmeterization of the particles. Therefore most many-body calculations are carried out in the lab frame, with matrix elements of the form

$$V_J(ab,cd) = \langle ab; J|\hat{V}|cd; J\rangle$$

We've written these out before as an integral. But if one is working in a harmonic oscillator basis, one can compute the matrix elements in the center-of-mass or relative frame and then have a finite transformation to the lab frame, as I'll explicate here.

Consider two particles, labeled a and b with coordinates $\vec{r}_a$ and $\vec{r}_b$, respectively; we'll leave off antisymmeterization until later. In the lab frame, the basis states for the (non-symmeterized) two-particle wavefunction will look like

$$\phi_a(\vec{r}_a)\phi_b(\vec{r}_b).$$

But one could also work in relative and center-of-mass coordinates, $\vec{r}$ and $\vec{R}$ respectively, and write basis states

$$\phi_{\rm rel}(\vec{r})\Phi_{\rm c.m.}(\vec{R}).$$

The key idea, of course, is to expand the lab frame wavefunction in terms of the relative and center-of-mass wavefunctions:

$$\phi_a(\vec{r}_a)\phi_b(\vec{r}_b) = \sum c_{ij}\phi_i(\vec{r})\Phi_j(\vec{R})$$

This change of basis is advantageous because any relative interaction will not change the center-of-mass wavefunction. To make this more clear, let's use the Dirac notation, but leave off angular momentum for the moment:

$$|a\rangle|b\rangle = \sum c(ab,ij)|i_{\rm rel}\rangle|j_{\rm c.m.}\rangle$$

and then the matrix element is expanded

$$V(ab,cd) = \langle a,b|\hat{V}|c,d\rangle = \sum c^*(ab,ij)c(cd,kl)\langle i_{\rm rel}, j_{\rm c.m.}|\hat{V}|\langle k_{\rm rel}, l_{\rm c.m.}\rangle \tag{17.135}$$

but as I just argued, if $\hat{V}$ is a relative operator, we must have $j_{\rm c.m.} = l_{\rm c.m.}$ and so simplify

$$V(ab,cd) = \langle a,b|\hat{V}|c,d\rangle = \sum c^*(ab,ij)c(cd,kj)\langle i_{\rm rel}|\hat{V}|\langle k_{\rm rel}\rangle \tag{17.136}$$

While one can do this in principle for any basis, for the harmonic oscillator the sum is finite, and the coefficients, known variously as the Brody-Moshinsky brackets or Talmi-Moshinsky brackets, can be computed analytically.

The key to understanding why the sum is finite is to recognize that the harmonic oscillator for a system of particles, alone among all systems, can be solved analytically in both the lab frame and in the relative / center-of-mass frame. Most of the work has already been done above, but let's redo it

Consider the Hamiltonian in the lab frame for two particles in a harmonic oscillator potential,

$$H = \frac{1}{2M}\vec{p}_1^2 + \frac{1}{2M}\vec{p}_2^2 + \frac{1}{2}M\Omega^2\vec{r}_1^2 + \frac{1}{2}M\Omega^2\vec{r}_2^2 \tag{17.137}$$

which we can solve immediately by separating into two lab frame Hamiltonians, $H = H_1 + H_2$, with

$$H_i = \frac{1}{2M}\vec{p}_i^2 + \frac{1}{2}M\Omega^2\vec{r}_i^2 \tag{17.138}$$

The eigenenergies of the Hamiltonian (17.137) are clearly

$$E = \hbar\Omega\left(N_1 + N_2 + 3\right) = \hbar\Omega\left(2n_1 + l_1 + 2n_2 + l_2 + 3\right) \tag{17.139}$$

where N_i, n_i, and l_i are the principal quantum number, radial nodal quantum number, and orbital angular momentum of particle i.

