Slides from PHY981

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Topics for Week 2, January 7-11

Introduction to the course and overview of observables

- Tuesday:
- Presentation of topics to be covered and introduction to nuclear structure physics
- Discussion of quantities like binding energies, masses, radii, separation energies, see chapters 1-4 of Alex Brown's (AB) 2011 lectures
- Definitions of various quantities
- Thursday:
- Single-particle degrees of freedom, discussion of data
- Hamiltonians and single-particle fields, see Suhonen (JS) chapter 3 and AB chapters 9 and 10. You can fetch JS's book from `http://link.springer.com.proxy2.cl.msu.edu/book/10.1007/978-3-540-48861-3/page/1`
- No exercises this week.

Lectures and exercise sessions

and syllabus (see next slide as well)

- Lectures: Tuesdays and Thursdays 1.00pm-2.20pm, seminar room 1341
- Exercise sessions: To be discussed.
- Detailed lecture notes, all exercises presented and projects can be found at the homepage of the course.
- Weekly plans and all other information are on the official webpage.

Lectures and exercise sessions

and syllabus (see next slide as well)

- Syllabus: Lecture notes, exercises and projects. Relevant chapters of Suhonen's text that cover parts of the material are chapters 3-9 and 11. Chapters 1-2 on angular momentum will be used as references for various derivations and only parts of these two chapters will be used. Alex Brown's lecture notes from 2011 can also be used, and the relevant chapters are 1-4, 6-29. Chapter 5 of Brown on angular momentum plays the same role as chapters 1-2 of Suhonen.

Main themes and reading suggestions

The various observables we will discuss in the course are thought to be understood via the following five major topics

1. Single particle properties and mean-field models, lecture notes, JS chapters 3-5 and AB chapters 7-10 and 14
2. Nuclear forces, covered by lecture notes
3. The nuclear shell-model, lecture notes, JS chapter 8 and AB chapters 11-22.
4. Particle-hole excitations, random-phase approximation and pairing, lecture notes and JS chapters 9 and 11.
5. Decays and one and two-body transition probabilities, lecture notes, JS chapters 6 and 7, AB chapters 23-29.

Plan for the semester

Projects, weekly exercises, deadlines and final oral exam

1. Two projects with a numerical content that count each 25%, weekly exercises that count 10% and a final oral exam which counts 40% of the final grade.
2. Project 1 will be available February 4 and has to be handed in on February 22.
3. Project 2 will be available March 25 and has to be handed in on April 12.
4. For the final oral exam (April 29 - May 1) you have to prepare a 20 minutes talk based on either a topic chosen by you or a topic defined towards the end of the semester. Duration of the examination is 40 minutes. The remaining 20 minutes are for questions from other topics as well.

Plan for the semester

Projects

1. Project 1 will deal with computing scattering phase shifts used to constrain nucleon-nucleon forces. The project will thus involved a comparison with experimental scattering data. Numerically, we need to compute inverses of matrices, where the matrices are discretizations on a grid of the nucleon-nucleon forces at study. All relevant auxiliary functions will be provided (such as computing the inverse of a matrix).
2. Project 2 will most likely deal with the build up of your own shell model code, and involves basically solving an eigenvalue problem. Again, all auxiliary functions will be provided.

Selected Texts on Nuclear Structure and Many-body theory

1. Heyde, *The Nuclear Shell Model*, Springer 1990
2. Lawson, *Theory of the Nuclear Shell Model*, Oxford 1980
3. Ring and Schuck, *Nuclear Many-Body Theory*, Springer 1980
4. Talmi, *Simple Models of Complex Nuclei: The Shell Model and Interacting Boson Model*, Harwood Academic Publishers 1993.
5. Blaizot and Ripka, *Quantum Theory of Finite systems*, MIT press 1986
6. Negele and Orland, *Quantum Many-Particle Systems*, Addison-Wesley, 1987.
7. Fetter and Walecka, *Quantum Theory of Many-Particle Systems*, McGraw-Hill, 1971.
8. Dickhoff and Van Neck, *Many-Body Theory Exposed*, World Scientific, 2006.

Masses and Binding energies

A basic quantity which can be measured for the ground states of nuclei is the atomic mass $M(N, Z)$ of the neutral atom with atomic mass number A and charge Z. The number of neutrons are N.
Atomic masses are usually tabulated in terms of the mass excess defined by

$$\Delta M(N, Z) = M(N, Z) - uA,$$

where u is the Atomic Mass Unit

$$u = M(^{12}\mathrm{C})/12 = 931.49386 \ \mathrm{MeV}/c^2.$$

In this course we will mainly use data from the 2003 compilation of Audi, Wapstra and Thibault.

Masses and Binding energies

The nucleon masses are

$$m_p = 938.27203(8)\ \mathrm{MeV}/c^2 = 1.00727646688(13)u,$$

and

$$m_n = 939.56536(8)\ \mathrm{MeV}/c^2 = 1.0086649156(6)u.$$

In the 2003 mass evaluation there are 2127 nuclei measured with an accuracy of 0.2 MeV or better, and 101 nuclei measured with an accuracy of greater than 0.2 MeV. For heavy nuclei one observes several chains of nuclei with a constant $N - Z$ value whose masses are obtained from the energy released in alpha decay.

Masses and Binding energies

Nuclear binding energy is defined as the energy required to break up a given nucleus into its constituent parts of N neutrons and Z protons. In terms of the atomic masses $M(N, Z)$ the binding energy is defined by:

$$BE(N, Z) = ZM_H c^2 + Nm_n c^2 - M(N, Z)c^2,$$

where M_H is the mass of the hydrogen atom and m_n is the mass of the neutron. In terms of the mass excess the binding energy is given by:

$$BE(N, Z) = Z\Delta_H c^2 + N\Delta_n c^2 - \Delta(N, Z)c^2,$$

where $\Delta_H c^2 = 7.2890$ MeV and $\Delta_n c^2 = 8.0713$ MeV.

Q-values and separation energies

We consider energy conservation for nuclear transformations that include, for example, the fusion of two nuclei a and b into the combined system c

$$^{N_a+Z_a}a + {}^{N_b+Z_b}b \rightarrow {}^{N_c+Z_c}c$$

or the decay of nucleus c into two other nuclei a and b

$$^{N_c+Z_c}c \rightarrow {}^{N_a+Z_a}a + {}^{N_b+Z_b}b$$

In general we have the reactions

$$\sum_i {}^{N_i+Z_i}i \rightarrow \sum_f {}^{N_f+Z_f}f$$

We require also that number of protons and neutrons are conserved in the initial stage and final stage, unless we have processes which violate baryon conservation,

$$\sum_i N_i = \sum_f N_f \quad \text{and} \quad \sum_i Z_i = \sum_f Z_f.$$

Q-values and separation energies

This process is characterized by an energy difference called the Q value:

$$Q = \sum_i M(N_i, Z_i)c^2 - \sum_f M(N_f, Z_f)c^2 = \sum_i BE(N_f, Z_f) - \sum_i BE(N_i, Z_i)$$

Spontaneous decay involves a single initial nuclear state and is allowed if $Q > 0$. In the decay, energy is released in the form of the kinetic energy of the final products. Reactions involving two initial nuclei and are endothermic (a net loss of energy) if $Q < 0$; the reactions are exothermic (a net release of energy) if $Q > 0$.

Q-values and separation energies

We can consider the Q values associated with the removal of one or two nucleons from a nucleus. These are conventionally defined in terms of the one-nucleon and two-nucleon separation energies

$$S_n = -Q_n = BE(N,Z) - BE(N-1,Z),$$

$$S_p = -Q_p = BE(N,Z) - BE(N,Z-1),$$

$$S_{2n} = -Q_{2n} = BE(N,Z) - BE(N-2,Z),$$

and

$$S_{2p} = -Q_{2p} = BE(N,Z) - BE(N,Z-2),$$

Radii

The root-mean-square (rms) charge radius has been measured for the ground states of many nuclei. For a spherical charge density, $\rho(\mathbf{r})$, the mean-square radius is defined by:

$$\langle r^2 \rangle = \frac{\int d\mathbf{r} \rho(\mathbf{r}) r^2}{\int d\mathbf{r} \rho(\mathbf{r})},$$

and the rms radius is the square root of this quantity denoted by

$$R = \sqrt{\langle r^2 \rangle}.$$

Radii

Radii for most stable nuclei have been deduced from electron scattering form factors and/or from the x-ray transition energies of muonic atoms. The relative radii for a series of isotopes can be extracted from the isotope shifts of atomic x-ray transitions. The rms radius for the nuclear point-proton density, R_p is obtained from the rms charge radius by:

$$R_p = \sqrt{R_{\rm ch}^2 - R_{\rm corr}^2},$$

where

$$R_{\rm corr}^2 = R_{\rm op}^2 + (N/Z)R_{\rm on}^2 + R_{\rm rel}^2,$$

where $R_{\rm op} = 0.875(7)$ fm is the rms radius of the proton, $R_{\rm on}^2 = 0.116(2)$ fm^2 is the mean-square radius of the neutron and $R_{\rm rel}^2 = 0.033$ fm^2 is the relativistic Darwin-Foldy correction. There are also smaller nucleus-dependent relativistic spin-orbit and mesonic-exchange corrections that should be included.

Definitions

An operator is defined as $\hat{O}$ throughout. Unless otherwise specified the number of particles is always A and d is the dimension of the system. In nuclear physics we normally define the total number of particles to be $A = N + Z$, where N is total number of neutrons and Z the total number of protons. In case of other baryons such isobars Δ or various hyperons such as Λ or Σ, one needs to add their definitions. Hereafter, A is reserved for the total number of particles, unless otherwise specificied. When we refer to a neutron we will use the label n and when we refer to a proton we will use the label p. Unless otherwise specified, we will call these particles for nucleons.

Definitions

The quantum numbers of a single-nucleon state in coordinate space are defined by the variable $x = (\mathbf{r}, \sigma)$, where $\mathbf{r} \in \mathbb{R}^d$with $d = 1, 2, 3$ represents the spatial coordinates and σ is the eigenspin of the nucleon. For fermions with eigenspin $1/2$ this means that

$$x \in \mathbb{R}^d \oplus (\frac{1}{2}),$$

and the integral

$$\int dx = \sum_{\sigma} \int d^d r = \sum_{\sigma} \int d\mathbf{r},$$

and

$$\int d^A x = \int dx_1 \int dx_2 \ldots \int dx_A.$$

Definitions

The quantum mechanical wave function of a given state with quantum numbers λ (encompassing all quantum numbers needed to specify the system), ignoring time, is

$$\Psi_\lambda = \Psi_\lambda(x_1, x_2, \ldots, x_A),$$

with $x_i = (\mathbf{r}_i, \sigma_i)$ and the projection of σ_i takes the values $\{-1/2, +1/2\}$ for nucleons with spin $1/2$. We will hereafter always refer to Ψ_λ as the exact wave function, and if the ground state is not degenerate we label it as

$$\Psi_0 = \Psi_0(x_1, x_2, \ldots, x_A).$$

Definitions

Since the solution Ψ_λ seldomly can be found in closed form, approximations are sought. In this text we define an approximative wave function or an ansatz to the exact wave function as

$$\Phi_\lambda = \Phi_\lambda(x_1, x_2, \ldots, x_A),$$

with

$$\Phi_0 = \Phi_0(x_1, x_2, \ldots, x_A),$$

being the ansatz to the ground state.

Definitions

The wave function Ψ_λ is sought in the Hilbert space of either symmetric or anti-symmetric A-body functions, namely

$$\Psi_\lambda \in \mathcal{H}_A := \mathcal{H}_1 \oplus \mathcal{H}_1 \oplus \cdots \oplus \mathcal{H}_1,$$

where the single-nucleon Hilbert space $\mathcal{H}_1$ is the space of square integrable functions over $\in \mathbb{R}^d \oplus (\sigma)$ resulting in

$$\mathcal{H}_1 := L^2(\mathbb{R}^d \oplus (\sigma)).$$

Definitions

Our Hamiltonian is invariant under the permutation (interchange) of two nucleons. Since we deal with fermions however, the total wave function is antisymmetric. Let $\hat{P}$ be an operator which interchanges two nucleons. Due to the symmetries we have ascribed to our Hamiltonian, this operator commutes with the total Hamiltonian,

$$[\hat{H}, \hat{P}] = 0,$$

meaning that $\Psi_\lambda(x_1, x_2, \dots, x_A)$ is an eigenfunction of $\hat{P}$ as well, that is

$$\hat{P}_{ij}\Psi_\lambda(x_1, x_2, \dots, x_i, \dots, x_j, \dots, x_A) = \beta\Psi_\lambda(x_1, x_2, \dots, x_j, \dots, x_i, \dots, x_A),$$

where β is the eigenvalue of $\hat{P}$. We have introduced the suffix ij in order to indicate that we permute nucleons i and j. The Pauli principle tells us that the total wave function for a system of fermions has to be antisymmetric, resulting in the eigenvalue $\beta = -1$.

Definitions and notations

The Schrödinger equation reads

$$\hat{H}(x_1, x_2, \ldots, x_A)\Psi_\lambda(x_1, x_2, \ldots, x_A) = E_\lambda \Psi_\lambda(x_1, x_2, \ldots, x_A), \tag{1}$$

where the vector x_i represents the coordinates (spatial and spin) of nucleon i, λ stands for all the quantum numbers needed to classify a given A-nucleon state and Ψ_λ is the pertaining eigenfunction. Throughout this course, Ψ refers to the exact eigenfunction, unless otherwise stated.

Definitions and notations

We write the Hamilton operator, or Hamiltonian, in a generic way

$$\hat{H} = \hat{T} + \hat{V}$$

where $\hat{T}$ represents the kinetic energy of the system

$$\hat{T} = \sum_{i=1}^{A} \frac{\mathbf{p}_i^2}{2m_i} = \sum_{i=1}^{A} \left(-\frac{\hbar^2}{2m_i} \nabla_{\mathbf{i}}{}^2 \right) = \sum_{i=1}^{A} t(x_i)$$

while the operator $\hat{V}$ for the potential energy is given by

$$\hat{V} = \sum_{i=1}^{A} \hat{u}_{\text{ext}}(x_i) + \sum_{ji=1}^{A} v(x_i, x_j) + \sum_{ijk=1}^{A} v(x_i, x_j, x_k) + \ldots \tag{2}$$

Hereafter we use natural units, viz. $\hbar = c = e = 1$, with e the elementary charge and c the speed of light. This means that momenta and masses have dimension energy.

Definitions and notations

If one does quantum chemistry, after having introduced the Born-Oppenheimer approximation which effectively freezes out the nucleonic degrees of freedom, the Hamiltonian for $N = n_e$ electrons takes the following form

$$\hat{H} = \sum_{i=1}^{n_e} t(x_i) - \sum_{i=1}^{n_e} k\frac{Z}{r_i} + \sum_{i<j}^{n_e} \frac{k}{r_{ij}},$$

with $k = 1.44$ eVnm

Definitions and notations

We can rewrite this as

$$\hat{H} = \hat{H}_0 + \hat{H}_I = \sum_{i=1}^{n_e} \hat{h}_0(x_i) + \sum_{i<j=1}^{n_e} \frac{1}{r_{ij}}, \tag{3}$$

where we have defined $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$ and

$$\hat{h}_0(x_i) = \hat{t}(x_i) - \frac{Z}{x_i}. \tag{4}$$

The first term of eq. (3), H_0, is the sum of the N *one-body* Hamiltonians $\hat{h}_0$. Each individual Hamiltonian $\hat{h}_0$ contains the kinetic energy operator of an electron and its potential energy due to the attraction of the nucleus. The second term, H_I, is the sum of the $n_e(n_e - 1)/2$ two-body interactions between each pair of electrons. Note that the double sum carries a restriction $i < j$.

Definitions and notations

The potential energy term due to the attraction of the nucleus defines the one-body field $u_i = u_{\rm ext}(x_i)$ of Eq. (2). We have moved this term into the $\hat{H}_0$ part of the Hamiltonian, instead of keeping it in $\hat{V}$ as in Eq. (2). The reason is that we will hereafter treat $\hat{H}_0$ as our non-interacting Hamiltonian. For a many-body wavefunction Φ_λ defined by an appropriate single-nucleon basis, we may solve exactly the non-interacting eigenvalue problem

$$\hat{H}_0\Phi_\lambda = w_\lambda\Phi_\lambda,$$

with w_λ being the non-interacting energy. This energy is defined by the sum over single-nucleon energies to be defined below. For atoms the single-nucleon energies could be the hydrogen-like single-nucleon energies corrected for the charge Z. For nuclei and quantum dots, these energies could be given by the harmonic oscillator in three and two dimensions, respectively.

Definitions and notations

We will assume that the interacting part of the Hamiltonian can be approximated by a two-body interaction. This means that our Hamiltonian is written as

$$\hat{H} = \hat{H}_0 + \hat{H}_I = \sum_{i=1}^{A} \hat{h}_0(x_i) + \sum_{i<j=1}^{A} \hat{v}(x_{ij}), \tag{5}$$

with

$$H_0 = \sum_{i=1}^{A} \hat{h}_0(x_i) = \sum_{i=1}^{A} \left(\hat{t}(x_i) + \hat{u}_{\rm ext}(x_i) \right). \tag{6}$$

The one-body part $u_{\rm ext}(x_i)$ is normally approximated by a harmonic oscillator potential or the Coulomb interaction an electron feels from the nucleus. However, other potentials are fully possible, such as one derived from the self-consistent solution of the Hartree-Fock equations or so-called Woods-Saxon potentials to be discussed in the next weeks.

The harmonic oscillator Hamiltonian

In the previous slide we defined

$$\hat{H} = \hat{H}_0 + \hat{H}_I = \sum_{i=1}^{A} \hat{h}_0(x_i) + \sum_{i<j=1}^{A} \hat{v}(x_{ij}),$$

with

$$H_0 = \sum_{i=1}^{A} \hat{h}_0(x_i) = \sum_{i=1}^{A} \left(\hat{t}(x_i) + \hat{u}_{\rm ext}(x_i) \right).$$

In nuclear physics the one-body part $u_{\rm ext}(x_i)$ is normally approximated by a harmonic oscillator potential. However, this is not fully correct, because as we have discussed, nuclei are self-bound systems and there is no external confining potential. The above Hamiltonian is thus not entirely correct for nuclear physics.

The harmonic oscillator Hamiltonian

What many people do then, is to add and subtract a harmonic oscillator potential, with

$$\hat{u}_{\rm ext}(x_i) = \hat{u}_{\rm ho}(x_i) = \frac{1}{2} m\omega^2 r_i^2,$$

where ω is the oscillator frequency. This leads to

$$\hat{H} = \hat{H}_0 + \hat{H}_I = \sum_{i=1}^{A} \hat{h}_0(x_i) + \sum_{i<j=1}^{A} \hat{v}(x_{ij}) - \sum_{i=1}^{A} \hat{u}_{\rm ho}(x_i),$$

with

$$H_0 = \sum_{i=1}^{A} \hat{h}_0(x_i) = \sum_{i=1}^{A} \left(\hat{t}(x_i) + \hat{u}_{\rm ho}(x_i) \right).$$

Many practitioners use this as the standard Hamiltonian when doing nuclear structure calculations. This is ok if the number of nucleons is large, but still with this Hamiltonian, we do not obey translational invariance. How can we cure this?

Translationally Invariant Hamiltonian

In setting up a translationally invariant Hamiltonian the following expressions are helpful. The center-of-mass (CoM) momentum is

$$P = \sum_{i=1}^{A} \boldsymbol{p}_i,$$

and we have that

$$\sum_{i=1}^{A} \boldsymbol{p}_i^2 = \frac{1}{A}\left[\boldsymbol{P}^2 + \sum_{i<j}(\boldsymbol{p}_i - \boldsymbol{p}_j)^2\right]$$

meaning that

$$\left[\sum_{i=1}^{A} \frac{\boldsymbol{p}_i^2}{2m} - \frac{\boldsymbol{P}^2}{2mA}\right] = \frac{1}{2mA}\sum_{i<j}(\boldsymbol{p}_i - \boldsymbol{p}_j)^2.$$

Translationally Invariant Hamiltonian

In a similar fashion we can define the CoM coordinate

$$\boldsymbol{R} = \frac{1}{A}\sum_{i=1}^{A} \boldsymbol{r}_i,$$

which yields

$$\sum_{i=1}^{A} \boldsymbol{r}_i^2 = \frac{1}{A}\left[A^2\boldsymbol{R}^2 + \sum_{i<j}(\boldsymbol{r}_i - \boldsymbol{r}_j)^2\right].$$

Translationally Invariant Hamiltonian

If we then introduce the harmonic oscillator one-body Hamiltonian

$$H_0 = \sum_{i=1}^{A} \left(\frac{\boldsymbol{p}_i^2}{2m} + \frac{1}{2} m\omega^2 \boldsymbol{r}_i^2 \right),$$

with ω the oscillator frequency, we can rewrite the latter as

$$H_{\rm HO} = \frac{\boldsymbol{P}^2}{2mA} + \frac{mA\omega^2 \boldsymbol{R}^2}{2} + \frac{1}{2mA} \sum_{i<j} (\boldsymbol{p}_i - \boldsymbol{p}_j)^2 + \frac{m\omega^2}{2A} \sum_{i<j} (\boldsymbol{r}_i - \boldsymbol{r}_j)^2.$$

Translationally Invariant Hamiltonian

Or we could write

$$H_{\mathrm{HO}} = H_{\mathrm{CoM}} + \frac{1}{2mA}\sum_{i<j}(\boldsymbol{p}_i - \boldsymbol{p}_j)^2 + \frac{m\omega^2}{2A}\sum_{i<j}(\boldsymbol{r}_i - \boldsymbol{r}_j)^2,$$

with

$$H_{\mathrm{CoM}} = \frac{\boldsymbol{P}^2}{2mA} + \frac{mA\omega^2\boldsymbol{R}^2}{2}.$$

Translationally Invariant Hamiltonian

The translationally invariant one- and two-body Hamiltonian reads for an A-nucleon system,

$$\hat{H} = \left[\sum_{i=1}^{A} \frac{\boldsymbol{p}_i^2}{2m} - \frac{\boldsymbol{P}^2}{2mA} \right] + \sum_{i<j}^{A} V_{ij} \ ,$$

where V_{ij} is the nucleon-nucleon interaction. Adding zero as her

$$\sum_{i=1}^{A} \frac{1}{2} m\omega^2 \boldsymbol{r}_i^2 - \frac{m\omega^2}{2A} \left[\boldsymbol{R}^2 + \sum_{i<j} (\boldsymbol{r}_i - \boldsymbol{r}_j)^2 \right] = 0.$$

we can then rewrite the Hamiltonian as

Translationally Invariant Hamiltonian

We can rewrite the Hamiltonian as

$$\hat{H} = \sum_{i=1}^{A} \left[\frac{\boldsymbol{p}_i^2}{2m} + \frac{1}{2} m\omega^2 \boldsymbol{r}_i^2 \right] + \sum_{i<j}^{A} \left[V_{ij} - \frac{m\omega^2}{2A} (\boldsymbol{r}_i - \boldsymbol{r}_j)^2 \right]$$

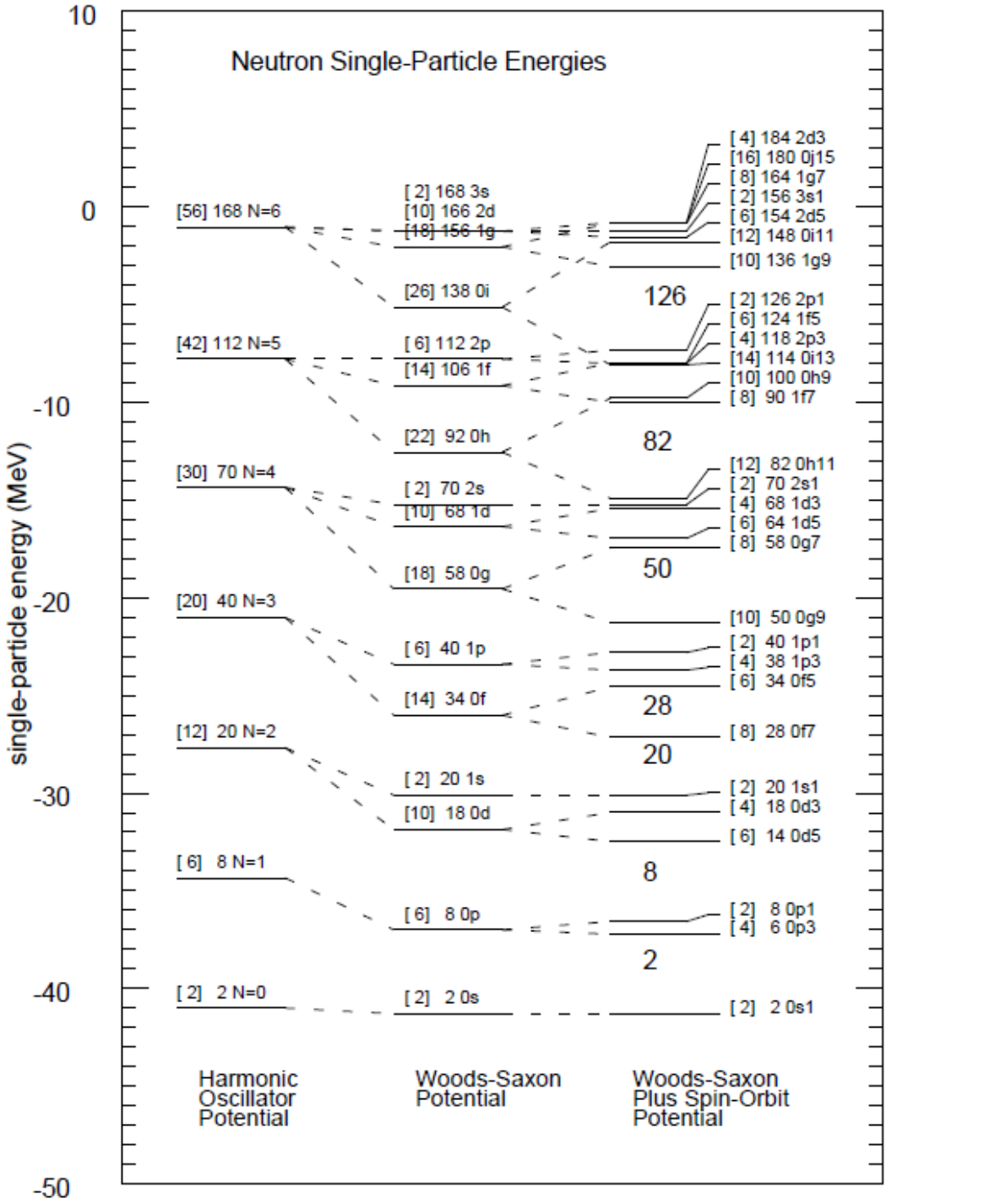
$$- H_{\mathrm{CoM}}.$$

Topics for Week 3, January 14-18

Single-particle fields and construction of many-body wave functions

- Tuesday:
- Repetition from last week
- Hamiltonians and single-particle fields, continued from last week
- Further discussion of basis functions and mentioning the Woods-Saxon potential (AB chapter 10 and JS chapter 3)
- Thursday:
- Hamiltonians and single-particle fields and start Hartree-Fock theory
- Exercises 1 and 2.