But we can transform to a different coordinate set, related to the usual relative and center-of-mass coordinates although for convenience with slightly different coefficients:

$$\vec{r} = \frac{1}{\sqrt{2}}\left(\vec{r}_1 - \vec{r}_2\right), \vec{R} = \frac{1}{\sqrt{2}}\left(\vec{r}_1 + \vec{r}_2\right), \tag{17.140}$$

$$\vec{p} = \frac{1}{\sqrt{2}}\left(\vec{p}_1 - \vec{p}_2\right), \vec{P} = \frac{1}{\sqrt{2}}\left(\vec{p}_1 + \vec{p}_2\right). \tag{17.141}$$

With these coordinates the Hamiltonian can also be written as

$$H = \frac{1}{2M}\vec{p}^2 + \frac{1}{2M}\vec{P}^2 + \frac{1}{2}M\Omega^2\vec{r}^2 + \frac{1}{2}M\Omega^2\vec{R}^2 = H_r + H_R \tag{17.142}$$

with

$$H_r = \frac{1}{2M}\vec{p}^2 + \frac{1}{2}M\Omega^2\vec{r}^2, H_R = \frac{1}{2M}\vec{P}^2 + \frac{1}{2}M\Omega^2\vec{R}^2, \tag{17.143}$$

and the energies are now

$$E = \hbar\Omega\left(N_r + N_R + 3\right) = \hbar\Omega\left(2n_r + l_r + 2n_R + l_R + 3\right). \tag{17.144}$$

(If we had not used the factor of $\sqrt{2}$ in the the transformation, the frequencies would be mismatched.)

Now comes the great but believeable leap: for any given two-particle wavefunction in the lab frame, which we write as $|n_a l_a, n_b l_b\rangle$, we can expand it in terms of wavefunctions in the 'relative' coordinate $\vec{r}$ and 'center-of-mass' coordinate $\vec{R}$, but the energies much match, that is

$$|n_a l_a, n_b l_b\rangle = \sum c(n_a l_a n_b l_b, n_r l_r n_R l_R)|n_r l_r, n_R l_R\rangle \tag{17.145}$$

but with the restriction that the energies match, that is

$$2(n_a + n_b) + l_a + l_b = 2(n_r + n_R) + l_r + l_R \tag{17.146}$$

One can do this in one-dimension easily enough using creation and annilation operators. The coefficient c are the Talmi-Brody-Moshinsky brackets, usually written in analogy to Clebsch-Gordan coefficients (for, like them, they are a unitary transformation based upon group theory)

$$\langle n_a l_a, n_b l_b; L | n_r l_r, n_R l_R; L \rangle \tag{17.147}$$

where one also has to account for the total orbital angular momentum L. There exist both tables of the coefficients as well as accessible routines for computing them.

We do have to worry about the relative coordinate. The matrix element in relative coordinates is

$$\langle n'_r l_r | (\vec{r}_1 - \vec{r}_2)^2 | n_r l_r \rangle = 2 \langle n'_r l_r | r^2 | n_r l_r \rangle \tag{17.148}$$

using Eq.(17.140). (We should also do this transformation for other interaction as well. For example, if we have a square well, so that $V = -V_0$ for $|\vec{r}_1 - \vec{r}_2| < R_0$ then it is also for $r < R_0/\sqrt{2}$.

The entire formula now is:

$$\begin{aligned} V_L(a,b,c,d) &= \langle n_a l_a, n_b l_b; L | \hat{V}(\vec{r}_1 - \vec{r}_2) | n_c l_c, n_d l_d; L \rangle \\ = \sum_{n_r l_r, n'_r, n_R n_R} & \langle n_a l_a, n_b l_b; L | n_r l_r, n_R l_R; L \rangle \langle n_c l_c, n_d l_d; L | n'_r l_r, n_R l_R; L \rangle \\ & \times \langle n_r l_r | V(\sqrt{2} r) | n'_r l_r | \rangle \end{aligned} \tag{17.149}$$

This is automatically antisymmetric. Note that we cannot change l_r because the interaction is a scalar, nor can we change n_R or l_R because those are center-of-mass coordinates.

Now let's test the two results against each other for simple cases. First, take the matrix elements where $a = b = c = d = 0s$. For computing in the lab frame, this arises strictly from the "single-particle" contribution, where $\langle 0s | r^2 | 0s \rangle = 3/2$. From Eq.(17.102) this has $V = 3$. From the relative frame, there is only one contribution, from $2\langle 00 | r^2 | 00 \rangle = 3$ as well. The Talmi-Brody-Moshinsky bracket is $\langle 0000, 0 | 0000, 0 \rangle = 1$ by inspection (because there can't be any other). So these two agree.