Suggested literature is AB chapters 9-11 and 14 and JS chapter 3 and 4


Neutron Single-Particle Energies
single-particle energy (MeV)
10
0
-10
-20
-30
-40
-50
[56] 168 N=6
[42] 112 N=5
[30] 70 N=4
[20] 40 N=3
[12] 20 N=2
[6] 8 N=1
[2] 2 N=0
[2] 168 3s
[10] 166 2d
[18] 156 1g
[26] 138 0i
[6] 112 2p
[14] 106 1f
[22] 92 0h
[2] 70 2s
[10] 68 1d
[18] 58 0g
[6] 40 1p
[14] 34 0f
[2] 20 1s
[10] 18 0d
[6] 8 0p
[2] 2 0s
[4] 184 2d3
[16] 180 0j15
[8] 164 1g7
[2] 156 3s1
[6] 154 2d5
[12] 148 0i11
[10] 136 1g9
126
[2] 126 2p1
[6] 124 1f5
[4] 118 2p3
[14] 114 0i13
[10] 100 0h9
[8] 90 1f7
82
[12] 82 0h11
[2] 70 2s1
[4] 68 1d3
[6] 64 1d5
[8] 58 0g7
50
[10] 50 0g9
[2] 40 1p1
[4] 38 1p3
[6] 34 0f5
28
[8] 28 0f7
20
[2] 20 1s1
[4] 18 0d3
[6] 14 0d5
8
[2] 8 0p1
[4] 6 0p3
2
[2] 2 0s1
Harmonic Oscillator Potential
Woods-Saxon Potential
Woods-Saxon Plus Spin-Orbit Potential

Definitions and notations

Our Hamiltonian is invariant under the permutation (interchange) of two nucleons. Since we deal with fermions, the total wave function is antisymmetric. Let $\hat{P}$ be an operator which interchanges two nucleons. Due to the symmetries we have ascribed to our Hamiltonian, this operator commutes with the total Hamiltonian,

$$[\hat{H}, \hat{P}] = 0,$$

meaning that $\Psi_\lambda(x_1, x_2, \dots, x_A)$ is an eigenfunction of $\hat{P}$ as well, that is

$$\hat{P}_{ij}\Psi_\lambda(x_1, x_2, \dots, x_i, \dots, x_j, \dots, x_A) = \beta\Psi_\lambda(x_1, x_2, \dots, x_i, \dots, x_j, \dots, x_A),$$

where β is the eigenvalue of $\hat{P}$. We have introduced the suffix *ij* in order to indicate that we permute nucleons *i* and *j*. The Pauli principle tells us that the total wave function for a system of fermions has to be antisymmetric, resulting in the eigenvalue $\beta = -1$.

Definitions and notations

In our case we assume that we can approximate the exact eigenfunction with a Slater determinant

$$\Phi(x_1, x_2, \ldots, x_A, \alpha, \beta, \ldots, \sigma) = \frac{1}{\sqrt{A!}} \begin{vmatrix} \psi_\alpha(x_1) & \psi_\alpha(x_2) & \ldots & \ldots & \psi_\alpha(x_A) \\ \psi_\beta(x_1) & \psi_\beta(x_2) & \ldots & \ldots & \psi_\beta(x_A) \\ \ldots & \ldots & \ldots & \ldots & \ldots \\ \ldots & \ldots & \ldots & \ldots & \ldots \\ \psi_\sigma(x_1) & \psi_\sigma(x_2) & \ldots & \ldots & \psi_\sigma(x_A) \end{vmatrix}, \tag{7}$$

where x_i stand for the coordinates and spin values of a nucleon i and $\alpha, \beta, \ldots, \gamma$ are quantum numbers needed to describe remaining quantum numbers.

Definitions and notations

The single-nucleon function $\psi_\alpha(x_i)$ are eigenfunctions of the one-body Hamiltonian, that is

$$\hat{h}_0(x_i) = \hat{t}(x_i) + \hat{u}_{\rm ho}(x_i),$$

with eigenvalues

$$\hat{h}_0(x_i)\psi_\alpha(x_i) = \left(\hat{t}(x_i) + \hat{u}_{\rm ho}(x_i)\right)\psi_\alpha(x_i) = \varepsilon_\alpha\psi_\alpha(x_i).$$

The energies ε_α are the so-called non-interacting single-nucleon energies, or unperturbed energies. The total energy is in this case the sum over all single-nucleon energies, if no two-body or more complicated many-body interactions are present.

Definitions and notations

Let us denote the ground state energy by E_0. According to the variational principle we have

$$E_0 \leq E[\Phi] = \int \Phi^* \hat{H} \Phi d\tau$$

where Φ is a trial function which we assume to be normalized

$$\int \Phi^* \Phi d\tau = 1,$$

where we have used the shorthand $d\tau = d\mathbf{x}_1 d\mathbf{x}_2 \ldots d\mathbf{x}_A$.

Definitions and notations

In the Hartree-Fock method the trial function is the Slater determinant of Eq. (7) which can be rewritten as

$$\Phi(x_1, x_2, \dots, x_A, \alpha, \beta, \dots, \nu) = \frac{1}{\sqrt{A!}} \sum_P (-)^P \hat{P} \psi_\alpha(x_1) \psi_\beta(x_2) \dots \psi_\nu(x_A) = \sqrt{A!} \mathcal{A} \Phi_H, \tag{8}$$

where we have introduced the antisymmetrization operator $\mathcal{A}$ defined by the summation over all possible permutations of two nucleons.

Definitions and notations

It is defined as

$$\mathcal{A} = \frac{1}{A!}\sum_{p}(-)^{p}\hat{P}, \tag{9}$$

with p standing for the number of permutations. We have introduced for later use the so-called Hartree-function, defined by the simple product of all possible single-nucleon functions

$$\Phi_H(x_1, x_2, \dots, x_A, \alpha, \beta, \dots, \nu) = \psi_\alpha(x_1)\psi_\beta(x_2)\dots\psi_\nu(x_A).$$

Definitions and notations

Both $\hat{H}_0$ and $\hat{\hat{H}}_I$ are invariant under all possible permutations of any two nucleons and hence commute with $\mathcal{A}$

$$[H_0, \mathcal{A}] = [H_I, \mathcal{A}] = 0. \tag{10}$$

Furthermore, $\mathcal{A}$ satisfies

$$\mathcal{A}^2 = \mathcal{A}, \tag{11}$$

since every permutation of the Slater determinant reproduces it.

Definitions and notations

The expectation value of $\hat{H}_0$

$$\int \Phi^* \hat{H}_0 \Phi d\tau = A! \int \Phi_H^* \mathcal{A} \hat{H}_0 \mathcal{A} \Phi_H d\tau$$

is readily reduced to

$$\int \Phi^* \hat{H}_0 \Phi d\tau = A! \int \Phi_H^* \hat{H}_0 \mathcal{A} \Phi_H d\tau,$$

where we have used eqs. (10) and (11). The next step is to replace the antisymmetrization operator by its definition Eq. (8) and to replace $\hat{H}_0$ with the sum of one-body operators

$$\int \Phi^* \hat{H}_0 \Phi d\tau = \sum_{i=1}^{A} \sum_{p} (-)^p \int \Phi_H^* \hat{h}_0 \hat{P} \Phi_H d\tau.$$

Definitions and notations

The integral vanishes if two or more nucleons are permuted in only one of the Hartree-functions Φ_H because the individual single-nucleon wave functions are orthogonal. We obtain then

$$\int \Phi^* \hat{H}_0 \Phi d\tau = \sum_{i=1}^{A} \int \Phi_H^* \hat{h}_0 \Phi_H d\tau.$$

Orthogonality of the single-nucleon functions allows us to further simplify the integral, and we arrive at the following expression for the expectation values of the sum of one-body Hamiltonians

$$\int \Phi^* \hat{H}_0 \Phi d\tau = \sum_{\mu=1}^{A} \int \psi_\mu^*(\mathbf{x}) \hat{h}_0 \psi_\mu(\mathbf{x}) d\mathbf{x}. \tag{12}$$

Definitions and notations

We introduce the following shorthand for the above integral

$$\langle \mu | \hat{h}_0 | \mu \rangle = \int \psi_\mu^*(\mathbf{x}) \hat{h}_0 \psi_\mu(\mathbf{x}) d\mathbf{x}.,$$

and rewrite Eq. (12) as

$$\int \Phi^* \hat{H}_0 \Phi d\tau = \sum_{\mu=1}^{A} \langle \mu | \hat{h}_0 | \mu \rangle. \tag{13}$$

Definitions and notations

The expectation value of the two-body part of the Hamiltonian (assuming a two-body Hamiltonian at most) is obtained in a similar manner. We have

$$\int \Phi^* \hat{H}_I \Phi d\tau = A! \int \Phi_H^* \mathcal{A} \hat{H}_I \mathcal{A} \Phi_H d\tau,$$

which reduces to

$$\int \Phi^* \hat{H}_I \Phi d\tau = \sum_{i \leq j=1}^{A} \sum_p (-)^p \int \Phi_H^* \hat{v}(x_{ij}) \hat{P} \Phi_H d\tau,$$

by following the same arguments as for the one-body Hamiltonian.

Definitions and notations

Because of the dependence on the inter-nucleon distance r_{ij}, permutations of any two nucleons no longer vanish, and we get

$$\int \Phi^* \hat{H}_I \Phi d\tau = \sum_{i<j=1}^{A} \int \Phi_H^* \hat{v}(x_{ij})(1 - P_{ij})\Phi_H d\tau.$$

where P_{ij} is the permutation operator that interchanges nucleon i and nucleon j. Again we use the assumption that the single-nucleon wave functions are orthogonal.

Definitions and notations

We obtain

$$\int \Phi^* \hat{H}_I \Phi d\tau = \frac{1}{2} \sum_{\mu=1}^{A} \sum_{\nu=1}^{A} \left[\int \psi_\mu^*(x_i) \psi_\nu^*(x_j) \hat{v}(x_{ij}) \psi_\mu(x_i) \psi_\nu(x_j) dx_i dx_j - \int \psi_\mu^*(x_i) \psi_\nu^*(x_j) \hat{v}(x_{ij}) \psi_\nu(x_i) \psi_\mu(x_j) dx_i dx_j \right]. \tag{14}$$

The first term is the so-called direct term. In Hartree-Fock theory it leads to the so-called Hartree term, while the second is due to the Pauli principle and is called the exchange term and in Hartree-Fock theory it defines the so-called xFock term. The factor $1/2$ is introduced because we now run over all pairs twice.

Definitions and notations

The last equation allows us to introduce some further definitions. The single-nucleon wave functions $\psi_\mu(\mathbf{x})$, defined by the quantum numbers μ and $\mathbf{x}$ (recall that $\mathbf{x}$ also includes spin degree, later we will also add isospin) are defined as the overlap

$$\psi_\alpha(x) = \langle x|\alpha\rangle.$$

Definitions and notations

We introduce the following shorthands for the above two integrals

$$\langle \mu\nu | V | \mu\nu \rangle = \int \psi_\mu^*(x_i)\psi_\nu^*(x_j)\hat{v}(x_{ij})\psi_\mu(x_i)\psi_\nu(x_j)dx_i dx_j,$$

and

$$\langle \mu\nu | V | \nu\mu \rangle = \int \psi_\mu^*(x_i)\psi_\nu^*(x_j)\hat{v}(x_{ij})\psi_\nu(x_i)\psi_\mu(x_j)dx_i dx_j.$$

Definitions and notations

The direct and exchange matrix elements can be brought together if we define the antisymmetrized matrix element

$$\langle \mu\nu | V | \mu\nu \rangle_{\mathrm{AS}} = \langle \mu\nu | V | \mu\nu \rangle - \langle \mu\nu | V | \nu\mu \rangle,$$

or for a general matrix element

$$\langle \mu\nu | V | \sigma\tau \rangle_{\mathrm{AS}} = \langle \mu\nu | V | \sigma\tau \rangle - \langle \mu\nu | V | \tau\sigma \rangle.$$

It has the symmetry property

$$\langle \mu\nu | V | \sigma\tau \rangle_{\mathrm{AS}} = -\langle \mu\nu | V | \tau\sigma \rangle_{\mathrm{AS}} = -\langle \nu\mu | V | \sigma\tau \rangle_{\mathrm{AS}}.$$

Definitions and notations

The antisymmetric matrix element is also hermitian, implying

$$\langle \mu\nu | V | \sigma\tau \rangle_{\mathrm{AS}} = \langle \sigma\tau | V | \mu\nu \rangle_{\mathrm{AS}}.$$

With these notations we rewrite Eq. (14) as

$$\int \Phi^* \hat{H}_I \Phi d\tau = \frac{1}{2} \sum_{\mu=1}^{A} \sum_{\nu=1}^{A} \langle \mu\nu | V | \mu\nu \rangle_{\mathrm{AS}}. \tag{15}$$

Definitions and notations

Combining Eqs. (13) and (18) we obtain the energy functional

$$E[\Phi] = \sum_{\mu=1}^{A} \langle \mu | \hat{h}_0 | \mu \rangle + \frac{1}{2} \sum_{\mu=1}^{A} \sum_{\nu=1}^{A} \langle \mu\nu | V | \mu\nu \rangle_{\mathrm{AS}}. \tag{16}$$

which we will use as our starting point for the Hartree-Fock calculations later in this course.

Hartree-Fock: our first many-body approach

HF theory is an algorithm for a finding an approximative expression for the ground state of a given Hamiltonian. The basic ingredients are

- Define a single-particle basis $\{\psi_\alpha\}$ so that

$$\hat{h}^{\mathrm{HF}}\psi_\alpha = \varepsilon_\alpha\psi_\alpha$$

  with

$$\hat{h}^{\mathrm{HF}} = \hat{t} + \hat{u}_{\mathrm{ext}} + \hat{u}^{\mathrm{HF}}$$

- where $\hat{u}^{\mathrm{HF}}$ is a single-particle potential to be determined by the HF algorithm.
- The HF algorithm means to choose $\hat{u}^{\mathrm{HF}}$ in order to have

$$\langle\hat{H}\rangle = E^{\mathrm{HF}} = \langle\Phi_0|\hat{H}|\Phi_0\rangle$$

  a local minimum with Φ_0 being the SD ansatz for the ground state.
- The variational principle ensures that $E^{\mathrm{HF}} \geq \tilde{E}_0$, $\tilde{E}_0$ the exact ground state energy.

Hartree-Fock:

Let us now compute the Hamiltonian matrix for a system consisting of a Slater determinant for the ground state $|\Phi_0\rangle$ and two 1p1h SDs $|\Phi_i^a\rangle$ and $|\Phi_j^b\rangle$. This can obviously be generalized to many more 1p1h SDs. We will show later that we get the following expectation values

$$\langle\Phi_0|\hat{H}|\Phi_0\rangle = E_0,$$

$$\langle\Phi_i^a|\hat{H}|\Phi_0\rangle = \langle a|\hat{f}|i\rangle,$$

$$\langle\Phi_j^b|\hat{H}|\Phi_0\rangle = \langle b|\hat{f}|j\rangle,$$

$$\langle\Phi_i^a|\hat{H}|\Phi_j^b\rangle = \langle aj|\hat{v}|ib\rangle,$$

and the diagonal elements

$$\langle\Phi_i^a|\hat{H}|\Phi_i^a\rangle = E_0 + \varepsilon_a - \varepsilon_i + \langle ai|\hat{v}|ia\rangle,$$

and

$$\langle\Phi_j^b|\hat{H}|\Phi_j^b\rangle = E_0 + \varepsilon_b - \varepsilon_j + \langle bj|\hat{v}|jb\rangle.$$

NOTE: These equations and those on the next slide will be derived during week 5 (end of january).

Hartree-Fock

We can then set up a Hamiltonian matrix to be diagonalized

$$\begin{pmatrix} E_0 & \langle i|\hat{f}|a\rangle & \langle j|\hat{f}|b\rangle \\ \langle a|\hat{f}|i\rangle & E_0 + \varepsilon_a - \varepsilon_i + \langle ai|\hat{v}|ia\rangle & \langle aj|\hat{v}|ib\rangle \\ \langle b|\hat{f}|j\rangle & \langle bi|\hat{v}|ja\rangle & E_0 + \varepsilon_b - \varepsilon_j + \langle bj|\hat{v}|jb\rangle \end{pmatrix}.$$

The HF method corresponds to finding a similarity transformation where the non-diagonal matrix elements

$$\langle i|\hat{f}|a\rangle = 0$$

. We will link this expectation value with the HF method, meaning that we want to find

$$\langle i|\hat{h}^{\mathrm{HF}}|a\rangle = 0$$

Topics for Week 4, January 21-25

Hartree-Fock theory and second-quantization

- Tuesday:
- Repetition from last week
- Derivation of the Hartree-Fock equations by varying the single-particle functions or the coefficients of the single-particle equations.
- Thursday:
- More discussion of Hartree-Fock and introduction of creation and annihilation operators
- Exercises 3 and 4.

Suggested literature is AB chapter 14 and JS chapter 4. For second quantization, I have added a lot of background material in the slides here.

Background material: Variational Calculus and Lagrangian Multiplier

The calculus of variations involves problems where the quantity to be minimized or maximized is an integral.
In the general case we have an integral of the type

$$E[\Phi] = \int_a^b f(\Phi(x), \frac{\partial \Phi}{\partial x}, x)dx,$$

where E is the quantity which is sought minimized or maximized. The problem is that although f is a function of the variables Φ, $\partial\Phi/\partial x$ and x, the exact dependence of Φ on x is not known. This means again that even though the integral has fixed limits a and b, the path of integration is not known. In our case the unknown quantities are the single-particle wave functions and we wish to choose an integration path which makes the functional $E[\Phi]$ stationary. This means that we want to find minima, or maxima or saddle points. In physics we search normally for minima. Our task is therefore to find the minimum of $E[\Phi]$ so that its variation δE is zero subject to specific constraints. In our case the constraints appear as the integral which expresses the orthogonality of the single-particle wave functions. The constraints can be treated via the technique of Lagrangian multipliers

Background material: Euler-Lagrange equations

We assume the existence of an optimum path, that is a path for which $E[\Phi]$ is stationary. There are infinitely many such paths. The difference between two paths $\delta\Phi$ is called the variation of Φ.
We call the variation $\eta(x)$ and it is scaled by a factor α. The function $\eta(x)$ is arbitrary except for

$$\eta(a) = \eta(b) = 0,$$

and we assume that we can model the change in Φ as

$$\Phi(x, \alpha) = \Phi(x, 0) + \alpha\eta(x),$$

and

$$\delta\Phi = \Phi(x, \alpha) - \Phi(x, 0) = \alpha\eta(x).$$

Background material: Euler-Lagrange equations

We choose $\Phi(x, \alpha = 0)$ as the unkonwn path that will minimize E. The value $\Phi(x, \alpha \neq 0)$ describes a neighbouring path.
We have

$$E[\Phi(\alpha)] = \int_a^b f(\Phi(x, \alpha), \frac{\partial \Phi(x, \alpha)}{\partial x}, x) dx.$$

In the slides I will use the shorthand

$$\Phi_x(x, \alpha) = \frac{\partial \Phi(x, \alpha)}{\partial x}.$$

In our case $a = 0$ and $b = \infty$ and we know the value of the wave function.

Background material: Euler-Lagrange equations

The condition for an extreme of

$$E[\Phi(\alpha)] = \int_a^b f(\Phi(x,\alpha), \Phi_x(x,\alpha), x)dx,$$

is

$$\left[\frac{\partial E[\Phi(\alpha)]}{\partial x}\right]_{\alpha=0} = 0.$$

The α dependence is contained in $\Phi(x,\alpha)$ and $\Phi_x(x,\alpha)$ meaning that

$$\left[\frac{\partial E[\Phi(\alpha)]}{\partial \alpha}\right] = \int_a^b \left(\frac{\partial f}{\partial \Phi}\frac{\partial \Phi}{\partial \alpha} + \frac{\partial f}{\partial \Phi_x}\frac{\partial \Phi_x}{\partial \alpha}\right) dx.$$

We have defined

$$\frac{\partial \Phi(x,\alpha)}{\partial \alpha} = \eta(x)$$

and thereby

$$\frac{\partial \Phi_x(x,\alpha)}{\partial \alpha} = \frac{d(\eta(x))}{dx}.$$

Background material: Euler-Lagrange equations

Using

$$\frac{\partial \Phi(x,\alpha)}{\partial \alpha} = \eta(x),$$

and

$$\frac{\partial \Phi_x(x,\alpha)}{\partial \alpha} = \frac{d(\eta(x))}{dx},$$

in the integral gives

$$\left[\frac{\partial E[\Phi(\alpha)]}{\partial \alpha}\right] = \int_a^b \left(\frac{\partial f}{\partial \Phi}\eta(x) + \frac{\partial f}{\partial \Phi_x}\frac{d(\eta(x))}{dx}\right) dx.$$

Integrate the second term by parts

$$\int_a^b \frac{\partial f}{\partial \Phi_x}\frac{d(\eta(x))}{dx}dx = \eta(x)\frac{\partial f}{\partial \Phi_x}|_a^b - \int_a^b \eta(x)\frac{d}{dx}\frac{\partial f}{\partial \Phi_x}dx,$$

and since the first term dissappears due to $\eta(a) = \eta(b) = 0$, we obtain

$$\left[\frac{\partial E[\Phi(\alpha)]}{\partial \alpha}\right] = \int_a^b \left(\frac{\partial f}{\partial \Phi} - \frac{d}{dx}\frac{\partial f}{\partial \Phi_x}\right)\eta(x)dx = 0.$$

Background material: Euler-Lagrange equations

$$\left[\frac{\partial E[\Phi(\alpha)]}{\partial \alpha}\right] = \int_a^b \left(\frac{\partial f}{\partial \Phi} - \frac{d}{dx}\frac{\partial f}{\partial \Phi_x}\right)\eta(x)dx = 0,$$

can also be written as

$$\alpha\left[\frac{\partial E[\Phi(\alpha)]}{\partial \alpha}\right]_{\alpha=0} = \int_a^b \left(\frac{\partial f}{\partial \Phi} - \frac{d}{dx}\frac{\partial f}{\partial \Phi_x}\right)\delta\Phi(x)dx = \delta E = 0.$$

The condition for a stationary value is thus a partial differential equation

$$\frac{\partial f}{\partial \Phi} - \frac{d}{dx}\frac{\partial f}{\partial \Phi_x} = 0,$$

known as Euler's equation. Can easily be generalized to more variables.

Background material: Lagrangian Multipliers

Consider a function of three independent variables $f(x, y, z)$. For the function f to be an extreme we have

$$df = 0.$$

A necessary and sufficient condition is

$$\frac{\partial f}{\partial x} = \frac{\partial f}{\partial y} = \frac{\partial f}{\partial z} = 0,$$

due to

$$df = \frac{\partial f}{\partial x} dx + \frac{\partial f}{\partial y} dy + \frac{\partial f}{\partial z} dz.$$

In physical problems the variables x, y, z are often subject to constraints (in our case Φ and the orthogonality constraint) so that they are no longer all independent. It is possible at least in principle to use each constraint to eliminate one variable and to proceed with a new and smaller set of independent varables.

Background material: Lagrangian Multipliers

The use of so-called Lagrangian multipliers is an alternative technique when the elimination of of variables is incovenient or undesirable. Assume that we have an equation of constraint on the variables x, y, z

$$\phi(x, y, z) = 0,$$

resulting in

$$d\phi = \frac{\partial \phi}{\partial x} dx + \frac{\partial \phi}{\partial y} dy + \frac{\partial \phi}{\partial z} dz = 0.$$

Now we cannot set anymore

$$\frac{\partial f}{\partial x} = \frac{\partial f}{\partial y} = \frac{\partial f}{\partial z} = 0,$$

if $df = 0$ is wanted because there are now only two independent variables! Assume x and y are the independent variables. Then dz is no longer arbitrary.

Background material: Lagrangian Multipliers

However, we can add to

$$df = \frac{\partial f}{\partial x}dx + \frac{\partial f}{\partial y}dy + \frac{\partial f}{\partial z}dz,$$

a multiplum of $d\phi$, viz. $\lambda d\phi$, resulting in

$$df + \lambda d\phi = (\frac{\partial f}{\partial z} + \lambda\frac{\partial \phi}{\partial x})dx + (\frac{\partial f}{\partial y} + \lambda\frac{\partial \phi}{\partial y})dy + (\frac{\partial f}{\partial z} + \lambda\frac{\partial \phi}{\partial z})dz = 0.$$

Our multiplier is chosen so that

$$\frac{\partial f}{\partial z} + \lambda\frac{\partial \phi}{\partial z} = 0.$$

Background material: Lagrangian Multipliers

However, we took dx and dy as to be arbitrary and thus we must have

$$\frac{\partial f}{\partial x} + \lambda \frac{\partial \phi}{\partial x} = 0,$$

and

$$\frac{\partial f}{\partial y} + \lambda \frac{\partial \phi}{\partial y} = 0.$$

When all these equations are satisfied, $df = 0$. We have four unknowns, x, y, z and λ. Actually we want only x, y, z, λ need not to be determined, it is therefore often called Lagrange's undetermined multiplier. If we have a set of constraints ϕ_k we have the equations

$$\frac{\partial f}{\partial x_i} + \sum_k \lambda_k \frac{\partial \phi_k}{\partial x_i} = 0.$$

Background material: Variational Calculus and Lagrangian Multipliers

Let us specialize to the expectation value of the energy for one particle in three-dimensions. This expectation value reads

$$E = \int dxdydz\psi^*(x,y,z)\hat{H}\psi(x,y,z),$$

with the constraint

$$\int dxdydz\psi^*(x,y,z)\psi(x,y,z) = 1,$$

and a Hamiltonian

$$\hat{H} = -\frac{1}{2}\nabla^2 + \hat{v}(x,y,z).$$

I will skip the variables x, y, z below, and write for example $\hat{v}(x,y,z) = V$.

Background material: Variational Calculus and Lagrangian Multiplier

The integral involving the kinetic energy can be written as, if we assume periodic boundary conditions or that the function ψ vanishes strongly for large values of x, y, z,

$$\int dxdydz\psi^* \left(-\frac{1}{2}\nabla^2\right)\psi dxdydz = \psi^*\nabla\psi| + \int dxdydz\frac{1}{2}\nabla\psi^*\nabla\psi.$$

Inserting this expression into the expectation value for the energy and taking the variational minimum we obtain

$$\delta E = \delta\left\{\int dxdydz\left(\frac{1}{2}\nabla\psi^*\nabla\psi + V\psi^*\psi\right)\right\} = 0.$$

Background material: Variational Calculus and Lagrangian Multiplier

The constraint appears in integral form as

$$\int dxdydz\psi^*\psi = \text{constant},$$

and multiplying with a Lagrangian multiplier λ and taking the variational minimum we obtain the final variational equation

$$\delta\left\{\int dxdydz\left(\frac{1}{2}\nabla\psi^*\nabla\psi + V\psi^*\psi - \lambda\psi^*\psi\right)\right\} = 0.$$

Introducing the function f

$$f = \frac{1}{2}\nabla\psi^*\nabla\psi + V\psi^*\psi - \lambda\psi^*\psi = \frac{1}{2}(\psi_x^*\psi_x + \psi_y^*\psi_y + \psi_z^*\psi_z) + V\psi^*\psi - \lambda\psi^*\psi,$$

where we have skipped the dependence on x, y, z and introduced the shorthand ψ_x, ψ_y and ψ_z for the various derivatives.

Background material: Variational Calculus and Lagrangian Multiplier

For ψ^* the Euler equation results in

$$\frac{\partial f}{\partial \psi^*} - \frac{\partial}{\partial x}\frac{\partial f}{\partial \psi_x^*} - \frac{\partial}{\partial y}\frac{\partial f}{\partial \psi_y^*} - \frac{\partial}{\partial z}\frac{\partial f}{\partial \psi_z^*} = 0,$$

which yields

$$-\frac{1}{2}(\psi_{xx} + \psi_{yy} + \psi_{zz}) + V\psi = \lambda\psi.$$

We can then identify the Lagrangian multiplier as the energy of the system. Then the last equation is nothing but the standard Schrödinger equation and the variational approach discussed here provides a powerful method for obtaining approximate solutions of the wave function.

Finding the Hartree-Fock functional $E[\Phi]$

We have the Hamiltonian

$$\hat{H} = \hat{H}_0 + \hat{H}_I = \sum_{i=1}^{A} \hat{h}_0(x_i) + \sum_{i<j=1}^{A} \hat{v}(r_{ij}),$$

$$\hat{h}_0(x_i) = -\frac{1}{2}\nabla_i^2 + \frac{1}{2}m\omega^2 r_i^2.$$

Finding the Hartree-Fock functional $E[\Phi]$

Let us denote the ground state energy by E_0. According to the variational principle we have

$$E_0 \leq E[\Phi] = \int \Phi^* \hat{H} \Phi d\tau$$

where Φ is a trial function which we assume to be normalized

$$\int \Phi^* \Phi d\tau = 1,$$

where we have used the shorthand $d\tau = dx_1 dx_2 \ldots dx_A$.

Finding the Hartree-Fock functional $E[\Phi]$

In the Hartree-Fock method the trial function is the Slater determinant which can be rewritten as

$$\Psi(x_1, x_2, \ldots, x_A, \alpha, \beta, \ldots, \nu) = \frac{1}{\sqrt{A!}} \sum_P (-)^P P \psi_\alpha(x_1)\psi_\beta(x_2)\ldots\psi_\nu(x_A) = \sqrt{A!}\mathcal{A}\Phi_H,$$

where we have introduced the anti-symmetrization operator $\mathcal{A}$ defined by the summation over all possible permutations of two fermions. It is defined as

$$\mathcal{A} = \frac{1}{A!} \sum_P (-)^P P,$$

with the the Hartree-function given by the simple product of all possible single-particle function

$$\Phi_H(x_1, x_2, \ldots, x_A, \alpha, \beta, \ldots, \nu) = \psi_\alpha(x_1)\psi_\beta(x_2)\ldots\psi_\nu(x_A).$$

Finding the Hartree-Fock functional $E[\Phi]$

Both $\hat{H}_0$ and $\hat{H}_I$ are invariant under permutations of fermions, and hence commute with $\mathcal{A}$

$$[H_0, \mathcal{A}] = [H_I, \mathcal{A}] = 0.$$

Furthermore, $\mathcal{A}$ satisfies

$$\mathcal{A}^2 = \mathcal{A},$$

since every permutation of the Slater determinant reproduces it.

Variational Calculus and Lagrangian Multiplier, back to Hartree-Fock

Our functional is written as

$$E[\Phi] = \sum_{\mu=1}^{A} \int \psi_\mu^*(x_i)\hat{h}_0(x_i)\psi_\mu(x_i)dx_i + \frac{1}{2}\sum_{\mu=1}^{A}\sum_{\nu=1}^{A}\left[\int \psi_\mu^*(x_i)\psi_\nu^*(x_j)\hat{v}(r_{ij})\psi_\mu(x_i)\psi_\nu(x_j)dx_i dx_j\right.$$

$$\left. - \int \psi_\mu^*(x_i)\psi_\nu^*(x_j)\hat{v}(r_{ij})\psi_\nu(x_i)\psi_\mu(x_j)dx_i dx_j\right]$$

The more compact version is

$$E[\Phi] = \sum_{\mu=1}^{A}\langle\mu|\hat{h}_0|\mu\rangle + \frac{1}{2}\sum_{\mu=1}^{A}\sum_{\nu=1}^{A}\left[\langle\mu\nu|\hat{v}(r_{ij})|\mu\nu\rangle - \langle\mu\nu|\hat{v}(r_{ij})|\nu\mu\rangle\right].$$

Hartree-Fock: Variational Calculus and Lagrangian Multiplier

If we generalize the Euler-Lagrange equations to more variables and introduce A^2 Lagrange multipliers which we denote by $\epsilon_{\mu\nu}$, we can write the variational equation for the functional of E

$$\delta E - \sum_{\mu=1}^{A}\sum_{\nu=1}^{A}\epsilon_{\mu\nu}\delta\int\psi_\mu^*\psi_\nu = 0.$$

For the orthogonal wave functions ψ_μ this reduces to

$$\delta E - \sum_{\mu=1}^{A}\epsilon_{\mu}\delta\int\psi_\mu^*\psi_\mu = 0.$$

Hartree-Fock: Variational Calculus and Lagrangian Multiplier

Variation with respect to the single-particle wave functions ψ_μ yields then

$$\sum_{\mu=1}^{A}\int \delta\psi_\mu^*\hat{h}_0(x_i)\psi_\mu dx_i + \frac{1}{2}\sum_{\mu=1}^{A}\sum_{\nu=1}^{A}\left[\int \delta\psi_\mu^*\psi_\nu^*\hat{v}(r_{ij})\psi_\mu\psi_\nu dx_i dx_j - \int \delta\psi_\mu^*\psi_\nu^*\frac{1}{r_{ij}}\psi_\nu\psi_\mu dx_i dx_j\right]$$

$$+\sum_{\mu=1}^{A}\int \psi_\mu^*\hat{h}_0(x_i)\delta\psi_\mu dx_i + \frac{1}{2}\sum_{\mu=1}^{A}\sum_{\nu=1}^{A}\left[\int \psi_\mu^*\psi_\nu^*\frac{1}{r_{ij}}\delta\psi_\mu\psi_\nu dx_i dx_j - \int \psi_\mu^*\psi_\nu^*\hat{v}(r_{ij})\psi_\nu\delta\psi_\mu dx_i dx_j\right]$$

$$-\sum_{\mu=1}^{A}E_\mu\int \delta\psi_\mu^*\psi_\mu dx_i - \sum_{\mu=1}^{A}E_\mu\int \psi_\mu^*\delta\psi_\mu dx_i$$

Hartree-Fock: Variational Calculus and Lagrangian Multiplier

Although the variations $\delta\psi$ and $\delta\psi^*$ are not independent, they may in fact be treated as such, so that the terms dependent on either $\delta\psi$ and $\delta\psi^*$ individually may be set equal to zero. To see this, simply replace the arbitrary variation $\delta\psi$ by $i\delta\psi$, so that $\delta\psi^*$ is replaced by $-i\delta\psi^*$, and combine the two equations. We thus arrive at the Hartree-Fock equations

$$\left[-\frac{1}{2}\nabla_i^2 - u_{\text{ext}}(x_i) + \sum_{\nu=1}^{A}\int \psi_\nu^*(x_j)\hat{v}(r_{ij})\psi_\nu(x_j)dx_j\right]\psi_\mu(x_i) - \left[\sum_{\nu=1}^{A}\int \psi_\nu^*(x_j)\hat{v}(r_{ij})\psi_\mu(x_j)dx_j\right]\psi_\nu(x_i) = \epsilon_\mu\psi_\mu(x_i).$$

Notice that the integration $\int dx_j$ implies an integration over the spatial coordinates $\mathbf{r_j}$ and a summation over the spin-coordinate of fermion j.

Hartree-Fock: Variational Calculus and Lagrangian Multiplier

The two first terms are the expectation value of the one-body operator. The third or *direct* term is the averaged field set up by all other nucleons. As written, the term includes the 'self-interaction' of nucleons when $i = j$. The self-interaction is cancelled in the fourth term, or the *exchange* term. The exchange term results from our inclusion of the Pauli principle and the assumed determinantal form of the wave-function. The effect of exchange is for nucleons of equal single-particle quantum numbers to avoid each other.

Hartree-Fock: Variational Calculus and Lagrangian Multiplier

A theoretically convenient form of the Hartree-Fock equation is to regard the direct and exchange operator defined through

$$V_\mu^d(x_i) = \int \psi_\mu^*(x_j)\psi_\mu(x_j)\hat{v}(r_{ij})dx_j$$

and

$$V_\mu^{ex}(x_i)g(x_i) = \left(\int \psi_\mu^*(x_j)\hat{v}(r_{ij})g(x_j)dx_j\right)\psi_\mu(x_i),$$

respectively.

Hartree-Fock: Variational Calculus and Lagrangian Multiplier

The function $g(x_i)$ is an arbitrary function, and by the substitution $g(x_i) = \psi_\nu(x_i)$ we get

$$V_\mu^{ex}(x_i)\psi_\nu(x_i) = \left(\int \psi_\mu^*(x_j)\hat{v}(r_{ij})\psi_\nu(x_j)dx_j \right) \psi_\mu(x_i).$$

Hartree-Fock: Variational Calculus and Lagrangian Multiplier

We may then rewrite the Hartree-Fock equations as

$$\hat{h}^{HF}(x_i)\psi_\nu(x_i) = \epsilon_\nu\psi_\nu(x_i),$$

with

$$\hat{h}^{HF}(x_i) = \hat{h}_0(x_i) + \sum_{\mu=1}^{A} V_\mu^d(x_i) - \sum_{\mu=1}^{A} V_\mu^{ex}(x_i),$$

and where $\hat{h}_0(i)$ is the one-body part. The latter is normally chosen as a part which yields solutions in closed form. The harmonic oscilltor is a classical problem thereof. We normally rewrite the last equation as

$$\hat{h}^{HF}(x_i) = \hat{h}_0(x_i) + \hat{u}^{HF}(x_i).$$

Rewriting the energy functional

The last equation

$$\hat{h}^{HF}(x_i) = \hat{h}_0(x_i) + \hat{u}^{HF}(x_i),$$

allows us to rewrite the ground state energy (adding and subtracting $\hat{u}^{HF}(x_i)$)

$$E_0^{HF} = \langle \Phi_0 | \hat{H} | \Phi_0 \rangle = \sum_{i \leq F}^{A} \langle i | \hat{h}_0 + \hat{u}^{HF} | j \rangle + \frac{1}{2} \sum_{i \leq F}^{A} \sum_{j \leq F}^{A} [\langle ij | \hat{v} | ij \rangle - \langle ij | \hat{v} | ji \rangle] - \sum_{i \leq F}^{A} \langle i | \hat{u}^{HF} | i \rangle,$$

as

$$E_0^{HF} = \sum_{i \leq F}^{A} \varepsilon_i + \frac{1}{2} \sum_{i \leq F}^{A} \sum_{j \leq F}^{A} [\langle ij | \hat{v} | ij \rangle - \langle ij | \hat{v} | ji \rangle] - \sum_{i \leq F}^{A} \langle i | \hat{u}^{HF} | i \rangle,$$

which is nothing but

$$E_0^{HF} = \sum_{i \leq F}^{A} \varepsilon_i - \frac{1}{2} \sum_{i \leq F}^{A} \sum_{j \leq F}^{A} [\langle ij | \hat{v} | ij \rangle - \langle ij | \hat{v} | ji \rangle] .$$

This form will be used in our discussion of for example Koopman's theorem.

Hartree-Fock by varying the coefficients of a wave function expansion

Another possibility is to expand the single-particle functions in a known basis and vary the coefficients, that is, the new single-particle wave function is written as a linear expansion in terms of a fixed chosen orthogonal basis (for example harmonic oscillator, Laguerre polynomials etc)

$$\psi_a = \sum_{\lambda} C_{a\lambda}\psi_{\lambda}. \tag{17}$$

In this case we vary the coefficients $C_{a\lambda}$. If the basis has infinitely many solutions, we need to truncate the above sum. In all our equations we assume a truncation has been made.
The single-particle wave functions $\psi_{\lambda}(\mathbf{r})$, defined by the quantum numbers λ and $\mathbf{r}$ are defined as the overlap

$$\psi_{\lambda}(\mathbf{r}) = \langle \mathbf{r}|\lambda\rangle.$$

Hartree-Fock by varying the coefficients of a wave function expansion

We will omit the radial dependence of the wave functions and introduce first the following shorthands for the Hartree and Fock integrals

$$\langle \mu\nu | V | \mu\nu \rangle = \int \psi^*_\mu(\mathbf{r}_i)\psi^*_\nu(\mathbf{r}_j) V(r_{ij}) \psi_\mu(\mathbf{r}_i)\psi_\nu(\mathbf{r}_j) d\mathbf{r}_i \mathbf{r}_j,$$

and

$$\langle \mu\nu | V | \nu\mu \rangle = \int \psi^*_\mu(\mathbf{r}_i)\psi^*_\nu(\mathbf{r}_j) V(r_{ij}) \psi_\nu(\mathbf{r}_i)\psi_\mu(\mathbf{r}_i) d\mathbf{r}_i \mathbf{r}_j.$$

Hartree-Fock by varying the coefficients of a wave function expansion

Since the interaction is invariant under the interchange of two particles it means for example that we have

$$\langle \mu\nu | V | \mu\nu \rangle = \langle \nu\mu | V | \nu\mu \rangle,$$

or in the more general case

$$\langle \mu\nu | V | \sigma\tau \rangle = \langle \nu\mu | V | \tau\sigma \rangle.$$

Hartree-Fock by varying the coefficients of a wave function expansion

The direct and exchange matrix elements can be brought together if we define the antisymmetrized matrix element

$$\langle\mu\nu|V|\mu\nu\rangle_{AS} = \langle\mu\nu|V|\mu\nu\rangle - \langle\mu\nu|V|\nu\mu\rangle,$$

or for a general matrix element

$$\langle\mu\nu|V|\sigma\tau\rangle_{AS} = \langle\mu\nu|V|\sigma\tau\rangle - \langle\mu\nu|V|\tau\sigma\rangle.$$

It has the symmetry property

$$\langle\mu\nu|V|\sigma\tau\rangle_{AS} = -\langle\mu\nu|V|\tau\sigma\rangle_{AS} = -\langle\nu\mu|V|\sigma\tau\rangle_{AS}.$$

The antisymmetric matrix element is also hermitian, implying

$$\langle\mu\nu|V|\sigma\tau\rangle_{AS} = \langle\sigma\tau|V|\mu\nu\rangle_{AS}.$$

Hartree-Fock by varying the coefficients of a wave function expansion

With have for the interaction part

$$\int \Phi^* \hat{H}_1 \Phi d\tau = \frac{1}{2} \sum_{\mu=1}^{A} \sum_{\nu=1}^{A} \langle \mu\nu | V | \mu\nu \rangle_{AS}. \tag{18}$$

Combining Eqs. (13) and (18) we obtain the energy functional

$$E[\Phi] = \sum_{\mu=1}^{N} \langle \mu | h | \mu \rangle + \frac{1}{2} \sum_{\mu=1}^{A} \sum_{\nu=1}^{A} \langle \mu\nu | V | \mu\nu \rangle_{AS}. \tag{19}$$

Hartree-Fock by varying the coefficients of a wave function expansion

If we vary the above energy functional with respect to the basis functions $|\mu\rangle$, this corresponds to what was done in the previous case. We are however interested in defining a new basis defined in terms of a chosen basis as defined in Eq. (17). We can then rewrite the energy functional as

$$E[\Psi] = \sum_{a=1}^{A} \langle a|h|a\rangle + \frac{1}{2}\sum_{ab=1}^{A} \langle ab|V|ab\rangle_{AS}, \tag{20}$$

where Ψ is the new Slater determinant defined by the new basis of Eq. (17).

Hartree-Fock by varying the coefficients of a wave function expansion

Using Eq. (17) we can rewrite Eq. (20) as

$$E[\Psi] = \sum_{a=1}^{A} \sum_{\alpha\beta} C_{a\alpha}^{*} C_{a\beta} \langle \alpha | h | \beta \rangle + \frac{1}{2} \sum_{ab=1}^{A} \sum_{\alpha\beta\gamma\delta} C_{a\alpha}^{*} C_{b\beta}^{*} C_{a\gamma} C_{b\delta} \langle \alpha\beta | V | \gamma\delta \rangle_{AS}. \quad (21)$$

Hartree-Fock by varying the coefficients of a wave function expansion

We wish now to minimize the above functional. We introduce again a set of Lagrange multipliers, noting that since $\langle a|b\rangle = \delta_{a,b}$ and $\langle \alpha|\beta\rangle = \delta_{\alpha,\beta}$, the coefficients $C_{a\gamma}$ obey the relation

$$\langle a|b\rangle = \delta_{a,b} = \sum_{\alpha\beta} C^*_{a\alpha} C_{a\beta} \langle \alpha|\beta\rangle = \sum_{\alpha} C^*_{a\alpha} C_{a\alpha},$$

which allows us to define a functional to be minimized that reads

$$E[\Psi] - \sum_{a=1}^{A} \epsilon_a \sum_{\alpha} C^*_{a\alpha} C_{a\alpha}. \tag{22}$$

Hartree-Fock by varying the coefficients of a wave function expansion

Minimizing with respect to $C^*_{k\alpha}$, remembering that $C^*_{k\alpha}$ and $C_{k\alpha}$ are independent, we obtain

$$\frac{d}{dC^*_{k\alpha}}\left[E[\Psi]-\sum_a \epsilon_a \sum_\alpha C^*_{a\alpha}C_{a\alpha}\right]=0, \tag{23}$$

which yields for every single-particle state k the following Hartree-Fock equations

$$\sum_\gamma C_{k\gamma}\langle\alpha|h|\gamma\rangle+\sum_{a=1}^{N}\sum_{\beta\gamma\delta}C^*_{a\beta}C_{a\delta}C_{k\gamma}\langle\alpha\beta|V|\gamma\delta\rangle_{AS}=\epsilon_k C_{k\alpha}. \tag{24}$$

Hartree-Fock by varying the coefficients of a wave function expansion

We can rewrite this equation as

$$\sum_{\gamma}\left\{\langle\alpha|h|\gamma\rangle+\sum_{a}^{A}\sum_{\beta\delta}C_{a\beta}^{*}C_{a\delta}\langle\alpha\beta|V|\gamma\delta\rangle_{AS}\right\}C_{k\gamma}=\epsilon_{k}C_{k\alpha}. \tag{25}$$

Note that the sums over greek indices run over the number of basis set functions (in principle an infinite number).

Hartree-Fock by varying the coefficients of a wave function expansion

Defining

$$h^{HF}_{\alpha\gamma} = \langle\alpha|h|\gamma\rangle + \sum_{a=1}^{N}\sum_{\beta\delta} C^{*}_{a\beta} C_{a\delta} \langle\alpha\beta|V|\gamma\delta\rangle_{AS},$$

we can rewrite the new equations as

$$\sum_{\gamma} h^{HF}_{\alpha\gamma} C_{k\gamma} = \epsilon_k C_{k\alpha}. \tag{26}$$

Note again that the sums over greek indices run over the number of basis set functions (in principle an infinite number).

Topics for Week 5, January 28-February 1

Second-quantization

- Tuesday:
- Repetition from last week
- Annihilation and creation operators, representation of Slater determinants, operators
- Thursday:
- Particle-hole formalism and Wick's theorem
- Exercises 5, 6, 7 and 8 are not to be handed in due to project work.

Suggested literature is JS chapter 4. For second quantization, I have added a lot of background material in the slides here.

Background material: Second quantization

Can we write our Slater determinants and operators in a more compact form and at the same time obtain a calculationla formalism that allows to easily compute expectation values? Yes, second quantization, or the number representation, offers this alternative!! See also later this week on a way to represent Slater determinants.
We introduce the time-independent operators $a_\alpha^\dagger$ and a_α which create and annihilate, respectively, a particle in the single-particle state φ_α. We define the fermion creation operator $a_\alpha^\dagger$

$$a_\alpha^\dagger|0\rangle \equiv |\alpha\rangle, \tag{27}$$

and

$$a_\alpha^\dagger|\alpha_1 \dots \alpha_n\rangle_{\rm AS} \equiv |\alpha\alpha_1 \dots \alpha_n\rangle_{\rm AS} \tag{28}$$

Background material: Second quantization

In Eq. (27) the operator $a_\alpha^\dagger$ acts on the vacuum state $|0\rangle$, which does not contain any particles. Alternatively, we could define a closed-shell nucleus or atom as our new vacuum, but then we need to introduce the particle-hole formalism, see the discussion to come.
In Eq. (28) $a_\alpha^\dagger$ acts on an antisymmetric n-particle state and creates an antisymmetric $(n+1)$-particle state, where the one-body state φ_α is occupied, under the condition that $\alpha \neq \alpha_1, \alpha_2, \ldots, \alpha_n$. It follows that we can express an antisymmetric state as the product of the creation operators acting on the vacuum state.

$$|\alpha_1 \ldots \alpha_n\rangle_{\mathrm{AS}} = a_{\alpha_1}^\dagger a_{\alpha_2}^\dagger \ldots a_{\alpha_n}^\dagger |0\rangle \tag{29}$$

Background material: Second quantization

It is easy to derive the commutation and anticommutation rules for the fermionic creation operators $a^\dagger_\alpha$. Using the antisymmetry of the states (29)

$$|\alpha_1 \ldots \alpha_i \ldots \alpha_k \ldots \alpha_n\rangle_{\rm AS} = -|\alpha_1 \ldots \alpha_k \ldots \alpha_i \ldots \alpha_n\rangle_{\rm AS} \tag{30}$$

we obtain

$$a^\dagger_{\alpha_i} a^\dagger_{\alpha_k} = -a^\dagger_{\alpha_k} a^\dagger_{\alpha_i} \tag{31}$$

Background material: Second quantization

Using the Pauli principle

$$|\alpha_1 \ldots \alpha_i \ldots \alpha_i \ldots \alpha_n\rangle_{\rm AS} = 0 \tag{32}$$

it follows that

$$a^\dagger_{\alpha_i} a^\dagger_{\alpha_i} = 0. \tag{33}$$

If we combine Eqs. (31) and (33), we obtain the well-known anti-commutation rule

$$a^\dagger_\alpha a^\dagger_\beta + a^\dagger_\beta a^\dagger_\alpha \equiv \{a^\dagger_\alpha, a^\dagger_\beta\} = 0 \tag{34}$$

Background material: Second quantization

The hermitian conjugate of $a_\alpha^\dagger$ is

$$a_\alpha = (a_\alpha^\dagger)^\dagger \tag{35}$$

If we take the hermitian conjugate of Eq. (34), we arrive at

$$\{a_\alpha, a_\beta\} = 0 \tag{36}$$

Background material: Second quantization

What is the physical interpretation of the operator a_α and what is the effect of a_α on a given state $|\alpha_1\alpha_2\ldots\alpha_n\rangle_{\rm AS}$? Consider the following matrix element

$$\langle\alpha_1\alpha_2\ldots\alpha_n|a_\alpha|\alpha'_1\alpha'_2\ldots\alpha'_m\rangle \tag{37}$$

where both sides are antisymmetric. We distinguish between two cases

1. $\alpha\in\{\alpha_i\}$. Using the Pauli principle of Eq. (32) it follows

$$\langle\alpha_1\alpha_2\ldots\alpha_n|a_\alpha = 0 \tag{38}$$

2. $\alpha\notin\{\alpha_i\}$. It follows that an hermitian conjugation

$$\langle\alpha_1\alpha_2\ldots\alpha_n|a_\alpha = \langle\alpha\alpha_1\alpha_2\ldots\alpha_n| \tag{39}$$

Background material: Second quantization

Eq. (39) holds for case (1) since the lefthand side is zero due to the Pauli principle. We write Eq. (37) as

$$\langle \alpha_1 \alpha_2 \dots \alpha_n | a_\alpha | \alpha'_1 \alpha'_2 \dots \alpha'_m \rangle = \langle \alpha_1 \alpha_2 \dots \alpha_n | \, \alpha \alpha'_1 \alpha'_2 \dots \alpha'_m \tag{40}$$

Here we must have $m = n + 1$ if Eq. (40) has to be trivially different from zero. Using Eqs. (38) and (38) we arrive at

$$\langle \alpha_1 \alpha_2 \dots \alpha_n | a_\alpha | \alpha'_1 \alpha'_2 \dots \alpha'_{n+1} \rangle = \left\{ \begin{array}{ll} 0 & \pm 1 \alpha \notin \{\alpha_i\} \cup \{\alpha \alpha_i\} = \{\alpha'_i\} \end{array} \right\}$$

Background material: Second quantization

For the last case, the minus and plus signs apply when the sequence $\alpha, \alpha_1, \alpha_2, \ldots, \alpha_n$ and $\alpha'_1, \alpha'_2, \ldots, \alpha'_{n+1}$ are related to each other via even and odd permutations. If we assume that $\alpha \notin \{\alpha_i\}$ we have from Eq. (**??**)

$$\langle \alpha_1 \alpha_2 \ldots \alpha_n | a_\alpha | \alpha'_1 \alpha'_2 \ldots \alpha'_{n+1} \rangle = 0 \tag{41}$$

when $\alpha \in \{\alpha'_i\}$. If $\alpha \notin \{\alpha'_i\}$, we obtain

$$a_\alpha \underbrace{| \alpha'_1 \alpha'_2 \ldots \alpha'_{n+1} \rangle}_{\neq \alpha} = 0 \tag{42}$$

and in particular

$$a_\alpha |0\rangle = 0 \tag{43}$$

Background material: Second quantization

If $\{\alpha\alpha_i\} = \{\alpha'_i\}$, performing the right permutations, the sequence $\alpha, \alpha_1, \alpha_2, \ldots, \alpha_n$ is identical with the sequence $\alpha'_1, \alpha'_2, \ldots, \alpha'_{n+1}$. This results in

$$\langle \alpha_1\alpha_2 \ldots \alpha_n | a_\alpha | \alpha\alpha_1\alpha_2 \ldots \alpha_n \rangle = 1 \tag{44}$$

and thus

$$a_\alpha | \alpha\alpha_1\alpha_2 \ldots \alpha_n \rangle = | \alpha_1\alpha_2 \ldots \alpha_n \rangle \tag{45}$$

Background material: Second quantization

The action of the operator a_α from the left on a state vector is to to remove one particle in the state α. If the state vector does not contain the single-particle state α, the outcome of the operation is zero. The operator a_α is normally called for a destruction or annihilation operator.