Now let's take the case $a = b = 0s, c = d = 0p, L = 0$. In the lab frame,

$$\langle 0s, 0s; L = 0 | (\vec{r}_1 - \vec{r}_2)^2 | 0p, 0p; L = 0 \rangle = \langle 0s, 0s | r_1^2 + r_2^2 - 2\vec{r}_1 \cdot \vec{r}_2 | 0p, 0p \rangle \tag{17.150}$$

but only the last term contributes (do you see why?). Then

$$-2 langle 0s, 0s | \vec{r}_1 \cdot \vec{r}_2 | 0p, 0p \rangle = +2 \left\{ \begin{array}{ccc} 0 & 0 & 0 \\ 1 & 1 & 1 \end{array} \right\} \langle 0s || \vec{r} || 0p \rangle^2 \tag{17.151}$$

(using Edmonds 7.1.6) and then by using (17.132) we get

$$+2\times 3\times \left\{ \begin{array}{ccc} 0 & 0 & 0 \\ 1 & 1 & 1 \end{array} \right\} \left(\begin{array}{ccc} 1 & 1 & 0 \\ 0 & 0 & 0 \end{array} \right)^2 \langle 0s|r|0p\rangle^2 \tag{17.152}$$

and we can look up each of these terms to get $-\sqrt{3}$. Antisymmeterization returns the same result, as we have two terms have the same value but we divide by 2 because $a = b$ and $c = d$.

Working from the relative frame, we have only have $n_r = 0$, $l_r = 0$, $n_R = 0$ and $l_R = 0$, but $n'_r = 1$. Then we have

$$\langle 00, 00; 0|00, 00; 0\rangle = 1; \tag{17.153}$$

$$\langle 01, 01; 0|20, 00; 0\rangle = +1/\sqrt{2}; \tag{17.154}$$

$$\langle 00|2r^2|10\rangle = -\sqrt{6} \tag{17.155}$$

so that the final result is $-\sqrt{3}$.

17.8 Calculation of the matrix elements in the relative frame: the general case

To make this suitable for nuclear physics, we have to put in spin. That is, we want the lab frame two-body matrix element

$$\langle n_a(l_a, 1/2)j_a, n_b(l_b, 1/2)j_b : JM|V_{\rm rel}|n_c(l_c, 1/2)j_c, n_d(l_d, 1/2)j_d : JM\rangle \tag{17.156}$$

in terms of relative matrix elements $\langle n'_r l'_r, S'; J_r|V(\sqrt{2}r)|n_r l_r, S; J_r\rangle$. We assume the relative interaction cannot change the total angular momentum, but it can change the spin S to S', and here one can change the relative angular momentum l_r. For a parity conserving interaction, $l'_r = l_r$ or $l_r \pm 2$, with the latter only as long as $S' = S = 1$. If we have a parity non-conserving interaction, then $l'_r = l_r \pm 1$ and at least one of S', S must be 1.

By transforming from j-j coupling to L-S coupling as in Eqn. (15.84),

$$\begin{aligned} &\langle n_a(l_a, 1/2)j_a, n_b(l_b, 1/2)j_b : J|\,\hat{H}\,|n_c(l_c, 1/2)j_b, n_d(l_d, 1/2)j_d : J\rangle = \\ &\qquad \sum_{L_{ab},S_{ab},L_{cd},S_{cd}} [j_a][j_b][L_{ab}][S_{ab}] \left\{ \begin{array}{ccc} l_a & 1/2 & j_a \\ l_b & 1/2 & j_b \\ L_{ab} & S_{ab} & J \end{array} \right\} \\ &\qquad\qquad [j_c]\,[j_d][L_{cd}][S_{cd}] \left\{ \begin{array}{ccc} l_c & 1/2 & j_c \\ l_d & 1/2 & j_d \\ L_{cd} & S_{cd} & J \end{array} \right\} \\ &\langle (n_a l_a, n_b l_b)L_{ab}, (1/2, 1/2)S_{ab} : J|\,\hat{H}\,|(n_c l_c, n_d l_d)L_{cd}, (1/2, 1/2)S_{cd} : J\rangle\,. \end{aligned} \tag{17.157}$$

The next step is to transform the spatial part to the relative frame using Talmi-Brody-Moshinsky brackets, but before that, we need to separate out the contributions from the spatial and spin parts. Towards this end, decompose the

interaction $\hat{H}$ into spatial and spin operators, of rank K each coupled up to an angular momentum scalar (total angular momentum zero), that is, we assume

$$\hat{H} = [\hat{O}^{\rm space}_K \otimes \hat{O}^{\rm spin}_K]_0 \tag{17.158}$$

and then [applying Edmonds 7.1.6, though modified]

$$\langle (n_a l_a, n_b l_b) L_{ab}, (1/2,1/2) S_{ab} : J | \, \hat{H} \, | (n_c l_c, n_d l_d) L_{cd}, (1/2,1/2) S_{cd} : J \rangle = \frac{[J]}{[k]} (-1)^{L_{cd}+S_{ab}+J+k} \left\{ \begin{array}{ccc} L_{ab} & L_{cd} & k \\ S_{cd} & S_{ab} & J \end{array} \right\} \times \langle (n_a l_a, n_b l_b) L_{ab} || \hat{O}^{\rm space}_K || (n_c l_c, n_d l_d) L_{cd} \rangle \langle (1/2,1/2) S_{ab} || \hat{O}^{\rm spin}_K || (1/2,1/2) S_{cd} \rangle . \tag{17.159}$$

Now apply the Talmi-Brody-Moshinsky brackets

$$\langle (n_a l_a, n_b l_b) L_{ab} || \hat{O}^{\rm space}_K || (n_c l_c, n_d l_d) L_{cd} \rangle = \sum_{n_R, L_R, n_r, n'_r, l_r, l'_r} \langle n'_r l'_r || \hat{O}^{\rm space}_K || n_r l_r \rangle \times \langle n_a l_a, n_b l_b : L_{ab} | n'_r l'_r, n_R l_R : L_{ab} \rangle \langle n_c l_c, n_d l_d : L_{cd} | n_r l_r, n_R l_R : L_{cd} \rangle \tag{17.160}$$

17.9 Summary

What you should get from this Chapter: a detailed discussion of the angular momentum (and isospin) coupling of scalar Hamiltonians, and methods and examples for computing the matrix elements.

17.10 Exercises

(18.x) Let $\hat{\pi}^\dagger_a, \hat{\nu}^\dagger_b$ be creation operators for protons and neutrons respectively, which means they both have $t = 1/2$ and $m_t = +1/2$ and $-1/2$ respectively. Ignoring angular momentum, one can introduce the two-body states

$$\hat{A}(ab)_{T=0,M_T=0} = \frac{1}{\sqrt{2}} \left(\hat{\pi}^\dagger_a \hat{\nu}^\dagger_b - \hat{\nu}^\dagger_a \hat{\pi}^\dagger_b \right),$$

$$\hat{A}(ab)_{T=1,M_T=1} = \hat{\pi}^\dagger_a \hat{\pi}^\dagger_b, \quad \hat{A}(ab)_{T=1,M_T=-1} = \hat{\nu}^\dagger_a \hat{\nu}^\dagger_b$$

$$\hat{A}(ab)_{T=1,M_T=0} = \frac{1}{\sqrt{2}} \left(\hat{\pi}^\dagger_a \hat{\nu}^\dagger_b + \hat{\nu}^\dagger_a \hat{\pi}^\dagger_b \right),$$

as well as the one-body operators

$$\hat{\rho}(ac)_{I=0,\mu_I=0} = \frac{1}{\sqrt{2}} \left(\hat{\pi}^\dagger_a \tilde{\nu}_b - \hat{\nu}^\dagger_a \tilde{\pi}_b \right) = -\frac{1}{\sqrt{2}} \left(\hat{\pi}^\dagger_a \hat{\pi}_b + \hat{\nu}^\dagger_a \hat{\nu}_b \right)$$

$$\hat{\rho}(ac)_{I=1,\mu_I=0} = \frac{1}{\sqrt{2}}\left(\hat{\pi}_a^\dagger \tilde{\nu}_b + \hat{\nu}_a^\dagger \tilde{\pi}_b\right) = -\frac{1}{\sqrt{2}}\left(\hat{\pi}_a^\dagger \hat{\pi}_b - \hat{\nu}_a^\dagger \hat{\nu}_b\right)$$

$$\hat{\rho}(ac)_{I=1,\mu_I=1} = \hat{\pi}_a^\dagger \tilde{\nu}_b = +\hat{\pi}_a^\dagger \hat{\pi}_b,$$

$$\hat{\rho}(ac)_{I=1,\mu_I=-1} = \hat{\nu}_a^\dagger \tilde{\pi}_b = -\hat{\nu}_a^\dagger \hat{\nu}_b.$$