The next step is to establish the commutator algebra of $a_\alpha^\dagger$ and a_β.

Background material: Second quantization

The action of the anti-commutator $\{a_\alpha^\dagger, a_\alpha\}$ on a given n-particle state is

$$
\begin{aligned}
a_\alpha^\dagger a_\alpha \underbrace{|\alpha_1 \alpha_2 \ldots \alpha_n\rangle}_{\neq \alpha} &= 0 \\
a_\alpha a_\alpha^\dagger \underbrace{|\alpha_1 \alpha_2 \ldots \alpha_n\rangle}_{\neq \alpha} &= a_\alpha \underbrace{|\alpha \alpha_1 \alpha_2 \ldots \alpha_n\rangle}_{\neq \alpha} = \underbrace{|\alpha_1 \alpha_2 \ldots \alpha_n\rangle}_{\neq \alpha}
\end{aligned}
\tag{46}
$$

if the single-particle state α is not contained in the state.

Background material: Second quantization

If it is present we arrive at

$$\begin{aligned} a_\alpha^\dagger a_\alpha |\alpha_1\alpha_2\ldots\alpha_k\alpha\alpha_{k+1}\ldots\alpha_{n-1}\rangle &= a_\alpha^\dagger a_\alpha (-1)^k |\alpha\alpha_1\alpha_2\ldots\alpha_{n-1}\rangle \\ = (-1)^k |\alpha\alpha_1\alpha_2\ldots\alpha_{n-1}\rangle &= |\alpha_1\alpha_2\ldots\alpha_k\alpha\alpha_{k+1}\ldots\alpha_{n-1}\rangle \\ a_\alpha a_\alpha^\dagger |\alpha_1\alpha_2\ldots\alpha_k\alpha\alpha_{k+1}\ldots\alpha_{n-1}\rangle &= 0 \end{aligned} \tag{47}$$

From Eqs. (46) and (47) we arrive at

$$\{a_\alpha^\dagger, a_\alpha\} = a_\alpha^\dagger a_\alpha + a_\alpha a_\alpha^\dagger = 1 \tag{48}$$

Background material: Second quantization

The action of $a^\dagger_\alpha, a_\beta$, with $\alpha \neq \beta$ on a given state yields three possibilities. The first case is a state vector which contains both α and β, then either α or β and finally none of them.

Background material: Second quantization

The first case results in

$$a_\alpha^\dagger a_\beta |\alpha\beta\alpha_1\alpha_2\ldots\alpha_{n-2}\rangle = 0$$
$$a_\beta a_\alpha^\dagger |\alpha\beta\alpha_1\alpha_2\ldots\alpha_{n-2}\rangle = 0 \tag{49}$$

while the second case gives

$$\begin{aligned} a_\alpha^\dagger a_\beta |\beta \underbrace{\alpha_1\alpha_2\ldots\alpha_{n-1}}_{\neq\alpha}\rangle &= |\alpha \underbrace{\alpha_1\alpha_2\ldots\alpha_{n-1}}_{\neq\alpha}\rangle \\ a_\beta a_\alpha^\dagger |\beta \underbrace{\alpha_1\alpha_2\ldots\alpha_{n-1}}_{\neq\alpha}\rangle &= a_\beta |\alpha\beta \underbrace{\beta\alpha_1\alpha_2\ldots\alpha_{n-1}}_{\neq\alpha}\rangle \\ &= -|\alpha \underbrace{\alpha_1\alpha_2\ldots\alpha_{n-1}}_{\neq\alpha}\rangle \end{aligned} \tag{50}$$

Background material: Second quantization

Finally if the state vector does not contain α and β

$$
\begin{aligned}
a_\alpha^\dagger a_\beta |\underbrace{\alpha_1\alpha_2\ldots\alpha_n}_{\neq\alpha,\beta}\rangle &= 0 \\
a_\beta a_\alpha^\dagger |\underbrace{\alpha_1\alpha_2\ldots\alpha_n}_{\neq\alpha,\beta}\rangle &= a_\beta|\alpha\underbrace{\alpha_1\alpha_2\ldots\alpha_n}_{\neq\alpha,\beta}\rangle = 0
\end{aligned}
\tag{51}
$$

For all three cases we have

$$
\{a_\alpha^\dagger, a_\beta\} = a_\alpha^\dagger a_\beta + a_\beta a_\alpha^\dagger = 0, \quad \alpha \neq \beta \tag{52}
$$

Background material: Second quantization

We can summarize our findings in Eqs. (48) and (52) as

$$\{a_\alpha^\dagger, a_\beta\} = \delta_{\alpha\beta} \tag{53}$$

with $\delta_{\alpha\beta}$ is the Kroenecker δ-symbol.
The properties of the creation and annihilation operators can be summarized as (for fermions)

$$a_\alpha^\dagger|0\rangle \equiv |\alpha\rangle,$$

and

$$a_\alpha^\dagger|\alpha_1 \ldots \alpha_n\rangle_{\rm AS} \equiv |\alpha\alpha_1 \ldots \alpha_n\rangle_{\rm AS}.$$

from which follows

$$|\alpha_1 \ldots \alpha_n\rangle_{\rm AS} = a_{\alpha_1}^\dagger a_{\alpha_2}^\dagger \ldots a_{\alpha_n}^\dagger|0\rangle.$$

Background material: Second quantization

The hermitian conjugate has the folowing properties

$$a_\alpha = (a_\alpha^\dagger)^\dagger.$$

Finally we found

$$a_\alpha \underbrace{|\alpha_1'\alpha_2'\ldots\alpha_{n+1}'\rangle}_{\neq\alpha} = 0, \quad \text{spesielt } a_\alpha|0\rangle = 0,$$

and

$$a_\alpha|\alpha\alpha_1\alpha_2\ldots\alpha_n\rangle = |\alpha_1\alpha_2\ldots\alpha_n\rangle,$$

and the corresponding commutator algebra

$$\{a_\alpha^\dagger, a_\beta^\dagger\} = \{a_\alpha, a_\beta\} = 0 \qquad \{a_\alpha^\dagger, a_\beta\} = \delta_{\alpha\beta}.$$

Background material: Operators in second quantization

A very useful operator is the so-called number-operator. Most physics cases we will study conserve the total number of particles. The number operator is therefore a useful quantity which allows us to test that our many-body formalism conserves the number of particles. In for example (d, p) or (p, d) reactions it is important to be able to describe quantum mechanical states where particles get added or removed. A creation operator $a_\alpha^\dagger$ adds one particle to the single-particle state α of a give many-body state vector, while an annihilation operator a_α removes a particle from a single-particle state α.

Operators in second quantization

Let us consider an operator proportional with $a^\dagger_\alpha a_\beta$ and $\alpha = \beta$. It acts on an n-particle state resulting in

$$a^\dagger_\alpha a_\alpha |\alpha_1 \alpha_2 \dots \alpha_n\rangle = \begin{cases} 0 & \alpha \notin \{\alpha_i\} \\ \\ |\alpha_1 \alpha_2 \dots \alpha_n\rangle & \alpha \in \{\alpha_i\} \end{cases} \tag{54}$$

Summing over all possible one-particle states we arrive at

$$\left(\sum_\alpha a^\dagger_\alpha a_\alpha \right) |\alpha_1 \alpha_2 \dots \alpha_n\rangle = n |\alpha_1 \alpha_2 \dots \alpha_n\rangle \tag{55}$$

Operators in second quantization

The operator

$$\hat{N} = \sum_{\alpha} a_{\alpha}^{\dagger} a_{\alpha} \tag{56}$$

is called the number operator since it counts the number of particles in a give state vector when it acts on the different single-particle states. It acts on one single-particle state at the time and falls therefore under category one-body operators. Next we look at another important one-body operator, namely $\hat{H}_0$ and study its operator form in the occupation number representation.

Operators in second quantization

We want to obtain an expression for a one-body operator which conserves the number of particles. Here we study the one-body operator for the kinetic energy plus an eventual external one-body potential. The action of this operator on a particular n-body state with its pertinent expectation value has already been studied in coordinate space. In coordinate space the operator reads

$$\hat{H}_0 = \sum_i \hat{h}_0(x_i) \tag{57}$$

and the anti-symmetric n-particle Slater determinant is defined as

$$\Phi(x_1, x_2, \dots, x_n, \alpha_1, \alpha_2, \dots, \alpha_n) = \frac{1}{\sqrt{n!}} \sum_p (-1)^p \psi_{\alpha_1}(x_1)\psi_{\alpha_2}(x_2)\dots\psi_{\alpha_n}(x_n). \tag{58}$$

Operators in second quantization

Defining

$$\hat{h}_0(x_i)\psi_{\alpha_i}(x_i) = \sum_{\alpha'_k} \psi_{\alpha'_k}(x_i)\langle\alpha'_k|\hat{h}_0|\alpha_k\rangle \tag{59}$$

we can easily evaluate the action of $\hat{H}_0$ on each product of one-particle functions in Slater determinant. From Eqs. (58) (59) we obtain the following result without permuting any particle pair

$$\begin{aligned}
& \left(\sum_i \hat{h}_0(x_i)\right)\psi_{\alpha_1}(x_1)\psi_{\alpha_2}(x_2)\ldots\psi_{\alpha_n}(x_n) \\
= & \sum_{\alpha'_1}\langle\alpha'_1|\hat{h}_0|\alpha_1\rangle\psi_{\alpha'_1}(x_1)\psi_{\alpha_2}(x_2)\ldots\psi_{\alpha_n}(x_n) \\
+ & \sum_{\alpha'_2}\langle\alpha'_2|\hat{h}_0|\alpha_2\rangle\psi_{\alpha_1}(x_1)\psi_{\alpha'_2}(x_2)\ldots\psi_{\alpha_n}(x_n) \\
+ & \ldots \\
+ & \sum_{\alpha'_n}\langle\alpha'_n|\hat{h}_0|\alpha_n\rangle\psi_{\alpha_1}(x_1)\psi_{\alpha_2}(x_2)\ldots\psi_{\alpha'_n}(x_n)
\end{aligned} \tag{60}$$

Operators in second quantization

If we interchange the positions of particle 1 and 2 we obtain

$$
\begin{aligned}
& \left(\sum_i \hat{h}_0(x_i)\right) \psi_{\alpha_1}(x_2)\psi_{\alpha_1}(x_2)\ldots\psi_{\alpha_n}(x_n) \\
= & \sum_{\alpha_2'} \langle \alpha_2' | \hat{h}_0 | \alpha_2 \rangle \psi_{\alpha_1}(x_2)\psi_{\alpha_2'}(x_1)\ldots\psi_{\alpha_n}(x_n) \\
+ & \sum_{\alpha_1'} \langle \alpha_1' | \hat{h}_0 | \alpha_1 \rangle \psi_{\alpha_1'}(x_2)\psi_{\alpha_2}(x_1)\ldots\psi_{\alpha_n}(x_n) \\
+ & \ldots \\
+ & \sum_{\alpha_n'} \langle \alpha_n' | \hat{h}_0 | \alpha_n \rangle \psi_{\alpha_1}(x_2)\psi_{\alpha_1}(x_2)\ldots\psi_{\alpha_n'}(x_n) \qquad (61)
\end{aligned}
$$

Operators in second quantization

We can continue by computing all possible permutations. We rewrite also our Slater determinant in its second quantized form and skip the dependence on the quantum numbers x_i. Summing up all contributions and taking care of all phases $(-1)^p$ we arrive at

$$\begin{aligned}
\hat{H}_0|\alpha_1,\alpha_2,\dots,\alpha_n\rangle &= \sum_{\alpha_1'}\langle\alpha_1'|\hat{h}_0|\alpha_1\rangle|\alpha_1'\alpha_2\dots\alpha_n\rangle \\
&+ \sum_{\alpha_2'}\langle\alpha_2'|\hat{h}_0|\alpha_2\rangle|\alpha_1\alpha_2'\dots\alpha_n\rangle \\
&+ \dots \\
&+ \sum_{\alpha_n'}\langle\alpha_n'|\hat{h}_0|\alpha_n\rangle|\alpha_1\alpha_2\dots\alpha_n'\rangle \qquad (62)
\end{aligned}$$

Operators in second quantization

In Eq. (62) we have expressed the action of the one-body operator of Eq. (57) on the n-body state of Eq. (58) in its second quantized form. This equation can be further manipulated if we use the properties of the creation and annihilation operator on each primed quantum number, that is

$$|\alpha_1\alpha_2\ldots\alpha'_k\ldots\alpha_n\rangle = a^\dagger_{\alpha'_k} a_{\alpha_k}|\alpha_1\alpha_2\ldots\alpha_k\ldots\alpha_n\rangle \tag{63}$$

Inserting this in the right-hand side of Eq. (62) results in

$$\begin{aligned}
\hat{H}_0|\alpha_1\alpha_2\ldots\alpha_n\rangle &= \sum_{\alpha'_1}\langle\alpha'_1|\hat{h}_0|\alpha_1\rangle a^\dagger_{\alpha'_1} a_{\alpha_1}|\alpha_1\alpha_2\ldots\alpha_n\rangle \\
&+ \sum_{\alpha'_2}\langle\alpha'_2|\hat{h}_0|\alpha_2\rangle a^\dagger_{\alpha'_2} a_{\alpha_2}|\alpha_1\alpha_2\ldots\alpha_n\rangle \\
&+ \ldots \\
&+ \sum_{\alpha'_n}\langle\alpha'_n|\hat{h}_0|\alpha_n\rangle a^\dagger_{\alpha'_n} a_{\alpha_n}|\alpha_1\alpha_2\ldots\alpha_n\rangle \\
&= \sum_{\alpha,\beta}\langle\alpha|\hat{h}_0|\beta\rangle a^\dagger_\alpha a_\beta|\alpha_1\alpha_2\ldots\alpha_n\rangle
\end{aligned} \tag{64}$$

Operators in second quantization

In the number occupation representation or second quantization we get the following expression for a one-body operator which conserves the number of particles

$$\hat{H}_0 = \sum_{\alpha\beta} \langle \alpha | \hat{h}_0 | \beta \rangle a_\alpha^\dagger a_\beta \tag{65}$$

Obviously, $\hat{H}_0$ can be replaced by any other one-body operator which preserved the number of particles. The stucture of the operator is therefore not limited to say the kinetic or single-particle energy only.

The opearator $\hat{H}_0$ takes a particle from the single-particle state β to the single-particle state α with a probability for the transition given by the expectation value $\langle \alpha | h | \beta \rangle$.

Operators in second quantization, another way to do exercise 2

It is instructive to verify Eq. (65) by computing the expectation value of $\hat{H}_0$ between two single-particle states (as we did in exercise 2)

$$\langle\alpha_1|\hat{H}_0|\alpha_2\rangle = \sum_{\alpha\beta}\langle\alpha|\hat{h}_0|\beta\rangle\langle 0|a_{\alpha_1}a^\dagger_\alpha a_\beta a^\dagger_{\alpha_2}|0\rangle \tag{66}$$

Using the commutation relations for the creation and annihilation operators we have

$$a_{\alpha_1}a^\dagger_\alpha a_\beta a^\dagger_{\alpha_2} = (\delta_{\alpha\alpha_1} - a^\dagger_\alpha a_{\alpha_1})(\delta_{\beta\alpha_2} - a^\dagger_{\alpha_2}a_\beta), \tag{67}$$

which results in

$$\langle 0|a_{\alpha_1}a^\dagger_\alpha a_\beta a^\dagger_{\alpha_2}|0\rangle = \delta_{\alpha\alpha_1}\delta_{\beta\alpha_2} \tag{68}$$

and

$$\langle\alpha_1|\hat{H}_0|\alpha_2\rangle = \sum_{\alpha\beta}\langle\alpha|\hat{h}_0|\beta\rangle\delta_{\alpha\alpha_1}\delta_{\beta\alpha_2} = \langle\alpha_1|\hat{h}_0|\alpha_2\rangle \tag{69}$$

as expected.

Operators in second quantization

Let us now derive the expression for our two-body interaction part, which also conserves the number of particles. We can proceed in exactly the same way as for the one-body operator. In the coordinate representation our two-body interaction part takes the following expression

$$\hat{H}_I = \sum_{i<j} V(x_i, x_j) \tag{70}$$

where the summation runs over distinct pairs. The term V can be an interaction model for the nucleon-nucleon interaction or the interaction between two electrons. It can also include additional two-body interaction terms.

Operators in second quantization

The action of this operator on a product of two single-particle functions is defined as

$$V(x_i, x_j)\psi_{\alpha_k}(x_i)\psi_{\alpha_l}(x_j) = \sum_{\alpha'_k \alpha'_l} \psi'_{\alpha_k}(x_i)\psi'_{\alpha_l}(x_j)\langle \alpha'_k \alpha'_l | V | \alpha_k \alpha_l \rangle \tag{71}$$

Operators in second quantization

We can now let $\hat{H}_I$ act on all terms in the linear combination for $|\alpha_1\alpha_2\ldots\alpha_n\rangle$. Without any permutations we have

$$\begin{aligned}
& \left(\sum_{i<j} V(x_i,x_j)\right)\psi_{\alpha_1}(x_1)\psi_{\alpha_2}(x_2)\ldots\psi_{\alpha_n}(x_n) \\
= & \sum_{\alpha_1'\alpha_2'}\langle\alpha_1'\alpha_2'|V|\alpha_1\alpha_2\rangle\psi'_{\alpha_1}(x_1)\psi'_{\alpha_2}(x_2)\ldots\psi_{\alpha_n}(x_n) \\
+ & \ldots \\
+ & \sum_{\alpha_1'\alpha_n'}\langle\alpha_1'\alpha_n'|V|\alpha_1\alpha_n\rangle\psi'_{\alpha_1}(x_1)\psi_{\alpha_2}(x_2)\ldots\psi'_{\alpha_n}(x_n) \\
+ & \ldots \\
+ & \sum_{\alpha_2'\alpha_n'}\langle\alpha_2'\alpha_n'|V|\alpha_2\alpha_n\rangle\psi_{\alpha_1}(x_1)\psi'_{\alpha_2}(x_2)\ldots\psi'_{\alpha_n}(x_n) \\
+ & \ldots
\end{aligned} \tag{72}$$

where on the rhs we have a term for each distinct pairs.

Operators in second quantization

For the other terms on the rhs we obtain similar expressions and summing over all terms we obtain

$$
\begin{aligned}
H_I|\alpha_1\alpha_2\ldots\alpha_n\rangle &= \sum_{\alpha_1',\alpha_2'}\langle\alpha_1'\alpha_2'|V|\alpha_1\alpha_2\rangle|\alpha_1'\alpha_2'\ldots\alpha_n\rangle \\
&+ \ldots \\
&+ \sum_{\alpha_1',\alpha_n'}\langle\alpha_1'\alpha_n'|V|\alpha_1\alpha_n\rangle|\alpha_1'\alpha_2\ldots\alpha_n'\rangle \\
&+ \ldots \\
&+ \sum_{\alpha_2',\alpha_n'}\langle\alpha_2'\alpha_n'|V|\alpha_2\alpha_n\rangle|\alpha_1\alpha_2'\ldots\alpha_n'\rangle \\
&+ \ldots
\end{aligned}
\tag{73}
$$

Operators in second quantization

We introduce second quantization via the relation

$$
\begin{aligned}
& a^\dagger_{\alpha'_k} a^\dagger_{\alpha'_l} a_{\alpha_l} a_{\alpha_k} |\alpha_1 \alpha_2 \ldots \alpha_k \ldots \alpha_l \ldots \alpha_n\rangle \\
= \quad & (-1)^{k-1}(-1)^{l-2} a^\dagger_{\alpha'_k} a^\dagger_{\alpha'_l} a_{\alpha_l} a_{\alpha_k} |\alpha_k \alpha_l \underbrace{\alpha_1 \alpha_2 \ldots \alpha_n}_{\neq \alpha_k, \alpha_l}\rangle \\
= \quad & (-1)^{k-1}(-1)^{l-2} |\alpha'_k \alpha'_l \underbrace{\alpha_1 \alpha_2 \ldots \alpha_n}_{\neq \alpha'_k, \alpha'_l}\rangle \\
= \quad & |\alpha_1 \alpha_2 \ldots \alpha'_k \ldots \alpha'_l \ldots \alpha_n\rangle \qquad (74)
\end{aligned}
$$

Operators in second quantization

Inserting this in (73) gives

$$
\begin{aligned}
H_I|\alpha_1\alpha_2\ldots\alpha_n\rangle &= \sum_{\alpha_1',\alpha_2'} \langle\alpha_1'\alpha_2'|V|\alpha_1\alpha_2\rangle a^\dagger_{\alpha_1'} a^\dagger_{\alpha_2'} a_{\alpha_2} a_{\alpha_1} |\alpha_1\alpha_2\ldots\alpha_n\rangle \\
&+ \quad \ldots \\
&= \sum_{\alpha_1',\alpha_n'} \langle\alpha_1'\alpha_n'|V|\alpha_1\alpha_n\rangle a^\dagger_{\alpha_1'} a^\dagger_{\alpha_n'} a_{\alpha_n} a_{\alpha_1} |\alpha_1\alpha_2\ldots\alpha_n\rangle \\
&+ \quad \ldots \\
&= \sum_{\alpha_2',\alpha_n'} \langle\alpha_2'\alpha_n'|V|\alpha_2\alpha_n\rangle a^\dagger_{\alpha_2'} a^\dagger_{\alpha_n'} a_{\alpha_n} a_{\alpha_2} |\alpha_1\alpha_2\ldots\alpha_n\rangle \\
&+ \quad \ldots \\
&= {\sum_{\alpha,\beta,\gamma,\delta}}' \langle\alpha\beta|V|\gamma\delta\rangle a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma |\alpha_1\alpha_2\ldots\alpha_n\rangle \qquad (75)
\end{aligned}
$$

Operators in second quantization

Here we let $\sum'$ indicate that the sums running over α and β run over all single-particle states, while the summations γ and δ run over all pairs of single-particle states. We wish to remove this restriction and since

$$\langle\alpha\beta|V|\gamma\delta\rangle = \langle\beta\alpha|V|\delta\gamma\rangle \tag{76}$$

we get

$$\sum_{\alpha,\beta}\langle\alpha\beta|V|\gamma\delta\rangle a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma = \sum_{\alpha,\beta}\langle\beta\alpha|V|\delta\gamma\rangle a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma \tag{77}$$

$$= \sum_{\alpha,\beta}\langle\beta\alpha|V|\delta\gamma\rangle a_\beta^\dagger a_\alpha^\dagger a_\gamma a_\delta \tag{78}$$

where we have used the anti-commutation rules.

Operators in second quantization

Changing the summation indices α and β in (78) we obtain

$$\sum_{\alpha,\beta}\langle\alpha\beta|V|\gamma\delta\rangle a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma = \sum_{\alpha,\beta}\langle\alpha\beta|V|\delta\gamma\rangle a_\alpha^\dagger a_\beta^\dagger a_\gamma a_\delta \tag{79}$$

From this it follows that the restriction on the summation over γ and δ can be removed if we multiply with a factor $\frac{1}{2}$, resulting in

$$\hat{H}_I = \frac{1}{2}\sum_{\alpha,\beta,\gamma,\delta}\langle\alpha\beta|V|\gamma\delta\rangle a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma \tag{80}$$

where we sum freely over all single-particle states α, β, γ og δ.