Show

$$\hat{\rho}(ac)_{I=0,\mu_T=0}\hat{\rho}(bd)_{I=0,\mu_T=0} =$$

$$\frac{1}{2}\hat{A}^\dagger(ab)_{T=0,M_T=0}\hat{A}(cd)_{T=1,M_T=0} + \frac{1}{2}\sum_{M_T=-1}^{1}\hat{A}^\dagger(ab)_{T=1,M_T}\hat{A}(cd)_{T=0,M_T}$$

and

$$\sum_{\mu_T=-1}^{1}\hat{\rho}(ac)_{I=1,\mu_T}\hat{\rho}(bd)_{I=1,\mu_T} =$$

$$\frac{1}{2}\hat{A}^\dagger(ab)_{T=0,M_T=0}\hat{A}(cd)_{T=0,M_T=0} - \frac{1}{6}\sum_{M_T=-1}^{1}\hat{A}^\dagger(ab)_{T=1,M_T}\hat{A}(cd)_{T=1,M_T}$$

This is a way to derive the isospin dependence in subsection 17.2.2.

(18.yy) Derive the induced valence single-particle energies from a filled core, that is, show

$$\epsilon_a = \frac{1}{2j_a+1}\sum_{b\in\text{core}}\sum_J (2J+1)V_J(ab,ab), \tag{17.161}$$

for valence orbit a. Show the generalization to protons and neutrons is

$$\epsilon_a = \frac{1}{2j_a+1}\sum_{b\in\text{core}}\sum_J \frac{2J+1}{2}\left(V_{J,T=0}(ab,ab) + 3V_{J,T=1}(ab,ab)\right). \tag{17.162}$$

Chapter 18

Master class problems and miscellaneous exercises

> We in science are spoiled by the success of mathematics. Mathematics is the study of problems so simple that they have good solutions.– *Whitfield Diffie*

18.1 Master class problem: particle-hole transformation

Back in Chapter 8 we looked at quasiparticles, admixtures of creation and annihilation operators, via the Bogoliubov transformation, i.e.,

$$\hat{c}^\dagger = u\hat{a}^\dagger - v\hat{a}, \tag{18.1}$$

etc.. If $u = 1$ and $v = 0$ then the quasiparticle is just a particle, but if $u = 0$ and $v = 1$ then the quasiparticle is a *hole*. Fermion holes have the same anticommunication relations as fermion particles; I won't consider bosons, but the generalization is straightforward. We can transform any problem from a particle representation to a hole representation, which is called a particle-hole transformation or a *Pandya* transformation. While the hole representation is mathematically equivalent to the particle representation, it can aid us either numerically or conceptually. For example, while ^{18}O can be considered as two particles outside a closed ^{16}O core, or magnesium as having two electrons outside a closed neon atom, ^{14}C can be considered as having two holes in a closed ^{16}O nucleus, or an oxygen atom as having two holes in a closed neon atom.

Deriving the Pandya transform is straightforward but requires mastery of both second quantization and angular momentum algebra. I will outline the problem and the steps and present the final answer; your task, should you choose to accept it, is to work out the intermediate steps in detail and convince yourselve my answers are correct.

For my notation, I use $\hat{a}^\dagger, \hat{a}$ for particle creation and annihilation operators, while I use $\hat{c}, \hat{c}^\dagger$ for hole annihilation and creation operators. Because destroying a particle with some set of quantum numbers, such as angular momentum j, m, is equivalent to creating a hole going backwards in time, I write

$$\hat{a}_{jm} = (-1)^{j+m} \hat{c}^\dagger_{j,\,-m}. \tag{18.2}$$

Let's begin with a general one-body operator,

$$\begin{aligned}\left[\hat{a}^\dagger_{j_a} \otimes \tilde{a}_{j_b}\right]_{J,M} &= \sum_{m_a,m_b} (j_a\, m_a, j_b m_b | JM) \hat{a}^\dagger_{j_a,m_a} (-1)^{j_b+m_b} \hat{a}_{j_b,\,-m_b} \qquad (18.3)\\ &= \sum_{m_a,m_b} (j_a\, m_a, j_b m_b | JM) (-1)^{j_a-m_a} \hat{c}_{j_a,\,-m_a} \hat{c}^\dagger_{j_b,\,+m_b}\end{aligned}$$

$$= \sum_{m_a,m_b} (j_a\, m_a, j_b m_b | JM) (-1)^{j_a-m_a} \left(\delta_{j_a j_b} \delta_{-m_a,\,m_b} - \hat{c}^\dagger_{j_b,\,+m_b} \hat{c}_{j_a,\,-m_a}\right).$$

Using $(-1)^{j-m} = (jm, j\ -m|00)\sqrt{2j+1}$, this simplifies to

$$\sqrt{2j_a+1}\delta_{ab}\delta_{J,0} - (-1)^{j_a-j_b-J} \left[\hat{c}^\dagger_{j_b} \otimes \tilde{c}_{j_a}\right]_{J,\,M} \tag{18.4}$$

The number operator for an orbit labeled by j_a is just

$$\hat{n}_a = \sqrt{2j_a+1}\left[\hat{a}^\dagger_{j_a} \otimes \tilde{a}_{j_a}\right]_{0,0},$$

so in hole space this becomes

$$(2j_a+1) - \hat{n}_{\tilde{a}}; \tag{18.5}$$

as $2j_a+1$ is the maximum number of particles in an orbit, we can intuitive see this answer is correct, i.e., the number of particles equals the maximum number of particles minus the number of holes.

18.2 Short problems

For simplicity, I'm going to consider just bosonic cases.

Example: in 1-D, KE + relative h.o.. Can find eigenmodes and simplify. Make more complicated by adding a repulsive delta-function

Example: the bosonic atom. Imagine electrons were bosons and not fermions. Assume they all fall into the same orbit. Compute the ground state energy as a function of Z. Importantly, compute the ionization potential.

Example: two spinless fermions in a h.o. well with delta-function potential. Use sine basis functions. (actually, save this for later because I'll need definitions of matrix elements...)

Exercise: work out in 3-D KE + trapping potential + repulsive delta function

Part IV

Appendices

Appendix A

Notes on the harmonic oscillator

Consider the harmonic oscillator potential $V(r) = \frac{1}{2}m\omega^2 r^2$. Assume the usual factorization of the wavefunction in spherical coordinates,

$$\Psi_{nlm}(r,\theta,\phi) = \frac{u_{nl}(r)}{r} Y_{lm}(\theta,\phi). \tag{A.1}$$

This yields the radial Schrödinger equation

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2} + \frac{1}{2}m\omega^2 r^2 - E\right) u_{nl}(r) = 0. \tag{A.2}$$

Introducing the oscillator length

$$b = \sqrt{\frac{\hbar}{m\omega}} \tag{A.3}$$

and the dimensionless variables $y = r/b$ and $\epsilon = E/\hbar\omega$, we get the scaled equation

$$\left(-\frac{1}{2}\frac{d^2}{dy^2} + \frac{1}{2}\frac{l(l+1)}{y^2} + \frac{1}{2}y^2 - \epsilon\right) u(y) = 0. \tag{A.4}$$

As a first step, let

$$u(y) = y^{l+1} f(y). \tag{A.5}$$

This transforms the equation to

$$\left(-\frac{1}{2}\frac{d^2}{dy^2} - \frac{l+1}{y}\frac{d}{dy} + \frac{1}{2}y^2 - \epsilon\right) f(y) = 0. \tag{A.6}$$

As a next step, let $x = y^2$, so that

$$\frac{d}{dy} = \frac{dx}{dy}\frac{d}{dx} = 2\sqrt{x}\frac{d}{dx}, \quad \frac{d^2}{dy^2} = 4x\frac{d^2}{dx^2} + 2\frac{d}{dx}, \tag{A.7}$$

yielding

$$\left(-2x\frac{d^2}{dx^2} - (2l+3)\frac{d}{dx} + \frac{1}{2}x - \epsilon\right) f(x) = 0 \tag{A.8}$$

The final step is to take

$$f(x) = \exp(-x/2)p(x) \tag{A.9}$$

which leads to

$$\left(x\frac{d^2}{dx^2} + (l+3/2-x)\frac{d}{dx} - \frac{1}{4}(2l+3-2\epsilon)\right) p(x) = 0. \tag{A.10}$$

One can solve this by a power series, but the power series are just associated Laguerre polynomials.