Operators in second quantization, exercise 2 again in another form

With this expression we can now verify that the second quantization form of $\hat{H}_I$ in Eq. (80) results in the same matrix between two anti-symmetrized two-particle states as its corresponding coordinate space representation (as we did in exercise 2). We have

$$\langle \alpha_1 \alpha_2 | \hat{H}_I | \beta_1 \beta_2 \rangle = \frac{1}{2} \sum_{\alpha\beta\gamma,\delta} \langle \alpha\beta | V | \gamma\delta \rangle \langle 0 | a_{\alpha_2} a_{\alpha_1} a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma a^\dagger_{\beta_1} a^\dagger_{\beta_2} | 0 \rangle. \tag{81}$$

Operators in second quantization

Using the commutation relations we get

$$
\begin{aligned}
& a_{\alpha_2} a_{\alpha_1} a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma a^\dagger_{\beta_1} a^\dagger_{\beta_2} \\
= \;& a_{\alpha_2} a_{\alpha_1} a^\dagger_\alpha a^\dagger_\beta (a_\delta \delta_{\gamma\beta_1} a^\dagger_{\beta_2} - a_\delta a^\dagger_{\beta_1} a_\gamma a^\dagger_{\beta_2}) \\
= \;& a_{\alpha_2} a_{\alpha_1} a^\dagger_\alpha a^\dagger_\beta (\delta_{\gamma\beta_1}\delta_{\delta\beta_2} - \delta_{\gamma\beta_1} a^\dagger_{\beta_2} a_\delta - a_\delta a^\dagger_{\beta_1} \delta_{\gamma\beta_2} + a_\delta a^\dagger_{\beta_1} a^\dagger_{\beta_2} a_\gamma) \\
= \;& a_{\alpha_2} a_{\alpha_1} a^\dagger_\alpha a^\dagger_\beta (\delta_{\gamma\beta_1}\delta_{\delta\beta_2} - \delta_{\gamma\beta_1} a^\dagger_{\beta_2} a_\delta \\
& \quad - \delta_{\delta\beta_1}\delta_{\gamma\beta_2} + \delta_{\gamma\beta_2} a^\dagger_{\beta_1} a_\delta + a_\delta a^\dagger_{\beta_1} a^\dagger_{\beta_2} a_\gamma)
\end{aligned}
\tag{82}
$$

Operators in second quantization

The vacuum expectation value of this product of operators becomes

$$\begin{aligned} & \langle 0|a_{\alpha_2} a_{\alpha_1} a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma a^\dagger_{\beta_1} a^\dagger_{\beta_2}|0\rangle \\ = \quad & (\delta_{\gamma\beta_1}\delta_{\delta\beta_2} - \delta_{\delta\beta_1}\delta_{\gamma\beta_2})\langle 0|a_{\alpha_2} a_{\alpha_1} a^\dagger_\alpha a^\dagger_\beta|0\rangle \\ = \quad & (\delta_{\gamma\beta_1}\delta_{\delta\beta_2} - \delta_{\delta\beta_1}\delta_{\gamma\beta_2})(\delta_{\alpha\alpha_1}\delta_{\beta\alpha_2} - \delta_{\beta\alpha_1}\delta_{\alpha\alpha_2}) \end{aligned} \tag{83}$$

Operators in second quantization

Insertion of Eq. (83) in Eq. (81) results in

$$\begin{aligned}\langle\alpha_1\alpha_2|\hat{H}_I|\beta_1\beta_2\rangle &= \frac{1}{2}\big[\langle\alpha_1\alpha_2|V|\beta_1\beta_2\rangle - \langle\alpha_1\alpha_2|V|\beta_2\beta_1\rangle \\ &\quad -\langle\alpha_2\alpha_1|V|\beta_1\beta_2\rangle + \langle\alpha_2\alpha_1|V|\beta_2\beta_1\rangle\big] \\ &= \langle\alpha_1\alpha_2|V|\beta_1\beta_2\rangle - \langle\alpha_1\alpha_2|V|\beta_2\beta_1\rangle \\ &= \langle\alpha_1\alpha_2|V|\beta_1\beta_2\rangle_{\mathrm{AS}}. \end{aligned} \tag{84}$$

Operators in second quantization

The two-body operator can also be expressed in terms of the anti-symmetrized matrix elements we discussed previously as

$$\begin{aligned}
\hat{H}_I &= \frac{1}{2}\sum_{\alpha\beta\gamma\delta}\langle\alpha\beta|V|\gamma\delta\rangle a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma \\
&= \frac{1}{4}\sum_{\alpha\beta\gamma\delta}\left[\langle\alpha\beta|V|\gamma\delta\rangle - \langle\alpha\beta|V|\delta\gamma\rangle\right] a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma \\
&= \frac{1}{4}\sum_{\alpha\beta\gamma\delta}\langle\alpha\beta|V|\gamma\delta\rangle_{\rm AS} a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma \qquad (85)
\end{aligned}$$

Operators in second quantization

The factors in front of the operator, either $\frac{1}{4}$ or $\frac{1}{2}$ tells whether we use antisymmetrized matrix elements or not.
We can now express the Hamiltonian operator for a many-fermion system in the occupation basis representation as

$$H = \sum_{\alpha,\beta} \langle \alpha | t + u | \beta \rangle a_\alpha^\dagger a_\beta + \frac{1}{4} \sum_{\alpha,\beta,\gamma,\delta} \langle \alpha\beta | V | \gamma\delta \rangle a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma . \tag{86}$$

This is form we will use in the rest of these lectures, assuming that we work with anti-symmetrized two-body matrix elements.

Wick's theorem

Wick's theorem is based on two fundamental concepts, namely *normal ordering* and *contraction*. The normal-ordered form of $\widehat{\mathbf{A}}\widehat{\mathbf{B}}..\widehat{\mathbf{X}}\widehat{\mathbf{Y}}$, where the individual terms are either a creation or annihilation operator, is defined as

$$\left\{\widehat{\mathbf{A}}\widehat{\mathbf{B}}..\widehat{\mathbf{X}}\widehat{\mathbf{Y}}\right\} \equiv (-1)^p \, [\text{creation operators}] \cdot [\text{annihilation operators}] \, . \tag{87}$$

The p subscript denotes the number of permutations that is needed to transform the original string into the normal-ordered form. A contraction between to arbitrary operators $\widehat{\mathbf{X}}$ and $\widehat{\mathbf{Y}}$ is defined as

$$\overbrace{\widehat{\mathbf{X}}\widehat{\mathbf{Y}}} \equiv \langle 0|\widehat{\mathbf{X}}\widehat{\mathbf{Y}}|0\rangle. \tag{88}$$

Wick's theorem

It is also possible to contract operators inside a normal ordered products. We define the original relative position between two operators in a normal ordered product as p, the so-called permutation number. This is the number of permutations needed to bring one of the two operators next to the other one. A contraction between two operators with $p \neq 0$ inside a normal ordered is defined as

$$\left\{ \widehat{\mathbf{A}}\widehat{\mathbf{B}}..\overbrace{\widehat{\mathbf{X}}\widehat{\mathbf{Y}}} \right\} = (-1)^p \left\{ \widehat{\mathbf{A}}\widehat{\mathbf{B}}..\widehat{\mathbf{X}}\widehat{\mathbf{Y}} \right\}. \tag{89}$$

In the general case with m contractions, the procedure is similar, and the prefactor changes to

$$(-1)^{p_1+p_2+..+p_m}. \tag{90}$$

Wick's theorem

Wick's theorem states that every string of creation and annihilation operators can be written as a sum of normalordered products with all possible ways of contractions,

$$\widehat{\mathbf{A}}\widehat{\mathbf{B}}\widehat{\mathbf{C}}\widehat{\mathbf{D}}..\widehat{\mathbf{R}}\widehat{\mathbf{X}}\widehat{\mathbf{Y}}\widehat{\mathbf{Z}} = \left\{\widehat{\mathbf{A}}\widehat{\mathbf{B}}\widehat{\mathbf{C}}\widehat{\mathbf{D}}..\widehat{\mathbf{R}}\widehat{\mathbf{X}}\widehat{\mathbf{Y}}\widehat{\mathbf{Z}}\right\} \tag{91}$$

$$+ \sum_{(1)} \left\{\overbrace{\widehat{\mathbf{A}}\widehat{\mathbf{B}}}\widehat{\mathbf{C}}\widehat{\mathbf{D}}..\widehat{\mathbf{R}}\widehat{\mathbf{X}}\widehat{\mathbf{Y}}\widehat{\mathbf{Z}}\right\} \tag{92}$$

$$+ \sum_{(2)} \left\{\overbrace{\widehat{\mathbf{A}}\widehat{\mathbf{B}}\widehat{\mathbf{C}}\widehat{\mathbf{D}}}..\widehat{\mathbf{R}}\widehat{\mathbf{X}}\widehat{\mathbf{Y}}\widehat{\mathbf{Z}}\right\} \tag{93}$$

$$+ \ldots \tag{94}$$

$$+ \sum_{\left[\frac{N}{2}\right]} \left\{\overbrace{\widehat{\mathbf{A}}\widehat{\mathbf{B}}\widehat{\mathbf{C}}\widehat{\mathbf{D}}}.. \overbrace{\widehat{\mathbf{R}}\widehat{\mathbf{X}}\widehat{\mathbf{Y}}\widehat{\mathbf{Z}}}\right\}. \tag{95}$$

Wick's theorem

The $\sum_{(m)}$ means the sum over all terms with m contractions, while $\left[\frac{N}{2}\right]$ means the largest integer that not do not exceeds $\frac{N}{2}$ where N is the number of creation and annihilation operators. When N is even,

$$\left[\frac{N}{2}\right] = \frac{N}{2}, \tag{96}$$

and the last sum in Eq. (91) is over fully contracted terms. When N is odd,

$$\left[\frac{N}{2}\right] \neq \frac{N}{2}, \tag{97}$$

and non of the terms in Eq. (91) are fully contracted. A proof will be included in the lecture notes.

Wick's theorem

An important extension of Wick's theorem allow us to define contractions between normal-ordered strings of operators. This is the so-called generalized Wick's theorem,

$$\left\{\hat{A}\hat{B}\hat{C}\hat{D}..\right\}\left\{\hat{R}\hat{X}\hat{Y}\hat{Z}..\right\} = \left\{\hat{A}\hat{B}\hat{C}\hat{D}..\hat{R}\hat{X}\hat{Y}\hat{Z}\right\} \tag{98}$$

$$+ \sum_{(1)} \left\{ \overbrace{\hat{A}\hat{B}\hat{C}\hat{D}..\hat{R}\hat{X}\hat{Y}\hat{Z}} \right\} \tag{99}$$

$$+ \sum_{(2)} \left\{ \overbrace{\hat{A}\hat{B}\hat{C}\hat{D}..\hat{R}\hat{X}\hat{Y}\hat{Z}} \right\} \tag{100}$$

$$+ \ldots \tag{101}$$

Wick's theorem

Turning back to the many-body problem, the vacuum expectation value of products of creation and annihilation operators can be written, according to Wick's theoren in Eq. (91), as a sum over normal ordered products with all possible numbers and combinations of contractions,

$$\langle 0|\hat{\mathbf{A}}\hat{\mathbf{B}}\hat{\mathbf{C}}\hat{\mathbf{D}}..\hat{\mathbf{R}}\hat{\mathbf{X}}\hat{\mathbf{Y}}\hat{\mathbf{Z}}|0\rangle = \langle 0|\left\{\hat{\mathbf{A}}\hat{\mathbf{B}}\hat{\mathbf{C}}\hat{\mathbf{D}}..\hat{\mathbf{R}}\hat{\mathbf{X}}\hat{\mathbf{Y}}\hat{\mathbf{Z}}\right\}|0\rangle \tag{102}$$

$$+\sum_{(1)}\langle 0|\left\{\overbrace{\hat{\mathbf{A}}\hat{\mathbf{B}}\hat{\mathbf{C}}\hat{\mathbf{D}}..\hat{\mathbf{R}}\hat{\mathbf{X}}\hat{\mathbf{Y}}\hat{\mathbf{Z}}}\right\}|0\rangle \tag{103}$$

$$+\sum_{(2)}\langle 0|\left\{\overbrace{\hat{\mathbf{A}}\hat{\mathbf{B}}\hat{\mathbf{C}}\hat{\mathbf{D}}..\hat{\mathbf{R}}\hat{\mathbf{X}}\hat{\mathbf{Y}}\hat{\mathbf{Z}}}\right\}|0\rangle \tag{104}$$

$$+\ldots \tag{105}$$

$$+\sum_{\left[\frac{N}{2}\right]}\langle 0|\left\{\overbrace{\hat{\mathbf{A}}\hat{\mathbf{B}}\hat{\mathbf{C}}\hat{\mathbf{D}}..}\ \overbrace{\hat{\mathbf{R}}\hat{\mathbf{X}}\hat{\mathbf{Y}}\hat{\mathbf{Z}}}\right\}|0\rangle. \tag{106}$$

Wick's theorem

All vacuum expectation values of normal ordered products without fully contracted terms are zero. Hence, the only contributions to the expectation value are those terms that *is* fully contracted,

$$\langle 0|\widehat{\mathbf{A}}\widehat{\mathbf{B}}\widehat{\mathbf{C}}\widehat{\mathbf{D}}..\widehat{\mathbf{R}}\widehat{\mathbf{X}}\widehat{\mathbf{Y}}\widehat{\mathbf{Z}}|0\rangle = \sum_{(all)} \langle 0| \left\{ \overbrace{\widehat{\mathbf{A}}\widehat{\mathbf{B}}\widehat{\mathbf{C}}\widehat{\mathbf{D}}}.. \overbrace{\widehat{\mathbf{R}}\widehat{\mathbf{X}}\widehat{\mathbf{Y}}\widehat{\mathbf{Z}}} \right\} |0\rangle \tag{107}$$

$$= \sum_{(all)} \overbrace{\widehat{\mathbf{A}}\widehat{\mathbf{B}}\widehat{\mathbf{C}}\widehat{\mathbf{D}}}.. \overbrace{\widehat{\mathbf{R}}\widehat{\mathbf{X}}\widehat{\mathbf{Y}}\widehat{\mathbf{Z}}}. \tag{108}$$

Wick's theorem

To obtain fully contracted terms, Eq. (96) must hold. When the number of creation and annihilation operators is odd, the vacuum expectation value can be set to zero at once. When the number is even, the expectation value is simply the sum of terms with all possible combinations of fully contracted terms. Observing that the only contractions that give nonzero contributions are

$$\overbrace{a_\alpha a^\dagger_\beta} = \delta_{\alpha\beta}, \tag{109}$$

the terms that contribute are reduced even more.

Wick's theorem provides us with an algebraic method for easy determine the terms that contribute to the matrix element. Our next step is the particle-hole formalism, which is a very useful formalism in many-body systems.

Second quantization and shell-model

Essentially most shell-model manipulations involve one and two-body operators with either one creation and one annihilation operators or two creation and two annihilations operators. Our Hamiltonian reads

$$\hat{H} = \sum_{\alpha\beta} \langle \alpha | t + u | \beta \rangle a_\alpha^\dagger a_\beta + \frac{1}{4} \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | V | \gamma\delta \rangle a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma .$$

This is form we have used in the shell model code, assuming that we work with anti-symmetrized two-body matrix elements. The two-body operator can be rewritten as

$$\hat{V} = \sum_{\alpha \leq \beta; \gamma \leq \delta} \langle \alpha\beta | V | \gamma\delta \rangle a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma .$$

Normally we have a diagonal one-body operator.

Creation and annihilation operators and shell model

In the build-up of a shell model code that is meant to tackle large dimensionalities is the action of the Hamiltonian $\hat{H}$ on a Slater determinant represented in second quantization as

$$|\alpha_1 \dots \alpha_n\rangle = a^\dagger_{\alpha_1} a^\dagger_{\alpha_2} \dots a^\dagger_{\alpha_n} |0\rangle.$$

The time consuming part stems from the action of the Hamiltonian on the above determinant,

$$\left(\sum_{\alpha\beta} \langle \alpha | t + u | \beta \rangle a^\dagger_\alpha a_\beta + \frac{1}{4} \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | V | \gamma\delta \rangle a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma \right) a^\dagger_{\alpha_1} a^\dagger_{\alpha_2} \dots a^\dagger_{\alpha_n} |0\rangle.$$

A practically useful way to implement this action is to encode a Slater determinant as a bit pattern.

Creation and annihilation operators and shell model

Assume that we have at our disposal n different single-particle orbits $\alpha_0, \alpha_2, \ldots, \alpha_{n-1}$ and that we can distribute among these orbits $N \leq n$ particles.
A Slater determinant can then be coded as an integer of n bits. As an example, if we have $n = 16$ single-particle states $\alpha_0, \alpha_1, \ldots, \alpha_{15}$ and $N = 4$ fermions occupying the states α_3, α_6, α_{10} and α_{13} we could write this Slater determinant as

$$\Phi_\Lambda = a^\dagger_{\alpha_3} a^\dagger_{\alpha_6} a^\dagger_{\alpha_{10}} a^\dagger_{\alpha_{13}} |0\rangle.$$

The unoccupied single-particle states have bit value 0 while the occupied ones are represented by bit state 1. In the binary notation we would write this 16 bits long integer as

α_0	α_1	α_2	α_3	α_4	α_5	α_6	α_7	α_8	α_9	α_{10}	α_{11}	α_{12}	α_{13}	α_{14}	α_{15}
0	0	0	1	0	0	1	0	0	0	1	0	0	1	0	0

which translates into the decimal number

$$2^3 + 2^6 + 2^{10} + 2^{13} = 9288.$$

We can thus encode a Slater determinant as a bit pattern.

Hilbert space dimensionality in shell model calculations

With N particles that can be distributed over n single-particle states, the total number of Slater determinats (and defining thereby the dimensionality of the system) is

$$\dim(\mathcal{H}) = \left(\begin{array}{c} n \\ N \end{array} \right).$$

The total number of bit patterns is 2^n.

Compact representation of Slater determinants

We assume again that we have at our disposal n different single-particle orbits $\alpha_0, \alpha_2, \ldots, \alpha_{n-1}$ and that we can distribute among these orbits $N \leq n$ particles. The ordering among these states is important as it defines the order of the creation operators. We will write the determinant

$$\Phi_\Lambda = a^\dagger_{\alpha_3} a^\dagger_{\alpha_6} a^\dagger_{\alpha_{10}} a^\dagger_{\alpha_{13}} |0\rangle,$$

in a more compact way as

$$\Phi_{3,6,10,13} = |0001001000100100\rangle.$$

The action of a creation operator is thus

$$a^\dagger_{\alpha_4} \Phi_{3,6,10,13} = a^\dagger_{\alpha_4} |0001001000100100\rangle = a^\dagger_{\alpha_4} a^\dagger_{\alpha_3} a^\dagger_{\alpha_6} a^\dagger_{\alpha_{10}} a^\dagger_{\alpha_{13}} |0\rangle,$$

which becomes

$$-a^\dagger_{\alpha_3} a^\dagger_{\alpha_4} a^\dagger_{\alpha_6} a^\dagger_{\alpha_{10}} a^\dagger_{\alpha_{13}} |0\rangle = -|0001101000100100\rangle.$$

Compact representation of Slater determinants

Similarly

$$a^\dagger_{\alpha_6}\Phi_{3,6,10,13} = a^\dagger_{\alpha_6}|0001001000100100\rangle = a^\dagger_{\alpha_6}a^\dagger_{\alpha_3}a^\dagger_{\alpha_6}a^\dagger_{\alpha_{10}}a^\dagger_{\alpha_{13}}|0\rangle,$$

which becomes

$$-a^\dagger_{\alpha_4}(a^\dagger_{\alpha_6})^2a^\dagger_{\alpha_{10}}a^\dagger_{\alpha_{13}}|0\rangle = 0!$$

This gives a simple recipe:

- If one of the bits b_j is 1 and we act with a creation operator on this bit, we return a null vector
- If $b_j = 0$, we set it to 1 and return a sign factor $(-1)^l$, where l is the number of bits set before bit j.

We see now the basic recipe for acting on a Slater determinant

Consider the action of $a^\dagger_{\alpha_2}$ on various slater determinants:

$$
\begin{aligned}
a^\dagger_{\alpha_2}\Phi_{00111} &= a^\dagger_{\alpha_2}|00111\rangle &&= 0 \times |00111\rangle \\
a^\dagger_{\alpha_2}\Phi_{01011} &= a^\dagger_{\alpha_2}|01011\rangle &&= (-1) \times |01111\rangle \\
a^\dagger_{\alpha_2}\Phi_{01101} &= a^\dagger_{\alpha_2}|01101\rangle &&= 0 \times |01101\rangle \\
a^\dagger_{\alpha_2}\Phi_{01110} &= a^\dagger_{\alpha_2}|01110\rangle &&= 0 \times |01110\rangle \\
a^\dagger_{\alpha_2}\Phi_{10011} &= a^\dagger_{\alpha_2}|10011\rangle &&= (-1) \times |10111\rangle \\
a^\dagger_{\alpha_2}\Phi_{10101} &= a^\dagger_{\alpha_2}|10101\rangle &&= 0 \times |10101\rangle \\
a^\dagger_{\alpha_2}\Phi_{10110} &= a^\dagger_{\alpha_2}|10110\rangle &&= 0 \times |10110\rangle \\
a^\dagger_{\alpha_2}\Phi_{11001} &= a^\dagger_{\alpha_2}|11001\rangle &&= (+1) \times |11101\rangle \\
a^\dagger_{\alpha_2}\Phi_{11010} &= a^\dagger_{\alpha_2}|11010\rangle &&= (+1) \times |11110\rangle
\end{aligned}
$$

What is the simplest way to obtain the phase when we act with one annihilation(creation) operator on the given Slater determinant representation?

Manipulating Slater determinants

We have an SD representation

$$\Phi_\Lambda = a^\dagger_{\alpha_0} a^\dagger_{\alpha_3} a^\dagger_{\alpha_6} a^\dagger_{\alpha_{10}} a^\dagger_{\alpha_{13}} |0\rangle,$$

in a more compact way as

$$\Phi_{0,3,6,10,13} = |1001001000100100\rangle.$$

The action of

$$a^\dagger_{\alpha_4} a_{\alpha_0} \Phi_{0,3,6,10,13} = a^\dagger_{\alpha_4} |0001001000100100\rangle = a^\dagger_{\alpha_4} a^\dagger_{\alpha_3} a^\dagger_{\alpha_6} a^\dagger_{\alpha_{10}} a^\dagger_{\alpha_{13}} |0\rangle,$$

which becomes

$$-a^\dagger_{\alpha_3} a^\dagger_{\alpha_4} a^\dagger_{\alpha_6} a^\dagger_{\alpha_{10}} a^\dagger_{\alpha_{13}} |0\rangle = -|0001101000100100\rangle.$$

Manipulating Slater determinants

The action

$$a_{\alpha_0}\Phi_{0,3,6,10,13} = |0001001000100100\rangle,$$

can be obtained by subtracting the logical sum (AND operation) of $\Phi_{0,3,6,10,13}$ and a word which represents only α_0, that is

$$|1000000000000000\rangle,$$

from $\Phi_{0,3,6,10,13} = |1001001000100100\rangle$.
This operation gives $|0001001000100100\rangle$.

Similarly, we can form $a^{\dagger}_{\alpha_4}a_{\alpha_0}\Phi_{0,3,6,10,13}$, say, by adding $|0000100000000000\rangle$ to $a_{\alpha_0}\Phi_{0,3,6,10,13}$, first checking that their logical sum is zero in order to make sure that orbital α_4 is not already occupied.

Manipulating Slater determinants, getting the phase

It is trickier however to get the phase $(-1)^l$. One possibility is as follows

- Let S_1 be a word that represents the $1-$bit to be removed and all others set to zero. In the previous example $S_1 = |1000000000000000\rangle$
- Define S_2 as the similar word that represents the bit to be added, that is in our case $S_2 = |0000100000000000\rangle$.
- Compute then $S = S_1 - S_2$, which here becomes

$$S = |0111000000000000\rangle$$

- Perform then the logical AND operation of S with the word containing

$$\Phi_{0,3,6,10,13} = |1001001000100100\rangle,$$

which results in $|0001000000000000\rangle$. Counting the number of $1-$bits gives the phase. Here you need however an algorithm for bitcounting. Several efficient ones available.

Particle-hole formalism

Second quantization is a useful and elegant formalism for constructing many-body states and quantum mechanical operators. As we will see later, one can express and translate many physical processes into simple pictures such as Feynman diagrams. Expecation values of many-body states are also easily calculated. However, although the equations are seemingly easy to set up, from a practical point of view, that is the solution of Schrödinger's equation, there is no particular gain. The many-body equation is equally hard to solve, irrespective of representation. The cliche that there is no free lunch brings us down to earth again. Note however that a transformation to a particular basis, for cases where the interaction obeys specific symmetries, can ease the solution of Schrödinger's equation.

Particle-hole formalism

But there is at least one important case where second quantization comes to our rescue. It is namely easy to introduce another reference state than the pure vacuum $|0\rangle$, where all single-particle are active. With many particles present it is often useful to introduce another reference state than the vacuum state $|0\rangle$. We will label this state $|c\rangle$ (c for core) and as we will see it can reduce considerably the complexity and thereby the dimensionality of the many-body problem. It allows us to sum up to infinite order specific many-body correlations. (add more stuff in the description below)

The particle-hole representation is one of these handy representations.

Particle-hole formalism

In the original particle representation these states are products of the creation operators $a^\dagger_{\alpha_i}$ acting on the true vacuum $|0\rangle$. Following (29) we have

$$|\alpha_1\alpha_2\ldots\alpha_{n-1}\alpha_n\rangle = a^\dagger_{\alpha_1}a^\dagger_{\alpha_2}\ldots a^\dagger_{\alpha_{n-1}}a^\dagger_{\alpha_n}|0\rangle \quad (110)$$

$$|\alpha_1\alpha_2\ldots\alpha_{n-1}\alpha_n\alpha_{n+1}\rangle = a^\dagger_{\alpha_1}a^\dagger_{\alpha_2}\ldots a^\dagger_{\alpha_{n-1}}a^\dagger_{\alpha_n}a^\dagger_{\alpha_{n+1}}|0\rangle \quad (111)$$

$$|\alpha_1\alpha_2\ldots\alpha_{n-1}\rangle = a^\dagger_{\alpha_1}a^\dagger_{\alpha_2}\ldots a^\dagger_{\alpha_{n-1}}|0\rangle \quad (112)$$

Particle-hole formalism

If we use Eq. (110) as our new reference state, we can simplify considerably the representation of this state

$$|c\rangle \equiv |\alpha_1\alpha_2\ldots\alpha_{n-1}\alpha_n\rangle = a^\dagger_{\alpha_1}a^\dagger_{\alpha_2}\ldots a^\dagger_{\alpha_{n-1}}a^\dagger_{\alpha_n}|0\rangle \tag{113}$$

The new reference states for the $n+1$ and $n-1$ states can then be written as

$$|\alpha_1\alpha_2\ldots\alpha_{n-1}\alpha_n\alpha_{n+1}\rangle = (-1)^n a^\dagger_{\alpha_{n+1}}|c\rangle \equiv (-1)^n|\alpha_{n+1}\rangle_c \tag{114}$$

$$|\alpha_1\alpha_2\ldots\alpha_{n-1}\rangle = (-1)^{n-1}a_{\alpha_n}|c\rangle \equiv (-1)^{n-1}|\alpha_{n-1}\rangle_c \tag{115}$$

Particle-hole formalism

The first state has one additional particle with respect to the new vacuum state $|c\rangle$ and is normally referred to as a one-particle state or one particle added to the many-body reference state. The second state has one particle less than the reference vacuum state $|c\rangle$ and is referred to as a one-hole state.