A.1 Associated Laguerre polynomials

Part of the trickiness of associated Laguerre polynomials is that there are two different conventions for normalization. Let me start first with the Laguerre polynomial $L_n(x)$, which has the differential equation

$$\left(x\frac{d^2}{dx^2} + (1-x)\frac{d}{dx} + n\right) L_n(x) = 0. \tag{A.11}$$

The Rodrigues representation has two different normalizations. The one frequently used in quantum mechanics is

$$L_n(x) = \frac{e^x}{n!}\frac{d^n}{dx^n}\left(x^n e^{-x}\right) \tag{A.12}$$

which has normalization $L_n(0) = 1$; but another normalization found in some mathematical methods books is

$$L_n(x) = e^x\frac{d^n}{dx^n}\left(x^n e^{-x}\right) \tag{A.13}$$

which has normalization $L_n(0) = n!$.

This discussion carries over to the associated Laguerre polynomials, which have the differential equation

$$\left(x\frac{d^2}{dx^2} + (k+1-x)\frac{d}{dx} + n\right) L_n^k(x) = 0. \tag{A.14}$$

where k does not have to be an integer (but $k = 0$ gives us the regular Laguerre polynomial); the two Rodrigues representations are

$$L_n^k(x) = \frac{x^{-k}e^x}{n!}\frac{d^n}{dx^n}\left(x^{n+k}e^{-x}\right) \tag{A.15}$$

which has normalization $L_n^k(0) = \Gamma(n+k+1)/n!\Gamma(k+1)$.

(There is an alternate definition and normalization,

$$L_n^k(x) = x^{-k}e^x \frac{d^n}{dx^n}\left(x^{n+k}e^{-x}\right) \tag{A.16}$$

which has normalization $L_n^k(0) = \Gamma(n+k+1)/\Gamma(k+1)$, but in the notes that follow I will write the solutions in terms of the first normalization convention.)

The associated Laguerre polynomial is, as a series,

$$L_n^k(x) = \sum_{m=0}^{n} (-1)^m \frac{1}{m!} \frac{\Gamma(n+k+1)}{\Gamma(n-m+1)\Gamma(k+m+1)} x^m. \tag{A.17}$$

Note that the associated Laguerre polynomial can be written in terms of confluent hypergeometric series.

The normalization integral for the associated Laguerre polynomial is

$$\int_0^\infty e^{-x}x^{k+1}\left(L_n^k(x)\right)^2 dx = \frac{\Gamma(n+k+1)}{n!}. \tag{A.18}$$

A.1.1 Recursion relations

It's useful to have various recursion relations. For example, examining (A.17) one finds

$$L_{n-1}^{k+1}(x) = -\frac{d}{dx}L_n^k(x). \tag{A.19}$$

Other useful recursion relations are

$$xL_n^k(x) = (2n+k+1)L_n^k(x) - (n+k)L_{n-1}^k(x) - (n+1)L_{n+1}^k(x) \tag{A.20}$$

which can also be rewritten as

$$(n+1)L_{n+1}^k(x) = (2n+k+1-x)L_n^k(x) - (n+k)L_{n-1}^k(x). \tag{A.21}$$

There is also the derivative recursion

$$x\frac{d}{dx}L_n^k(x) = nL_n^k(x) - (n+k)L_{n-1}^k(k). \tag{A.22}$$

Alternately, one can use a generating function

$$\frac{\exp(-xz/(1-z))}{(1-z)^{k+1}} = \sum_{n=0}^{\infty} L_n^k(x)z^n \tag{A.23}$$

which leads to

$$\sum_{n=0}^{\infty} L_n^{k+1}(x)z^n = \frac{1}{1-z}\sum_{n=0}^{\infty} L_n^k(x)z^n \tag{A.24}$$

or the following recursion relations:

$$L_n^k(x) = L_n^{k+1} - L_{n-1}^{k+1}, \tag{A.25}$$

$$L_n^{k+1}(x) = \sum_{i=0}^{n} L_i^k(x). \tag{A.26}$$

A.2 Application to the 3D harmonic oscillator

Looking back at Eq. A.10, if we define $\epsilon = 2n+l+3/2$, then we get the associated Laguerre equation A.14 with $k = l + 1/2$. Then we get the special form

$$L_n^{l+1/2}(x) = \sum_{m=0}^{n} (-1)^m \frac{1}{m!} \frac{\Gamma(n+l+1+1/2)}{\Gamma(n-m+1)\Gamma(l+m+1+1/2)} x^m. \tag{A.27}$$

For this we use $\Gamma(j+1/2) = \sqrt{\pi}\frac{(2j-1)!!}{2^j}$ to get

$$L_n^{l+1/2}(x) = \sum_{m=0}^{n} (-1)^m \frac{1}{m!} \frac{(2n+2l+1)!!}{2^{n-m}(n-m)!(2m+2l+1)!!} x^m. \tag{A.28}$$

To get for arbitrary n, one should use the recursion (A.21), starting with

$$L_0^{l+1/2}(x) = 1, \tag{A.29}$$

$$L_1^{l+1/2}(x) = l + \frac{3}{2} - x, \tag{A.30}$$

and then recurse up to n.

Finally, the radial wavefunction is, up to a normalization

$$u_{nl}(r) = N_{nl}(r/b)^{l+1} \exp(-\frac{1}{2}(r/b)^2) L_n^{l+1/2}((r/b)^2) \tag{A.31}$$

This must be normalized by

$$\int_0^\infty |u_{nl}(r)|^2 dr = 1. \tag{A.32}$$

If we let $z = (r/b)^2$, then we have the normalization condition

$$\frac{1}{2} N_{nl}^2 b^3 \int_0^\infty e^{-z} z^{l+1/2} \left(L_n^{l+1/2}(z)\right)^2 dz = 1 \tag{A.33}$$

which, using the normalization integral (A.18) for the associated Laguerre polynomial, gives

$$N_{nl} = \sqrt{\frac{2n!}{b^3 \Gamma(n+l+3/2)}}, \tag{A.34}$$

or, using the double-factorial,

$$N_{nl} = \sqrt{\frac{2^{n+l+2} n!}{b^3 \sqrt{\pi}(2n+2l+1)!!}}, \tag{A.35}$$

A.3 Matrix elements

I can use the recursion relations and definitions of the h.o. radial wavefunction to compute various matrix elements I need.

For example, one can derive that

$$rR_{nl} = \frac{N_{nl}}{N_{n,l+1}} R_{n,l+1} - \frac{N_{nl}}{N_{n-1,l+1}} R_{n-1,l+1}. \tag{A.36}$$

Then one easily gets the following:

$$\langle n, l+1 | r | nl \rangle = \frac{N_{nl}}{N_{n,l+1}} = \sqrt{n+l+3/2}, \tag{A.37}$$

$$\langle n-1, l+1 | r | nl \rangle = -\frac{N_{nl}}{N_{n-1,l+1}} = -\sqrt{n}. \tag{A.38}$$

Similarly, I need the matrix element

$$\left\langle n', l+1 \left| \frac{d}{dr} - \frac{l}{r} \right| n, l \right\rangle \tag{A.39}$$

Using the above one can show that

$$\left(\frac{d}{dr} - \frac{l}{r} \right) R_{nl} = -rR_{nl} - 2\frac{N_{nl}}{N_{n-1,l+1}} R_{n-1,l+1} \tag{A.40}$$

which yield

$$\left\langle n, l+1 \left| \frac{d}{dr} - \frac{l}{r} \right| n, l \right\rangle = -\sqrt{n+l+3/2}, \tag{A.41}$$

$$\left\langle n-1, l+1 \left| \frac{d}{dr} - \frac{l}{r} \right| n, l \right\rangle = -\sqrt{n} \tag{A.42}$$

Appendix B

Recommended resources

There are a number of books and review articles on the configuration-interaction shell model. We focus on those in nuclear physics. One of the best, but nowadays difficult to get, is Brussard and Glaudemans [1977]. Some other useful references, in historical order, are [De-Shalit and Talmi, 2013], Towner [1977], Lawson [1980] (thorough, but be aware his phase conventions differ from most others), Talmi [1993], Heyde [1994], Suhonen [2007], and others. A particular useful review article touching on many of the ideas here Caurier et al. [2005]; the review article Brown and Wildenthal [1988] is older but has useful information on applications of the shell model. The no-core shell model and other *ab initio* methods are a rapidly evolving field, but good overviews of the topic are Navrátil et al. [2000] and Barrett et al. [2013].

For angular momentum coupling a widely used reference is the slim volume by Edmonds [1996]. If you can't find what you need in Edmonds, you can almost certainly find it in Varshalovich et al. [1988]. Sadly, neither are good pedagogical introductions to the topic of angular momentum algebra.

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