Particle-hole formalism

When dealing with a new reference state it is often convenient to introduce new creation and annihilation operators since we have from Eq. (115)

$$a_\alpha |c\rangle \neq 0 \tag{116}$$

since α is contained in $|c\rangle$, while for the true vacuum we have $a_\alpha |0\rangle = 0$ for all α.

Particle-hole formalism

The new reference state leads to the definition of new creation and annihilation operators which satisfy the following relations

$$b_\alpha|c\rangle = 0 \tag{117}$$

$$\{b^\dagger_\alpha, b^\dagger_\beta\} = \{b_\alpha, b_\beta\} = 0$$

$$\{b^\dagger_\alpha, b_\beta\} = \delta_{\alpha\beta} \tag{118}$$

We assume also that the new reference state is properly normalized

$$\langle c|c\rangle = 1 \tag{119}$$

Particle-hole formalism

The physical interpretation of these new operators is that of so-called quasiparticle states. This means that a state defined by the addition of one extra particle to a reference state $|c\rangle$ may not necesseraly be interpreted as one particle coupled to a core.

Particle-hole formalism

We define now new creation operators that act on a state α creating a new quasiparticle state

$$b_\alpha^\dagger|c\rangle = \begin{cases} a_\alpha^\dagger|c\rangle = |\alpha\rangle, & \alpha > F \\ a_\alpha|c\rangle = |\alpha^{-1}\rangle, & \alpha \leq F \end{cases} \tag{120}$$

where F is the Fermi level representing the last occupied single-particle orbit of the new reference state $|c\rangle$.

Particle-hole formalism

The annihilation is the hermitian conjugate of the creation operator

$$b_\alpha = (b_\alpha^\dagger)^\dagger,$$

resulting in

$$b_\alpha^\dagger = \begin{cases} a_\alpha^\dagger & \alpha > F \\ a_\alpha & \alpha \leq F \end{cases} \qquad b_\alpha = \begin{cases} a_\alpha & \alpha > F \\ a_\alpha^\dagger & \alpha \leq F \end{cases} \tag{121}$$

Particle-hole formalism

With the new creation and annihilation operator we can now construct many-body quasiparticle states, with one-particle-one-hole states, two-particle-two-hole states etc in the same fashion as we previously constructed many-particle states. We can write a general particle-hole state as

$$|\beta_1\beta_2\dots\beta_{n_p}\gamma_1^{-1}\gamma_2^{-1}\dots\gamma_{n_h}^{-1}\rangle \equiv \underbrace{b^\dagger_{\beta_1}b^\dagger_{\beta_2}\dots b^\dagger_{\beta_{n_p}}}_{>F}\underbrace{b^\dagger_{\gamma_1}b^\dagger_{\gamma_2}\dots b^\dagger_{\gamma_{n_h}}}_{\leq F}|c\rangle \tag{122}$$

Particle-hole formalism

We can now rewrite our one-body and two-body operators in terms of the new creation and annihilation operators. The number operator becomes

$$\hat{N} = \sum_{\alpha} a_{\alpha}^{\dagger} a_{\alpha} = \sum_{\alpha > F} b_{\alpha}^{\dagger} b_{\alpha} + n_c - \sum_{\alpha \leq F} b_{\alpha}^{\dagger} b_{\alpha} \tag{123}$$

where n_c is the number of particle in the new vacuum state $|c\rangle$. The action of $\hat{N}$ on a many-body state results in

$$N|\beta_1 \beta_2 \dots \beta_{n_p} \gamma_1^{-1} \gamma_2^{-1} \dots \gamma_{n_h}^{-1}\rangle = (n_p + n_c - n_h)|\beta_1 \beta_2 \dots \beta_{n_p} \gamma_1^{-1} \gamma_2^{-1} \dots \gamma_{n_h}^{-1}\rangle \tag{124}$$

Particle-hole formalism

Here $n = n_p + n_c - n_h$ is the total number of particles in the quasi-particle state of Eq. (122). Note that $\hat{N}$ counts the total number of particles present

$$N_{qp} = \sum_{\alpha} b_{\alpha}^{\dagger} b_{\alpha}, \tag{125}$$

gives us the number of quasi-particles as can be seen by computing

$$N_{qp} = |\beta_1 \beta_2 \ldots \beta_{n_p} \gamma_1^{-1} \gamma_2^{-1} \ldots \gamma_{n_h}^{-1}\rangle = (n_p + n_h)|\beta_1 \beta_2 \ldots \beta_{n_p} \gamma_1^{-1} \gamma_2^{-1} \ldots \gamma_{n_h}^{-1}\rangle \tag{126}$$

where $n_{qp} = n_p + n_h$ is the total number of quasi-particles.

Particle-hole formalism

We express the one-body operator $\hat{H}_0$ in terms of the quasi-particle creation and annihilation operators, resulting in

$$\begin{aligned}\hat{H}_0 &= \sum_{\alpha\beta>F} \langle\alpha|h|\beta\rangle b^\dagger_\alpha b_\beta + \sum_{\substack{\alpha>F \\ \beta\leq F}} \left[\langle\alpha|h|\beta\rangle b^\dagger_\alpha b^\dagger_\beta + \langle\beta|h|\alpha\rangle b_\beta b_\alpha\right] \\ &+ \sum_{\alpha\leq F} \langle\alpha|h|\alpha\rangle - \sum_{\alpha\beta\leq F} \langle\beta|h|\alpha\rangle b^\dagger_\alpha b_\beta \qquad (127)\end{aligned}$$

Particle-hole formalism

The first term gives contribution only for particle states, while the last one contributes only for holestates. The second term can create or destroy a set of quasi-particles and the third term is the contribution from the vacuum state $|c\rangle$. The physical meaning of these terms will be discussed in the next section, where we attempt at a diagrammatic representation.

Particle-hole formalism

Before we continue with the expressions for the two-body operator, we introduce a nomenclature we will use for the rest of this text. It is inspired by the notation used in coupled cluster theories. We reserve the labels $i, j, k, \ldots$ for hole states and $a, b, c, \ldots$ for states above F, viz. particle states. This means also that we will skip the constraint $\leq F$ or $> F$ in the summation symbols. Our operator $\hat{H}_0$ reads now

$$\begin{aligned} \hat{H}_0 &= \sum_{ab} \langle a|h|b\rangle b_a^\dagger b_b + \sum_{ai} \left[\langle a|h|i\rangle b_a^\dagger b_i^\dagger + \langle i|h|a\rangle b_i b_a \right] \\ &+ \sum_{i} \langle i|h|i\rangle - \sum_{ij} \langle j|h|i\rangle b_i^\dagger b_j \end{aligned} \tag{128}$$

Particle-hole formalism

The two-particle operator in the particle-hole formalism is more complicated since we have to translate four indices $\alpha\beta\gamma\delta$ to the possible combinations of particle and hole states. When performing the commutator algebra we can regroup the operator in five different terms

$$\hat{H}_I = \hat{H}_I^{(a)} + \hat{H}_I^{(b)} + \hat{H}_I^{(c)} + \hat{H}_I^{(d)} + \hat{H}_I^{(e)} \tag{129}$$

Using anti-symmetrized matrix elements, the term $\hat{H}_I^{(a)}$ is

$$\hat{H}_I^{(a)} = \frac{1}{4} \sum_{abcd} \langle ab|V|cd\rangle b_a^\dagger b_b^\dagger b_d b_c \tag{130}$$

Particle-hole formalism

The next term $\hat{H}_I^{(b)}$ reads

$$\hat{H}_I^{(b)} = \frac{1}{4}\sum_{abci}\left(\langle ab|V|ci\rangle b_a^\dagger b_b^\dagger b_i^\dagger b_c + \langle ai|V|cb\rangle b_a^\dagger b_i b_b b_c\right) \tag{131}$$

This term conserves the number of quasiparticles but creates or removes a three-particle-one-hole state. For $\hat{H}_I^{(c)}$ we have

$$\begin{aligned}\hat{H}_I^{(c)} &= \frac{1}{4}\sum_{abij}\left(\langle ab|V|ij\rangle b_a^\dagger b_b^\dagger b_j^\dagger b_i^\dagger + \langle ij|V|ab\rangle b_a b_b b_j b_i\right) + \\ &\frac{1}{2}\sum_{abij}\langle ai|V|bj\rangle b_a^\dagger b_j^\dagger b_b b_i + \frac{1}{2}\sum_{abi}\langle ai|V|bi\rangle b_a^\dagger b_b. \end{aligned} \tag{132}$$

Particle-hole formalism

The first line stands for the creation of a two-particle-two-hole state, while the second line represents the creation to two one-particle-one-hole pairs while the last term represents a contribution to the particle single-particle energy from the hole states, that is an interaction between the particle states and the hole states within the new vacuum state. The fourth term reads

$$\begin{aligned}\hat{H}_I^{(d)} &= \frac{1}{4}\sum_{aijk}\left(\langle ai|V|jk\rangle b_a^\dagger b_k^\dagger b_j^\dagger b_i + \langle ji|V|ak\rangle b_k^\dagger b_j b_i b_a\right) + \\ &\quad \frac{1}{4}\sum_{aij}\left(\langle ai|V|ji\rangle b_a^\dagger b_j^\dagger + \langle ji|V|ai\rangle - \langle ji|V|ia\rangle b_j b_a\right). \qquad (133)\end{aligned}$$

Particle-hole formalism

The terms in the first line stand for the creation of a particle-hole state interacting with hole states, we will label this as a two-hole-one-particle contribution. The remaining terms are a particle-hole state interacting with the holes in the vacuum state. Finally we have

$$\hat{H}_I^{(e)} = \frac{1}{4}\sum_{ijkl}\langle kl|V|ij\rangle b_i^\dagger b_j^\dagger b_l b_k + \frac{1}{2}\sum_{ijk}\langle ij|V|kj\rangle b_k^\dagger b_i + \frac{1}{2}\sum_{ij}\langle ij|V|ij\rangle \tag{134}$$

The first terms represents the interaction between two holes while the second stands for the interaction between a hole and the remaining holes in the vacuum state. It represents a contribution to single-hole energy to first order. The last term collects all contributions to the energy of the ground state of a closed-shell system arising from hole-hole correlations.

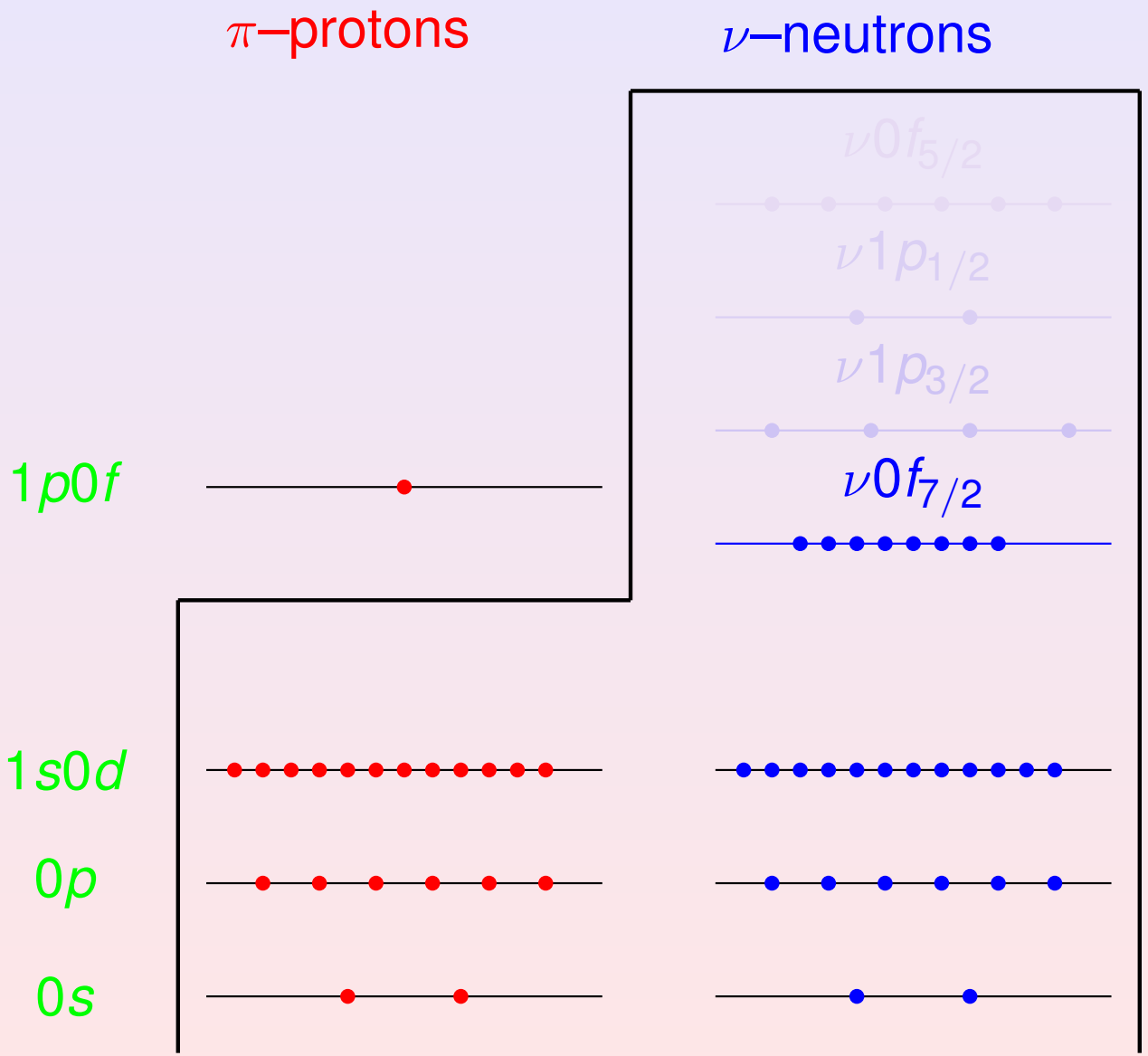
Topics for Week 6, February 4-8

Second-quantization and nuclear forces

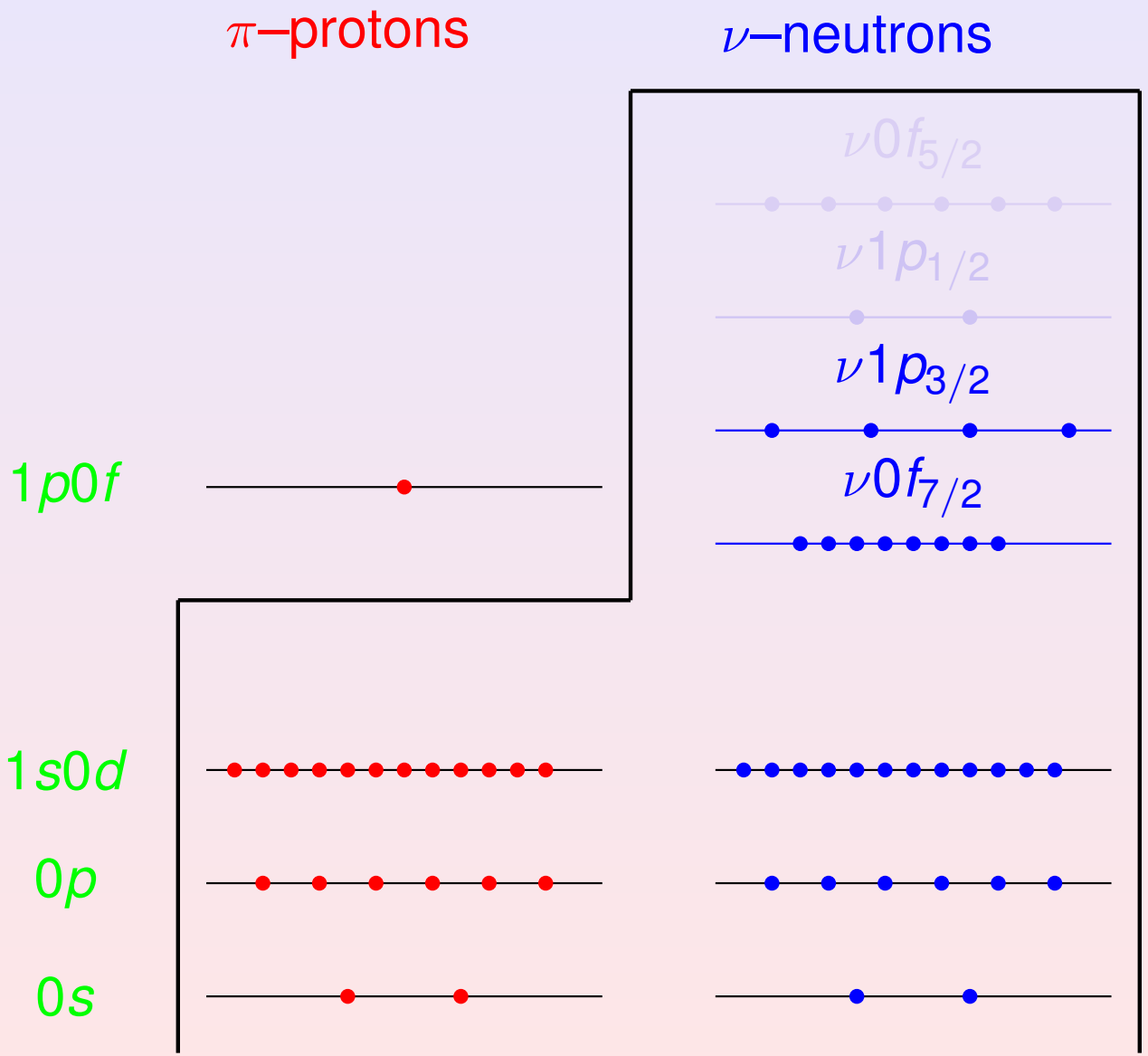
- Tuesday:
- Repetition from last week on second quantization and examples
- Quantum numbers for one-particle and two-particle systems
- Phenomenology of nuclear forces
- Thursday:
- Phenomenology of nuclear forces
- Discussion of central, spin-orbit and tensor forces

Suggested literature is JS chapters 4 and 5 for the usage of second quantization. For quantum numbers, chapter 1 on angular momentum and chapter 5 of Suhonen. See also chapters 5, 12 and 13 of Alex Brown.

Example of single-particle systems, one proton in the *fp* shell on top of ^{48,52,54,60}Ca cores



Example of single-particle systems, one proton in the *fp* shell on top of ^{48,52,54,60}Ca cores



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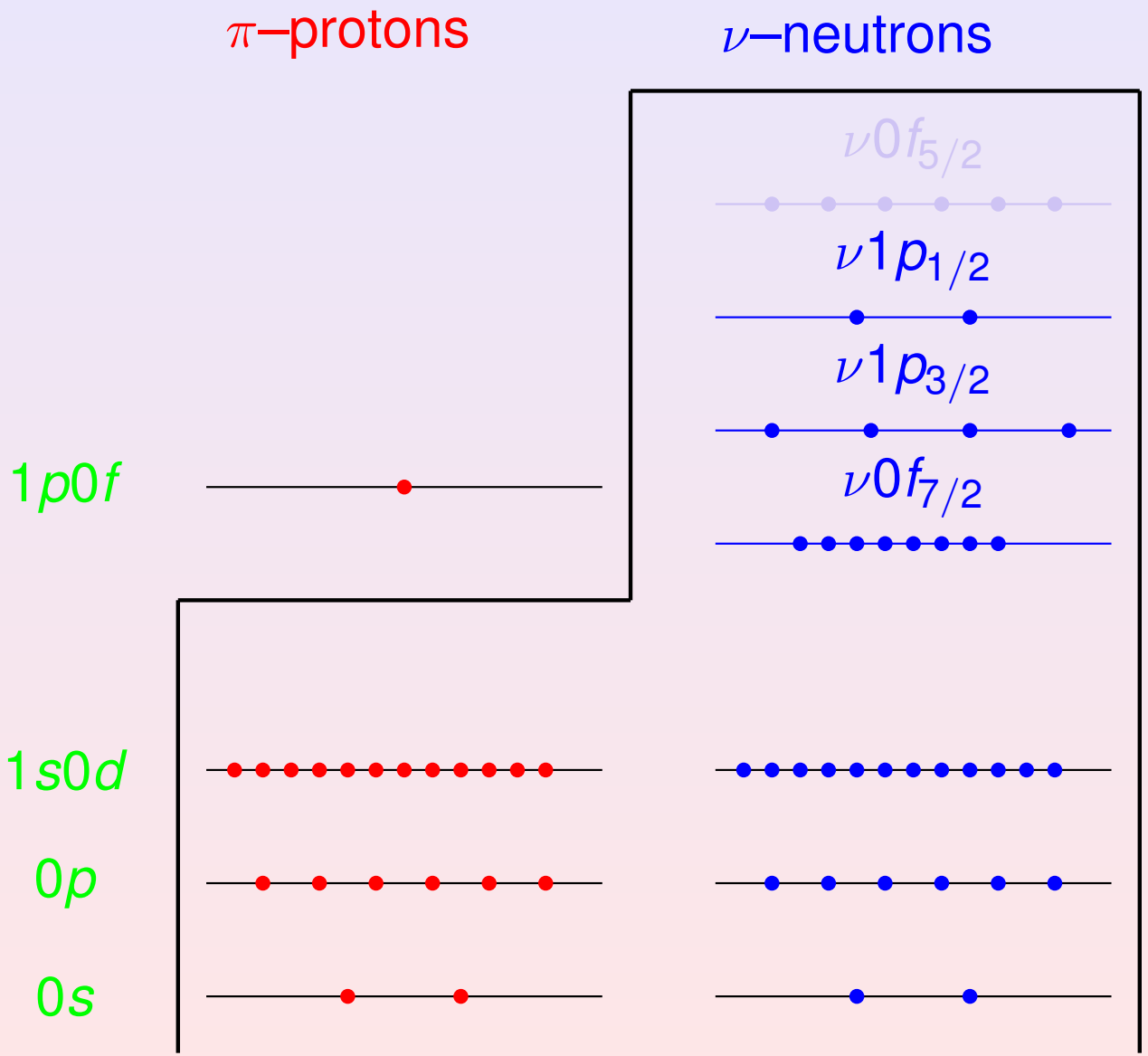
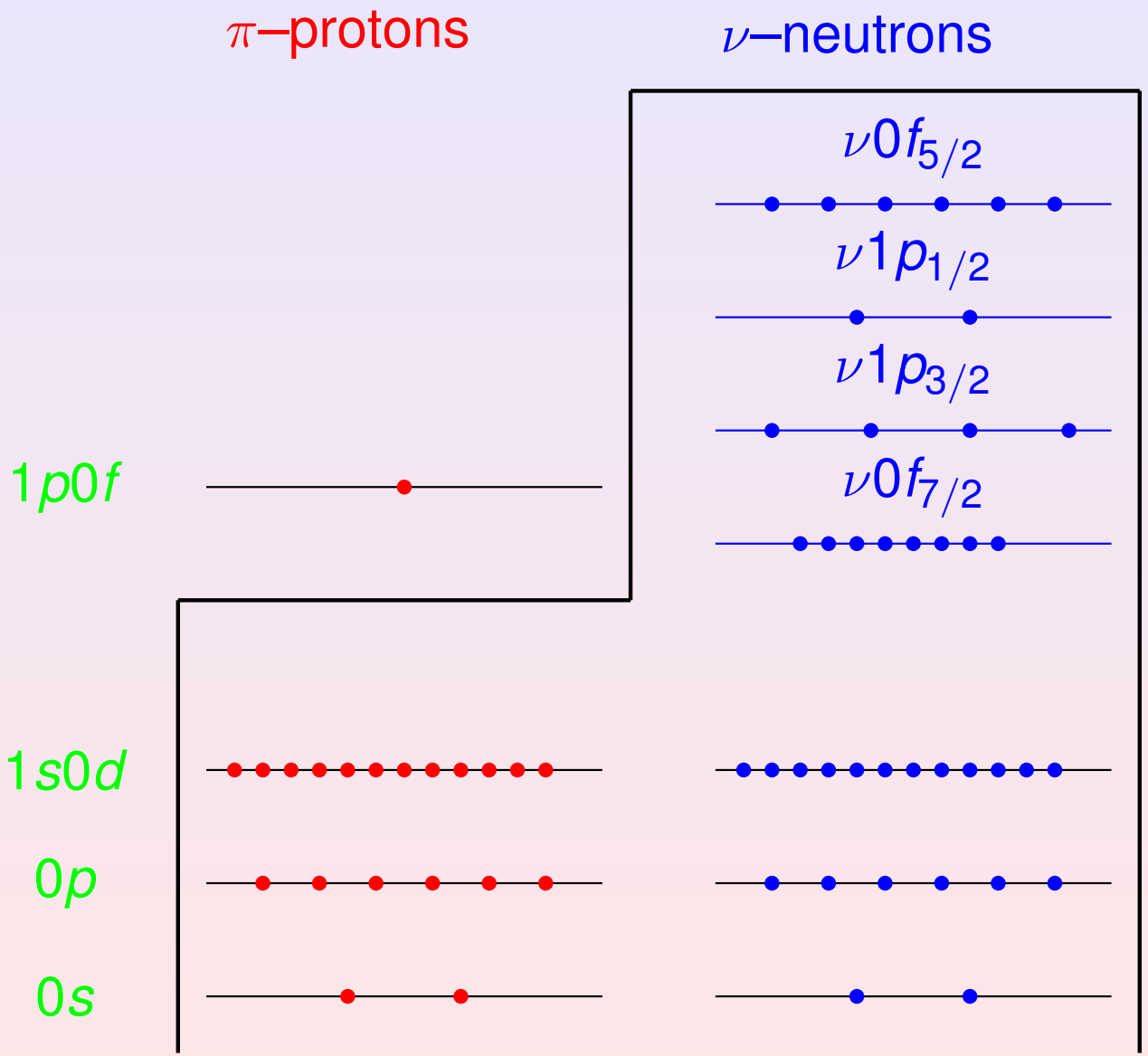
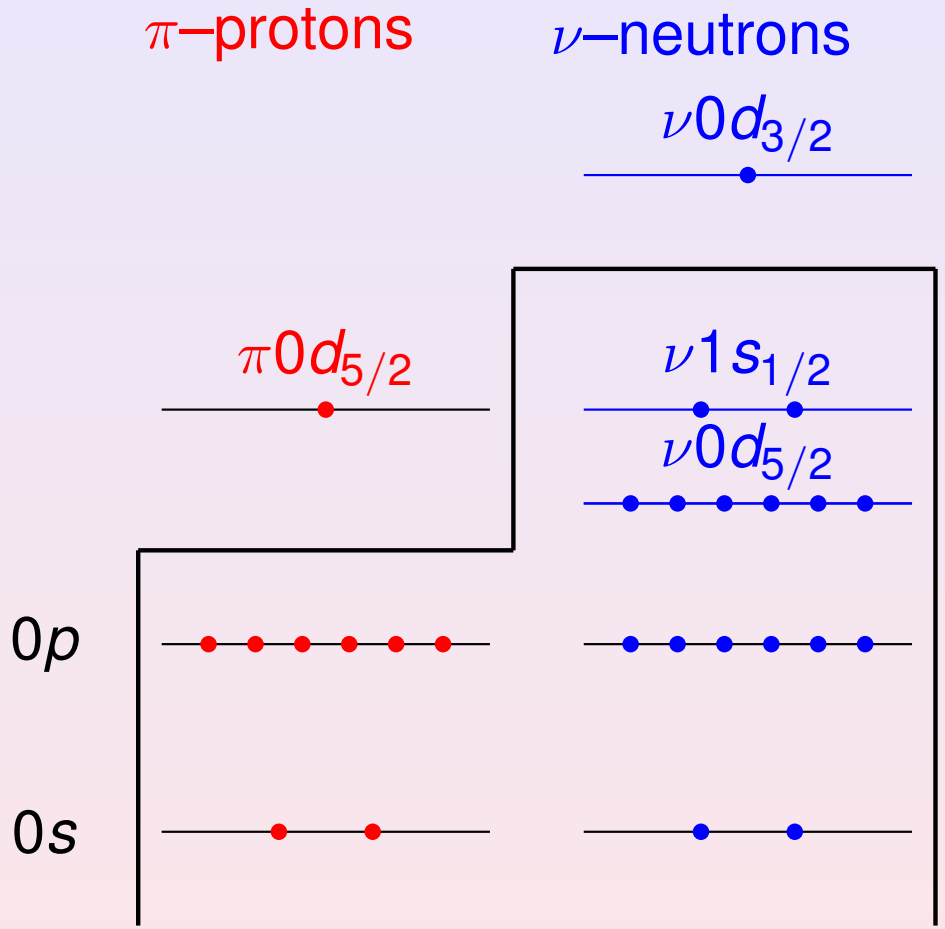


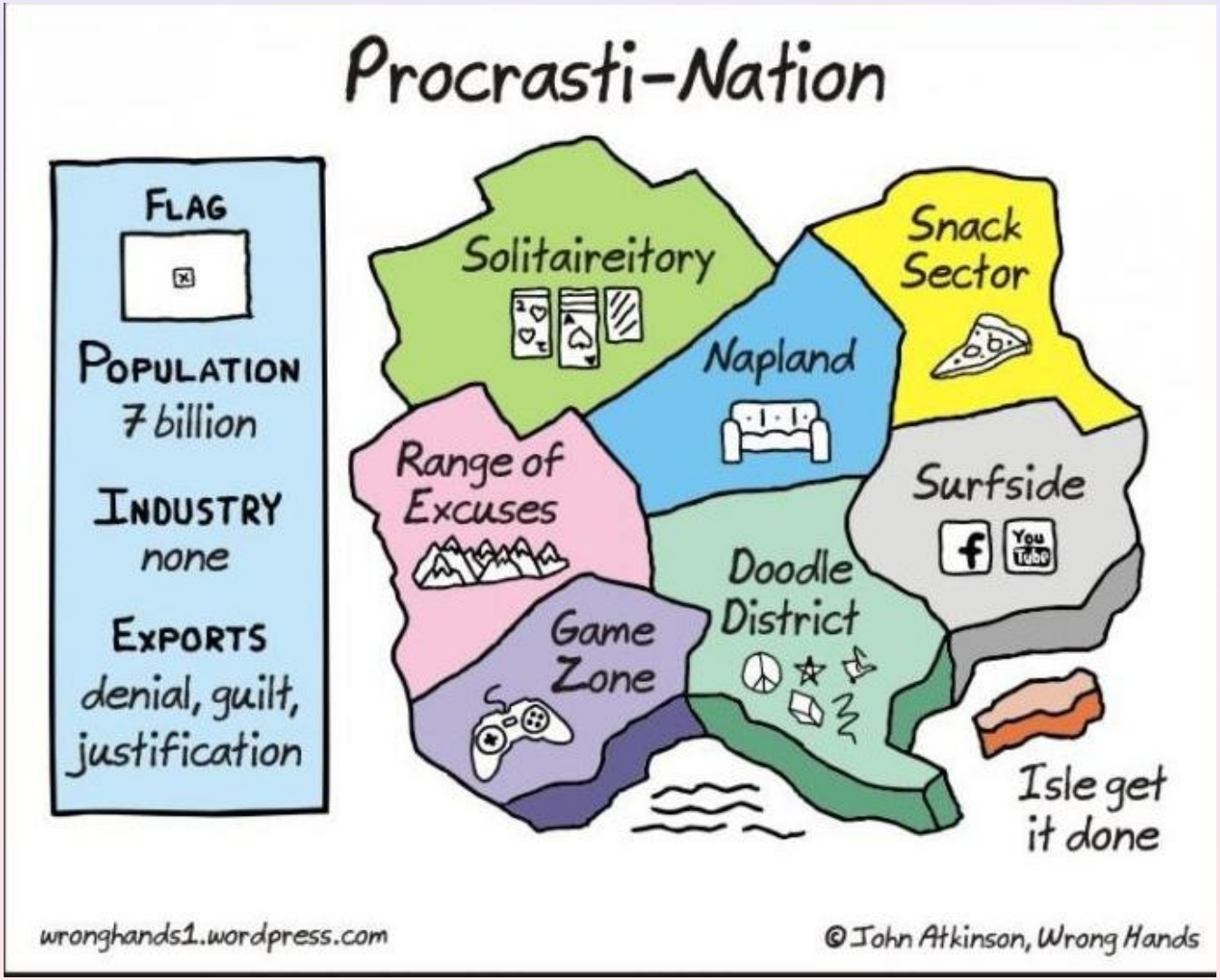
Example of single-particle systems, one proton in the *fp* shell on top of ^{48,52,54,60}Ca cores



Example of two-particle system, one proton and one neutron in the *sd* shell on top of a ^{24}O



Project 1, some hints and tips



Project 1, exercise a

We have defined

$$J_{\pm} = \sum_{p} a^{\dagger}_{p\pm} a_{p\mp}, \tag{135}$$

$$J_z = \frac{1}{2} \sum_{p,\sigma} \sigma a^{\dagger}_{p\sigma} a_{p\sigma}, \tag{136}$$

$$J^2 = J_+ J_- + J_z^2 - J_z, \tag{137}$$

and we wish to compute the commutators

$$[J_z, J_{\pm}], \quad [J_+, J_-], \quad [J^2, J_{\pm}] \quad \text{and} \quad [J^2, J_z].$$

Project 1, exercise a

Let us begin with the first and set in for J_z and $J_\pm$ given by equations (136) and (135):

$$
\begin{aligned}
[J_z, J_\pm] &= J_z J_\pm - J_\pm J_z \\
&= \left(\frac{1}{2} \sum_{p,\sigma} \sigma a^\dagger_{p\sigma} a_{p\sigma} \right) \left(\sum_{p'} a^\dagger_{p'\pm} a_{p'\mp} \right) - \left(\sum_{p'} a^\dagger_{p'\pm} a_{p'\mp} \right) \left(\frac{1}{2} \sum_{p,\sigma} \sigma a^\dagger_{p\sigma} a_{p\sigma} \right) \\
&= \frac{1}{2} \sum_{p,p',\sigma} \sigma \left(a^\dagger_{p\sigma} a_{p\sigma} a^\dagger_{p'\pm} a_{p'\mp} - a^\dagger_{p'\pm} a_{p'\mp} a^\dagger_{p\sigma} a_{p\sigma} \right).
\end{aligned}
$$

Project 1, exercise a

We use then the anti-commutation relations for creation and annihilation operators

$$\{a_l, a_k\} = 0, \tag{138}$$

$$\{a_l^\dagger, a_k^\dagger\} = 0, \tag{139}$$

$$\{a_l^\dagger, a_k\} = \delta_{lk}, \tag{140}$$

and we obtain

$$\begin{aligned}[J_z, J_\pm] &= \frac{1}{2}\sum_{p,p',\sigma} \sigma \left(a^\dagger_{p\sigma} a_{p\sigma} a^\dagger_{p'\pm} a_{p'\mp} - a^\dagger_{p'\pm}\left(\delta_{p'p}\delta_{\mp\sigma} - a^\dagger_{p\sigma} a_{p'\mp}\right) a_{p\sigma}\right) \\ &= \frac{1}{2}\sum_{p,p',\sigma} \sigma \left(a^\dagger_{p\sigma} a_{p\sigma} a^\dagger_{p'\pm} a_{p'\mp} - a^\dagger_{p'\pm}\delta_{p'p}\delta_{\mp\sigma} a_{p\sigma} + a^\dagger_{p'\pm} a^\dagger_{p\sigma} a_{p'\mp} a_{p\sigma}\right),\end{aligned}$$

which can be manipulated to give

$$\begin{aligned}[J_z, J_\pm] &= \frac{1}{2}\sum_p \left((\pm 1) a^\dagger_{p\pm} a_{p\mp} - (\mp 1) a^\dagger_{p\pm} a_{p\mp}\right) = \pm\frac{1}{2}\sum_p \left(a^\dagger_{p\pm} a_{p\mp} + (\pm 1) a^\dagger_{p\pm} a_{p\mp}\right) \\ &= \pm\sum_p a^\dagger_{p\pm} a_{p\mp} = \pm J_\pm,\end{aligned}$$

Project 1, constructing states

We have the state

$$|2,-2\rangle = a^\dagger_{1\_} a^\dagger_{2\_} a^\dagger_{3\_} a^\dagger_{4\_} |0\rangle \tag{141}$$

with $J_z = -2$ and $J = 2$ (I write these states as $|J, J_z\rangle$). The other states with total $J = 2$ are those with $J_z = -1, 0, 1, 2$. In addition, we have the relations

$$J_+|J, J_z\rangle = \sqrt{J(J+1) - J_z(J_z+1)}|J, J_z+1\rangle, \tag{142}$$

$$J_-|J, J_z\rangle = \sqrt{J(J+1) - J_z(J_z-1)}|J, J_z-1\rangle. \tag{143}$$

Project 1, constructing states

We can thence construct the other states with $J = 2$ by using J_+ on $|2, -2\rangle$:

$$J_+|2,-2\rangle = \sqrt{2(2+1)-(-2)(-2+1)}|2,-2+1\rangle = \sqrt{6-2}|2,-1\rangle = 2|2,-1\rangle,$$

which gives

$$\begin{aligned}
|2,-1\rangle &= \frac{1}{2}J_+|2,-2\rangle \\
&= \frac{1}{2}\sum_p a^\dagger_{p+}a_{p-}a^\dagger_{1-}a^\dagger_{2-}a^\dagger_{3-}a^\dagger_{4-}|0\rangle \\
&= \frac{1}{2}\left(a^\dagger_{1+}a^\dagger_{2-}a^\dagger_{3-}a^\dagger_{4-} + a^\dagger_{1-}a^\dagger_{2+}a^\dagger_{3-}a^\dagger_{4-} + a^\dagger_{1-}a^\dagger_{2-}a^\dagger_{3+}a^\dagger_{4-} + a^\dagger_{1-}a^\dagger_{2-}a^\dagger_{3-}a^\dagger_{4+}\right)|0\rangle.
\end{aligned} \tag{144}$$

We can then proceed like this for the other states as well.

Single-particle and two-particle quantum numbers

In order to understand the basics of the nucleon-nucleon interaction, we need to define the relevant quantum numbers and how we build up a single-particle state and a two-body state.

1. For the single-particle states, due to the fact that we have spin-orbit force, then the quantum numbers for for the project of orbital momentum l, that is m_l, and for spin s, that is m_s, are no longer so-called good quantum numbers. The total angular momentum j and its projection m_j are then so-called good quantum number.
2. This means that the operator $\hat{J}^2$ does not commute with $\hat{L}_z$ or $\hat{S}_z$.
3. We also start normally with single-particle state functions defined using say the harmonic oscillator. For these functions, we have no explicit dependence on j. How can we introduce single-particle wave functions which have j and its projection m_j as quantum numbers?

Single-particle and two-particle quantum numbers, brief review on angular momenta etc

We have that the operators for the orbital momentum are given by

$$L_x = -i\hbar(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}) = yp_z - zp_y,$$

$$L_y = -i\hbar(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}) = zp_x - xp_z,$$

$$L_z = -i\hbar(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}) = xp_y - yp_x.$$

Single-particle and two-particle quantum numbers, brief review on angular momenta etc

Since we have a spin orbit force which is strong, it is easy to show that the total angular momentum operator

$$\hat{\mathbf{J}} = \hat{\mathbf{L}} + \hat{\mathbf{S}}$$

does not commute with $\hat{\mathbf{L}}_z$ and $\hat{\mathbf{S}}_z$. To see this, we calculate for example

$$\begin{aligned} [\hat{\mathbf{L}}_z, \hat{\mathbf{J}}^2] &= [\hat{\mathbf{L}}_z, (\hat{\mathbf{L}} + \hat{\mathbf{S}})^2] \\ &= [\hat{\mathbf{L}}_z, \hat{\mathbf{L}}^2 + \hat{\mathbf{S}}^2 + 2\hat{\mathbf{L}}\hat{\mathbf{S}}] \\ &= [\hat{\mathbf{L}}_z, \hat{\mathbf{L}}\hat{\mathbf{S}}] = [\hat{\mathbf{L}}_z, \hat{\mathbf{L}}_x\hat{\mathbf{S}}_x + \hat{\mathbf{L}}_y\hat{\mathbf{S}}_y + \hat{\mathbf{L}}_z\hat{\mathbf{S}}_z] \neq 0, \end{aligned} \tag{145}$$

since we have that $[\hat{\mathbf{L}}_z, \hat{\mathbf{L}}_x] = i\hbar\hat{\mathbf{L}}_y$ and $[\hat{\mathbf{L}}_z, \hat{\mathbf{L}}_y] = i\hbar\hat{\mathbf{L}}_x$.

Single-particle and two-particle quantum numbers, brief review on angular momenta etc

We have also

$$|\widehat{\mathbf{J}}| = \hbar\sqrt{J(J+1)},$$

with the the following degeneration

$$M_J = -J, -J+1, \ldots, J-1, J.$$

With a given value of L and S we can then determine the possible values of J by studying the z component of $\widehat{\mathbf{J}}$. It is given by

$$\widehat{\mathbf{J}}_z = \widehat{\mathbf{L}}_z + \widehat{\mathbf{S}}_z.$$

The operators $\widehat{\mathbf{L}}_z$ and $\widehat{\mathbf{S}}_z$ have the quantum numbers $L_z = M_L\hbar$ and $S_z = M_S\hbar$, respectively, meaning that

$$M_J\hbar = M_L\hbar + M_S\hbar,$$

or

$$M_J = M_L + M_S.$$

Since the max value of M_L is L and for M_S is S we obtain

$$(M_J)_{\text{maks}} = L + S.$$

Single-particle and two-particle quantum numbers, brief review on angular momenta etc

For nucleons we have that the maximum value of $M_S = m_s = 1/2$, yielding

$$(m_j)_{\max} = l + \frac{1}{2}.$$

Using this and the fact that the maximum value of $M_J = m_j$ is j we have

$$j = l + \frac{1}{2}, l - \frac{1}{2}, l - \frac{3}{2}, l - \frac{5}{2}, \ldots$$

To decide where this series terminates, we use the vector inequality

$$|\widehat{\mathbf{L}} + \widehat{\mathbf{S}}| \geq \left| |\widehat{\mathbf{L}}| - |\widehat{\mathbf{S}}| \right|.$$

Using $\widehat{\mathbf{J}} = \widehat{\mathbf{L}} + \widehat{\mathbf{S}}$ we get

$$|\widehat{\mathbf{J}}| \geq |\widehat{\mathbf{L}}| - |\widehat{\mathbf{S}}|,$$

or

$$|\widehat{\mathbf{J}}| = \hbar\sqrt{J(J+1)} \geq |\hbar\sqrt{L(L+1)} - \hbar\sqrt{S(S+1)}|.$$

Single-particle and two-particle quantum numbers, brief review on angular momenta etc

If we limit ourselves to nucleons only with $s = 1/2$ we find that

$$|\widehat{\mathbf{J}}| = \hbar\sqrt{j(j+1)} \geq |\hbar\sqrt{l(l+1)} - \hbar\sqrt{\frac{1}{2}(\frac{1}{2}+1)}|.$$

It is then easy to show that for nucleons there are only two possible values of j which satisfy the inequality, namely

$$j = l + \frac{1}{2} \text{ or } j = l - \frac{1}{2},$$

and with $l = 0$ we get

$$j = \frac{1}{2}.$$

Single-particle and two-particle quantum numbers, brief review on angular momenta etc

Let us study some selected examples. We need also to keep in mind that parity is conserved. The strong and electromagnetic Hamiltonians conserve parity. Thus the eigenstates can be broken down into two classes of states labeled by their parity $\pi = +1$ or $\pi = -1$. The nuclear interactions do not mix states with different parity. For nuclear structure the total parity originates from the intrinsic parity of the nucleon which is $\pi_{\mathrm{intrinsic}} = +1$ and the parities associated with the orbital angular momenta $\pi_l = (-1)^l$. The total parity is the product over all nucleons
$\pi = \prod_i \pi_{\mathrm{intrinsic}}(i)\pi_l(i) = \prod_i (-1)^{l_i}$
The basis states we deal with are constructed so that they conserve parity and have thus a definite parity.

Single-particle and two-particle quantum numbers

Consider now the single-particle orbits of the $1s0d$ shell. For a $0d$ state we have the quantum numbers $l = 2$, $m_l = -2, -1, 0, 1, 2$, $s + 1/2$, $m_s = \pm 1/2$, $n = 0$ (the number of nodes of the wave function). This means that we have positive parity and

$$j = \frac{3}{2} = l - s \qquad m_j = -\frac{3}{2}, -\frac{1}{2}, \frac{1}{2}, \frac{3}{2}.$$

and

$$j = \frac{5}{2} = l + s \qquad m_j = -\frac{5}{2}, -\frac{3}{2}, -\frac{1}{2}, \frac{1}{2}, \frac{3}{2}, \frac{5}{2}.$$

Single-particle and two-particle quantum numbers

Our single-particle wave functions, if we use the harmonic oscillator, do however not contain the quantum numbers j and m_j. Normally what we have is an eigenfunction for the one-body problem defined as

$$\phi_{nlm_l sm_s}(r,\theta,\phi) = R_{nl}(r)Y_{lm_l}(\theta,\phi)\xi_{sm_s},$$

where we have used spherical coordinates (with a spherically symmetric potential) and the spherical harmonics

$$Y_{lm_l}(\theta,\phi) = P(\theta)F(\phi) = \sqrt{\frac{(2l+1)(l-m_l)!}{4\pi(l+m_l)!}}P_l^{m_l}(cos(\theta))\exp(im_l\phi),$$

with $P_l^{m_l}$ being the so-called associated Legendre polynomials. Examples are

$$Y_{00} = \sqrt{\frac{1}{4\pi}},$$

for $l = m_l = 0$,

$$Y_{10} = \sqrt{\frac{3}{4\pi}}cos(\theta),$$

for $l = 1$ and $m_l = 0$,

$$Y_{1\pm 1} = \sqrt{\frac{3}{8\pi}}sin(\theta)exp(\pm i\phi),$$

for $l = 1$ and $m_l = \pm 1$,

$$Y_{20} = \sqrt{\frac{5}{16\pi}}(3cos^2(\theta) - 1)$$

for $l = 2$ and $m_l = 0$ etc.

Single-particle and two-particle quantum numbers

How can we get a function in terms of j and m_j? Define now

$$\phi_{nlm_l sm_s}(r,\theta,\phi) = R_{nl}(r)Y_{lm_l}(\theta,\phi)\xi_{sm_s},$$

and

$$\psi_{njm_j;lm_l sm_s}(r,\theta,\phi),$$

as the state with quantum numbers jm_j. Operating with

$$\hat{\mathbf{j}}^2 = (\hat{\mathbf{l}}+\hat{\mathbf{s}})^2 = \hat{\mathbf{l}}^2 + \hat{\mathbf{s}}^2 + 2\hat{\mathbf{l}}_z\hat{\mathbf{s}}_z + \hat{\mathbf{l}}_+\hat{\mathbf{s}}_- + \hat{\mathbf{l}}_-\hat{\mathbf{s}}_+,$$

on the latter state we will obtain admixtures from possible $\phi_{nlm_l sm_s}(r,\theta,\phi)$ states.

Single-particle and two-particle quantum numbers

To see this, we consider the following example and fix

$$j = \frac{3}{2} = l - s \qquad m_j = \frac{3}{2}.$$

and

$$j = \frac{5}{2} = l + s \qquad m_j = \frac{3}{2}.$$

It means we can have, with $l = 2$ and $s = 1/2$ being fixed, in order to have $m_j = 3/2$ either $m_l = 1$ and $m_s = 1/2$ or $m_l = 2$ and $m_s = -1/2$. The two states

$$\psi_{n=0j=5/2m_j=3/2;l=2s=1/2}$$

and

$$\psi_{n=0j=3/2m_j=3/2;l=2s=1/2}$$

will have admixtures from $\phi_{n=0l=2m_l=2s=1/2m_s=-1/2}$ and $\phi_{n=0l=2m_l=1s=1/2m_s=1/2}$. How do we find these admixtures? Note that we don't specify the values of m_l and m_s in the functions ψ since $\widehat{\mathbf{j}}^2$ does not commute with $\widehat{\mathbf{L}}_z$ and $\widehat{\mathbf{S}}_z$.

Single-particle and two-particle quantum numbers

We operate with

$$\hat{\mathbf{j}}^2 = (\hat{\mathbf{l}} + \hat{\mathbf{s}})^2 = \hat{\mathbf{l}}^2 + \hat{\mathbf{s}}^2 + 2\hat{\mathbf{l}}_z\hat{\mathbf{s}}_z + \hat{\mathbf{l}}_+\hat{\mathbf{s}}_- + \hat{\mathbf{l}}_-\hat{\mathbf{s}}_+$$

on the two jm_j states, that is

$$\hat{\mathbf{j}}^2\psi_{n=0j=5/2m_j=3/2;l=2s=1/2} = \alpha\hbar^2[l(l+1) + \frac{3}{4} + 2m_l m_s]\phi_{n=0l=2m_l=2s=1/2m_s=-1/2} +$$

$$\beta\hbar^2\sqrt{l(l+1) - m_l(m_l-1)}\phi_{n=0l=2m_l=1s=1/2m_s=1/2},$$

and

$$\hat{\mathbf{j}}^2\psi_{n=0j=5/2m_j=3/2;l=2s=1/2} = \alpha\hbar^2[l(l+1) + \frac{3}{4} + 2m_l m_s] + \phi_{n=0l=2m_l=1s=1/2m_s=1/2} +$$

$$\beta\hbar^2\sqrt{l(l+1) - m_l(m_l+1)}\phi_{n=0l=2m_l=2s=1/2m_s=-1/2}.$$

Single-particle and two-particle quantum numbers

This means that the eigenvectors $\phi_{n=0l=2m_l=2s=1/2m_s=-1/2}$ etc are not eigenvectors of $\widehat{\mathbf{j}}^2$. The above problems gives a 2×2 matrix that mixes the vectors $\psi_{n=0j=5/2m_j3/2;l=2m_ls=1/2m_s}$ and $\psi_{n=0j=5/2m_j3/2;l=2m_ls=1/2m_s}$ with the states $\phi_{n=0l=2m_l=2s=1/2m_s=-1/2}$ and $\phi_{n=0l=2m_l=1s=1/2m_s=1/2}$. The unknown coefficients α and β results from eigenvectors of this matrix. That is inserting all values m_l, l, m_s, s we obtain the matrix

$$\begin{bmatrix} 19/4 & 2 \\ 2 & 31/4 \end{bmatrix}$$

whose eigenvectors are the columns of

$$\begin{bmatrix} 2/\sqrt{5} & 1/\sqrt{5} \\ 1/\sqrt{5} & -2/\sqrt{5} \end{bmatrix}$$

These numbers define the so-called Clebsch-Gordan coupling coefficients (the overlaps between the two basis sets). We can thus write

$$\psi_{njm_j;ls} = \sum_{m_l m_s} \langle lm_l sm_s | jm_j \rangle \phi_{nlm_l sm_s},$$

where the coefficients $\langle lm_l sm_s | jm_j \rangle$ are the so-called Clebsch-Gordan coeffficients.

Clebsch-Gordan coefficients

The Clebsch-Gordan coeffficients $\langle lm_l sm_s | jm_j \rangle$ have some interesting properties for us, like the following orthogonality relations

$$\sum_{m_1 m_2} \langle j_1 m_1 j_2 m_2 | JM \rangle \langle j_1 m_1 j_2 m_2 | J' M' \rangle = \delta_{J,J'} \delta_{M,M'},$$

$$\sum_{JM} \langle j_1 m_1 j_2 m_2 | JM \rangle \langle j_1 m_1' j_2 m_2' | JM \rangle = \delta_{m_1,m_1'} \delta_{m_2,m_2'},$$

$$\langle j_1 m_1 j_2 m_2 | JM \rangle = (-1)^{j_1+j_2-J} \langle j_2 m_2 j_1 m_1 | JM \rangle,$$

and many others. The latter will turn extremely useful when we are going to define two-body states and interactions in a coupled basis.

The two-body case

See whiteboard!! To be filled in later!!

From Yukawa to Lattice QCD and Effective Field Theory

1930's

Chadwick (1932) discovers the neutron and Heisenberg (1932) proposes the first Phenomenology (Isospin). Yukawa (1935) and his Meson Hypothesis

1940's

Discovery of the pion in cosmic ray (1947) and in the Berkeley Cyclotron Lab (1948). Nobelprize awarded to Yukawa (1949). Rabi (1948) measures quadrupole moment of the deuteron.

1950's

Taketani, Nakamura, Sasaki (1951): 3 ranges. One-Pion-Exchange (OPE): o.k. Multi-pion exchanges: Problems! Taketani, Machida, Onuma (1952); "Pion Theories" Brueckner, Watson (1953).

From Yukawa to Lattice QCD and Effective Field Theory

1960's

Many pions = multi-pion resonances: $\sigma(600)$, $\rho(770)$, $\omega(782)$
etc.One-Boson-Exchange Model. Refined Meson Theories

1970's

Sophisticated models for two-pion exchange: Paris Potential (Lacombe et al., Phys. Rev. C **21**, 861 (1980)) Bonn potential (Machleidt et al., Phys. Rep. **149**, 1 (1987))

1980's

Quark cluster models. Begin of effective field theory studies.

From Yukawa to Lattice QCD and Effective Field Theory

1990's

1993-2001: High-precision NN potentials: Nijmegen I, II, '93, Reid93 (Stoks et al. 1994), Argonne V18 (Wiringa et al, 1995), CD-Bonn (Machleidt et al. 1996 and 2001. Advances in effective field theory: Weinberg (1990); Ordonez, Ray, van Kolck and many more.

3rd Millenium

Another "pion theory"; but now right: constrained by chiral symmetry. Three-body and higher-body forces appear naturally at a given order of the chiral expansion.

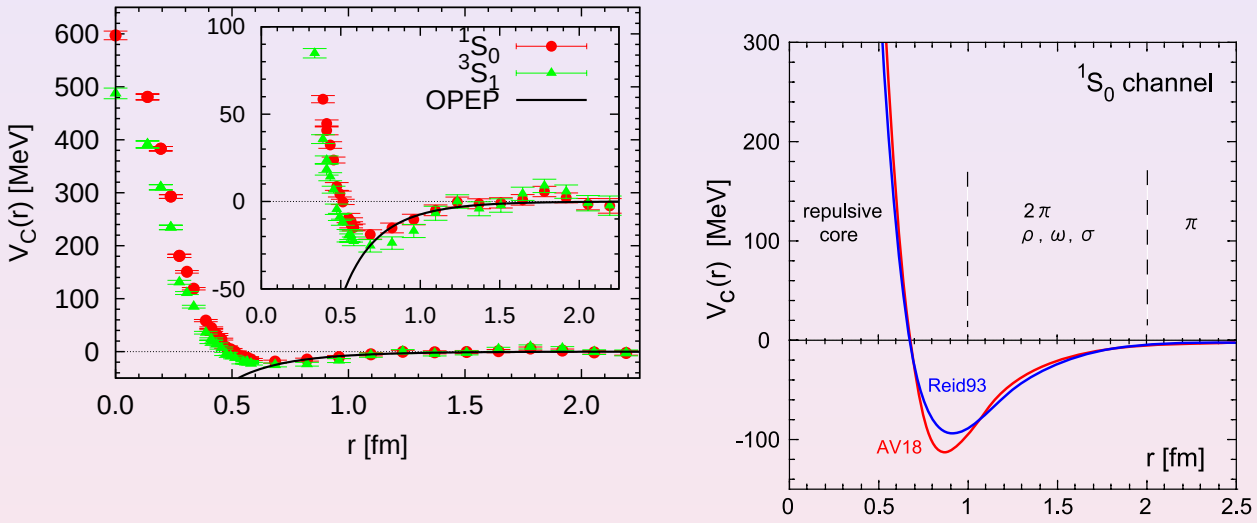
2006

Nucleon-nucleon interaction from Lattice QCD, final confirmation of meson hypothesis of Yukawa?

Progress in our QCD understanding of the NN force

- Explore the limits of our understanding of the atomic nuclei based on nucleonic and mesonic degrees of freedom. CEBAF, J-Parc, FAIR and LHC offer such perspectives.
- Experimental plans aim at identifying and exploring the transition from the nucleon/meson description of nuclei to the underlying quark and gluon description.
- Test the short-range behavior of the NN interaction via deep inelastic scattering
- Effective field theory has made progress in constructing NN and NNN forces from the underlying symmetries of QCD
- Three-body and higher-body forces emerge naturally and have explicit expressions at every order in the chiral expansion.
- Recent progress in Lattice QCD (LQCD) may hold great promise for constraining effective field theories.
- LQCD will be able to tell us about the interactions of systems that cannot be probed experimentally, but have relevance to astrophysics (nucleon-hyperon interactions), meson-meson and meson-baryon interactions, and other fields of nuclear physics.

Lattice QCD, Ishii *et al*, PRL 2007



The nucleon-nucleon interaction, Phenomenology vs Lattice calculations.

Features of the Nucleon-Nucleon (NN) Force

The aim is to give you an overview over central features of the nucleon-nucleon interaction and how it is constructed, with both technical and theoretical approaches.

1. The existence of the deuteron with $J^\pi = 1^+$ indicates that the force between protons and neutrons is attractive at least for the ${}^3S_1$ partial wave. Interference between Coulomb and nuclear scattering for the proton-proton partial wave ${}^1S_0$ shows that the NN force is attractive at least for the ${}^1S_0$ partial wave.
2. It has a short range and strong intermediate attraction.
3. Spin dependent, scattering lengths for triplet and singlet states are different,
4. Spin-orbit force. Observation of large polarizations of scattered nucleons perpendicular to the plane of scattering.

Features of the Nucleon-Nucleon (NN) Force, continued

1. Strongly repulsive core. The s-wave phase shift becomes negative at ≈ 250 MeV implying that the singlet S has a hard core with range $0.4 - 0.5$ fm.
2. Charge independence (almost). Two nucleons in a given two-body state always (almost) experience the same force. Modern interactions break charge and isospin symmetry lightly. That means that the pp, neutron-neutron and pn parts of the interaction will be different for the same quantum numbers.
3. Non-central. There is a tensor force. First indications from the quadrupole moment of the deuteron pointing to an admixture in the ground state of both $l = 2$ ($^3D_1$) and $l = 0$ ($^3S_1$) orbital momenta.

Short Range Evidence

Comparison of the binding energies of ^{2}H (deuteron), ^{3}H (triton), ^{4}He (alpha - particle) show that the nuclear force is of finite range ($1 - 2$ fm) and very strong within that range. For nuclei with $A > 4$, the energy saturates: Volume and binding energies of nuclei are proportional to the mass number A (as we saw from exercise 1).
Nuclei are also bound. The average distance between nucleons in nuclei is about 2 fm which must roughly correspond to the range of the attractive part.

Charge Dependence

- After correcting for the electromagnetic interaction, the forces between nucleons (pp, nn, or np) in the same state are almost the same.
- ”Almost the same”: Charge-independence is slightly broken.
- Equality between the pp and nn forces: Charge symmetry.
- Equality between pp/nn force and np force: Charge independence.
- Better notation: Isospin symmetry, invariance under rotations in isospin

Charge Dependence, ${}^1S_0$ Scattering Lengths

Charge-symmetry breaking (CSB), after electromagnetic effects have been removed:

- $a_{pp} = -17.3 \pm 0.4\text{fm}$
- $a_{nn} = -18.8 \pm 0.5\text{fm}$. Note however discrepancy from *nd* breakup reactions resulting in $a_{nn} = -18.72 \pm 0.13 \pm 0.65\text{fm}$ and $\pi^- + d \to \gamma + 2n$ reactions giving $a_{nn} = -18.93 \pm 0.27 \pm 0.3\text{fm}$.

Charge-independence breaking (CIB)

- $a_{pn} = -23.74 \pm 0.02\text{fm}$

Symmetries of the Nucleon-Nucleon (NN) Force

1. Translation invariance
2. Galilean invariance
3. Rotation invariance in space
4. Space reflection invariance
5. Time reversal invariance
6. Invariance under the interchange of particle 1 and 2
7. Almost isospin symmetry

$$V(\mathbf{r}) = \left\{ C_c + C_\sigma \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 + C_T \left(1 + \frac{3}{m_\alpha r} + \frac{3}{(m_\alpha r)^2} \right) S_{12}(\hat{r}) \right.$$

$$\left. + C_{SL} \left(\frac{1}{m_\alpha r} + \frac{1}{(m_\alpha r)^2} \right) \mathbf{L} \cdot \mathbf{S} \right\} \frac{e^{-m_\alpha r}}{m_\alpha r}$$

How do we derive such terms? (Note: no isospin dependence)

References for Various Phenomenological Interactions

Potentials which are based upon the standard non-relativistic operator structure are called ”Phenomenological Potentials” Some historically important examples are

- Gammel-Thaler potential (Phys. Rev. **107**, 291, 1339 (1957) and the Â· Hamada-Johnston potential, Nucl. Phys. **34**, 382 (1962)), bot with a hard core. core.
- Reid potential (Ann. Phys. (N.Y.) **50**, 411 (1968)), soft core.
- Argonne V_{14} potential (Wiringa et al., Phys. Rev. C **29**, 1207 (1984)) with 14 operators and the Argonne V_{18} potential (Wiringa et al., Phys. Rev. C **51**, 38 (1995)), uses 18 operators
- A good reference: R. Machleidt, Adv. Nucl. Phys **19**, 189 (1989).

Effective Degrees of Freedom, History

1. From 1950 till approximately 2000: One-Boson-Exchange (OBE) models dominate. These are models which typically include several low-mass mesons, that is with masses below 1 GeV.
2. Now: models based on chiral perturbation theory. These are effective models with nucleons and pions as degrees of freedom only. The other mesons which appeared in standard one-boson model appear as multi-pion resonances.

Topics for Week 7, February 11-15

Nuclear forces

- Tuesday:
- Repetion from last week
- Phenomenology of nuclear forces
- Definitions and derivation of the Lippman-Schwinger equation for scattering problems
- How to construct a Nucleon-nucleon force from data
- Thursday:
- No lecture, only project work

Next week we will discuss more explicitely the various operators of the nucleon-nucleon interaction such as the central force, spin-orbit and tensor force.

Quantum numbers and the Schödinger equation in relative and CM coordinates

Last week we discussed single-particle quantum numbers and two-particle quantum numbers. For the single-particle case, we have the following eigenfunctions

$$\psi_{njm_j;ls} = \sum_{m_l m_s} \langle lm_l sm_s | jm_j \rangle \phi_{nlm_l sm_s},$$

where the coefficients $\langle lm_l sm_s | jm_j \rangle$ are the so-called Clebsch-Gordan coeffficients. The relevant quantum numbers are n (related to the principal quantum number and the number of nodes of the wave function) and

$$\hat{\mathbf{j}}^2 \psi_{njm_j;ls} = \hbar^2 j(j+1)\psi_{njm_j;ls},$$

$$\hat{\mathbf{j}}_z \psi_{njm_j;ls} = \hbar m_j \psi_{njm_j;ls},$$

$$\hat{\mathbf{l}}^2 \psi_{njm_j;ls} = \hbar^2 l(l+1)\psi_{njm_j;ls},$$

$$\hat{\mathbf{s}}^2 \psi_{njm_j;ls} = \hbar^2 s(s+1)\psi_{njm_j;ls},$$

but s_z and l_z do not result in good quantum numbers in a basis where we use the angular momentum j.

Quantum numbers and the Schödinger equation in relative and CM coordinates

For a two-body state where we couple two angular momenta j_1 and j_2 to a final angular momentum J with projection M_J, we can define a similar transformation in terms of the Clebsch-Gordan coeffficients

$$\psi_{(j_1 j_2)JM_J} = \sum_{m_{j_1} m_{j_2}} \langle j_1 m_{j_1} j_2 m_{j_2} | JM_J \rangle \psi_{n_1 j_1 m_{j_1}; l_1 s_1} \psi_{n_2 j_2 m_{j_2}; l_2 s_2}.$$

We will write these functions in a more compact form hereafter, namely,

$$|(j_1 j_2)JM_J\rangle = \psi_{(j_1 j_2)JM_J},$$

and

$$|j_i m_{j_i}\rangle = \psi_{n_i j_i m_{j_i}; l_i s_i},$$

where we have skipped the explicit reference to l, s and n. The spin of a nucleon is always $1/2$ while the value of l can be deduced from the parity of the state. It is thus normal to label a state with a given total angular momentum as j^π, where $\pi = \pm 1$.

Quantum numbers and the Schödinger equation in relative and CM coordinates

Our two-body state can thus be written as

$$|(j_1 j_2)JM_J\rangle = \sum_{m_{j_1} m_{j_2}} \langle j_1 m_{j_1} j_2 m_{j_2} | JM_J\rangle |j_1 m_{j_1}\rangle |j_2 m_{j_2}\rangle.$$

Due to the coupling order of the Clebsch-Gordan coefficient it reads as j_1 coupled to j_2 to yield a final angular momentum J. If we invert the order of coupling we would have

$$|(j_2 j_1)JM_J\rangle = \sum_{m_{j_1} m_{j_2}} \langle j_2 m_{j_2} j_1 m_{j_1} | JM_J\rangle |j_1 m_{j_1}\rangle |j_2 m_{j_2}\rangle,$$

and due to the symmetry properties of the Clebsch-Gordan coefficient we have

$$|(j_2 j_1)JM_J\rangle = (-1)^{j_1+j_2-J} \sum_{m_{j_1} m_{j_2}} \langle j_1 m_{j_1} j_2 m_{j_2} | JM_J\rangle |j_1 m_{j_1}\rangle |j_2 m_{j_2}\rangle = (-1)^{j_1+j_2-J} |(j_1 j_2)JM_J\rangle.$$

We call the basis $|(j_1 j_2)JM_J\rangle$ for the **coupled basis**, or just j-coupled basis/scheme. The basis formed by the simple product of single-particle eigenstates $|j_1 m_{j_1}\rangle |j_2 m_{j_2}\rangle$ is called the **uncoupled-basis**, or just the m-scheme basis.

Quantum numbers

We have thus the coupled basis

$$|(j_1 j_2)JM_J\rangle = \sum_{m_{j_1} m_{j_2}} \langle j_1 m_{j_1} j_2 m_{j_2} | JM_J\rangle |j_1 m_{j_1}\rangle |j_2 m_{j_2}\rangle.$$

and the uncoupled basis

$$|j_1 m_{j_1}\rangle |j_2 m_{j_2}\rangle.$$

The latter can easily be generalized to many single-particle states whereas the first needs specific coupling coefficients and definitions of coupling orders. The *m*-scheme basis is easy to implement numerically and is used in most standard shell-model codes. Our coupled basis obeys also the following relations

$$\widehat{\mathbf{J}}^2 |(j_1 j_2)JM_J\rangle = \hbar^2 J(J+1)|(j_1 j_2)JM_J\rangle$$

$$\widehat{\mathbf{J}}_z |(j_1 j_2)JM_J\rangle = \hbar M_J |(j_1 j_2)JM_J\rangle,$$

Relative and CoM system

What follows now is a more technical discussion of how we can solve the two-nucleon problem. This will lead us to the so-called Lippman-Schwinger equation for the scattering problem and a rewrite of Schrödinger's equation in relative and center-of-mass coordinates.
Let us define the latter first. As we did earlier this semester, we define the center-of-mass (CoM) momentum as

$$\boldsymbol{K} = \sum_{i=1}^{A} \boldsymbol{k}_i,$$

with $\hbar = c = 1$ the wave number $k_i = p_i$, with p_i the pertinent momentum of a single-particle state. We have also the relative momentum

$$\boldsymbol{k}_{ij} = \frac{1}{2}(\boldsymbol{k}_i - \boldsymbol{k}_j).$$

We will below skip the indices ij and simply write $\boldsymbol{k}$
In a similar fashion we can define the CoM coordinate

$$\boldsymbol{R} = \frac{1}{A}\sum_{i=1}^{A} \boldsymbol{r}_i,$$

and the relative distance

$$\boldsymbol{r}_{ij} = (\boldsymbol{r}_i - \boldsymbol{r}_j).$$

Relative and CoM system

With the definitions

$$\boldsymbol{K} = \sum_{i=1}^{A} \boldsymbol{k}_i,$$

and

$$\boldsymbol{k}_{ij} = \frac{1}{2}(\boldsymbol{k}_i - \boldsymbol{k}_j).$$

we can rewrite the two-particle kinetic energy (note that we use $\hbar = c = 1$ as

$$\frac{\boldsymbol{k}_1^2}{2m_n} + \frac{\boldsymbol{k}_2^2}{2m_n} = \frac{\boldsymbol{k}^2}{m_n} + \frac{\boldsymbol{K}^2}{4m_n},$$

where m_n is the average of the proton and the neutron masses. Since the two-nucleon interaction depends only on the relative distance, this means that we can separate Schrödinger's equation in an equation for the center-of-mass motion and one for the relative motion.

Relative and CoM system

With an equation for the relative motion only and a separate one for the center-of-mass motion we need to redefine the two-body quantum numbers.
Previously we had a two-body state vector defined as $|(j_2 j_1)JM_J\rangle$ in a coupled basis.
We will now define the quantum numbers for the relative motion. Here we need to define new orbital momenta (since these are the quantum numbers which change). We define

$$\widehat{\mathbf{l}}_1 + \widehat{\mathbf{l}}_2 = \widehat{\lambda} = \widehat{\mathbf{l}} + \widehat{\mathbf{L}},$$

where $\widehat{\mathbf{l}}$ is the orbital momentum associated with the relative motion and $\widehat{\mathbf{L}}$ the corresponding one linked with the CoM. The total spin S is unchanged since it acts in a different space. We have thus that

$$\widehat{\mathbf{J}} = \widehat{\mathbf{l}} + \widehat{\mathbf{L}} + \widehat{\mathbf{S}},$$

which allows us to define the angular momentum of the relative motion

$$\mathcal{J} = \widehat{\mathbf{l}} + \widehat{\mathbf{S}},$$

where $\mathcal{J}$ is the total angular momentum of the relative motion.

How to construct a nucleon-nucleon force: Mathematical Intermezzo, two-body Schrödinger in k-space

Before we break down the Schrödinger equation into a partial wave decomposition, we derive now the so-called Lippman-Schwinger equation. We will do this in an operator form first. Thereafter, we rewrite it in terms of various quantum numbers such as relative momenta, orbital momenta etc. The Schrödinger equation in abstract vector representation is

$$\left(\hat{H}_0 + \hat{V}\right)|\psi_n\rangle = E_n|\psi_n\rangle.$$

In our case for the two-body problem $\hat{H}_0$ is just the kinetic energy. We rewrite it as

$$\left(\hat{H}_0 - E_n\right)|\psi_n\rangle = -\hat{V}|\psi_n\rangle.$$

We assume that the invers of $\left(\hat{H}_0 - E_n\right)$ exists and rewrite this equation as

$$|\psi_n\rangle = \frac{1}{\left(E_n - \hat{H}_0\right)}\hat{V}|\psi_n\rangle.$$

How to construct a nucleon-nucleon force: Mathematical Intermezzo, two-body Schrödinger in k-space

The equation

$$|\psi_n\rangle = \frac{1}{\left(E_n - \hat{H}_0\right)} \hat{V}|\psi_n\rangle,$$

is normally solved in an iterative fashion. We assume first that

$$|\psi_n\rangle = |\phi_n\rangle,$$

where $|\phi_n\rangle$ are the eigenfunctions of

$$\hat{H}_0|\phi_n\rangle = \omega_n|\phi_n\rangle$$

the so-called unperturbed problem. In our case, these will simply be the kinetic energies of the relative motion.

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Inserting $|\phi_n\rangle$ on the right-hand side of

$$|\psi_n\rangle = \frac{1}{(E_n - \hat{H}_0)}\hat{V}|\psi_n\rangle,$$

yields

$$|\psi_n\rangle = |\phi_n\rangle + \frac{1}{\left(E_n - \hat{H}_0\right)}\hat{V}|\phi_n\rangle,$$

as our first iteration. Reinserting again gives

$$|\psi_n\rangle = |\phi_n\rangle + \frac{1}{\left(E_n - \hat{H}_0\right)}\hat{V}|\phi_n\rangle + \frac{1}{(E_n - \hat{H}_0)}\hat{V}\frac{1}{\left(E_n - \hat{H}_0\right)}\hat{V}|\phi_n\rangle,$$

and continuing we obtain

$$|\psi_n\rangle = \sum_{i=0}^{\infty}\left[\frac{1}{(E_n - \hat{H}_0)}\hat{V}\right]^i|\phi_n\rangle.$$

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It is easy to see that

$$|\psi_n\rangle = \sum_{i=0}^{\infty} \left[\frac{1}{(E_n - \hat{H}_0)} \hat{V} \right]^i |\phi_n\rangle,$$

can be rewritten as

$$|\psi_n\rangle = |\phi_n\rangle + \frac{1}{(E_n - \hat{H}_0)} \hat{V} \left(1 + \frac{1}{(E_n - \hat{H}_0)} \hat{V} + \frac{1}{(E_n - \hat{H}_0)} \hat{V} \frac{1}{(E_n - \hat{H}_0)} \hat{V} + \ldots \right] |\phi_n\rangle,$$

which we rewrite as

$$|\psi_n\rangle = |\phi_n\rangle + \frac{1}{(E_n - \hat{H}_0)} \hat{V} |\psi_n\rangle.$$

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In operator form we have thus

$$|\psi_n\rangle = |\phi_n\rangle + \frac{1}{(E_n - \hat{H}_0)}\hat{V}|\psi_n\rangle.$$

We multiply from the left with $\hat{V}$ and $\langle\phi_m|$ and obtain

$$\langle\phi_m|\hat{V}|\psi_n\rangle = \langle\phi_m|\hat{V}|\phi_n\rangle + \langle\phi_m|\hat{V}\frac{1}{(E_n - \hat{H}_0)}\hat{V}|\psi_n\rangle.$$

We define thereafter the so-called T-matrix as

$$\langle\phi_m|\hat{T}|\phi_n\rangle = \langle\phi_m|\hat{V}|\psi_n\rangle.$$

We can rewrite our equation as

$$\langle\phi_m|\hat{T}|\phi_n\rangle = \langle\phi_m|\hat{V}|\phi_n\rangle + \langle\phi_m|\hat{V}\frac{1}{(E_n - \hat{H}_0)}\hat{T}|\phi_n\rangle.$$

How to construct a nucleon-nucleon force: Mathematical Intermezzo, two-body Schrödinger in k-space

The equation

$$\langle\phi_m|\hat{T}|\phi_n\rangle = \langle\phi_m|\hat{V}|\phi_n\rangle + \langle\phi_m|\hat{V}\frac{1}{(E_n - \hat{H}_0)}\hat{T}|\phi_n\rangle,$$

is called the Lippman-Schwinger equation. Inserting the completeness relation

$$\mathbf{1} = \sum_n |\phi_n\rangle\langle\phi_n|, \;\; \langle\phi_n|\phi_{n'}\rangle = \delta_{n,n'}$$

we have

$$\langle\phi_m|\hat{T}|\phi_n\rangle = \langle\phi_m|\hat{V}|\phi_n\rangle + \sum_k \langle\phi_m|\hat{V}|\phi_k\rangle \frac{1}{(E_n - \omega_k)}\langle\phi_k|\hat{T}|\phi_n\rangle,$$

which is (when we specify the state $|\phi_n\rangle$) an integral equation that can actually be solved by matrix inversion easily! The unknown quantity is the T-matrix.

How to construct a nucleon-nucleon force: Mathematical Intermezzo, two-body Schrödinger in k-space

Now we wish to introduce a partial wave decomposition in order to solve the Lippman-Schwinger equation. With a partial wave decomposition we can reduce a three-dimensional integral equation to a one-dimensional one.
Let us continue with our Schrödinger equation in the abstract vector representation

$$(T + V)\,|\psi_n\rangle = E_n|\psi_n\rangle \tag{146}$$

Here T is the kinetic energy operator and V is the potential operator. The eigenstates form a complete orthonormal set according to

$$\mathbf{1} = \sum_n |\psi_n\rangle\langle\psi_n|, \;\; \langle\psi_n|\psi_{n'}\rangle = \delta_{n,n'}$$

Mathematical Intermezzo, two-body Schrödinger in k-space

The most commonly used representations of equation 146 are the coordinate and the momentum space representations. They define the completeness relations

$$\mathbf{1} = \int d\mathbf{r}\, |\mathbf{r}\rangle\langle\mathbf{r}|, \;\; \langle\mathbf{r}|\mathbf{r}'\rangle = \delta(\mathbf{r}-\mathbf{r}') \tag{147}$$

$$\mathbf{1} = \int d\mathbf{k}\, |\mathbf{k}\rangle\langle\mathbf{k}|, \;\; \langle\mathbf{k}|\mathbf{k}'\rangle = \delta(\mathbf{k}-\mathbf{k}') \tag{148}$$

Here the basis states in both **r**- and **k**-space are dirac-delta function normalized. From this it follows that the plane-wave states are given by,

$$\langle\mathbf{r}|\mathbf{k}\rangle = \left(\frac{1}{2\pi}\right)^{3/2} \exp\left(i\mathbf{k}\cdot\mathbf{r}\right) \tag{149}$$

which is a transformation function defining the mapping from the abstract $|\mathbf{k}\rangle$ to the abstract $|\mathbf{r}\rangle$ space.

Mathematical Intermezzo, two-body Schrödinger in k-space

That the **r**-space basis states are delta-function normalized follows from

$$\delta(\mathbf{r}-\mathbf{r}') = \langle \mathbf{r}|\mathbf{r}'\rangle = \langle \mathbf{r}|\mathbf{1}|\mathbf{r}'\rangle = \int \mathrm{d}\mathbf{k}\ \langle \mathbf{r}|\mathbf{k}\rangle\langle \mathbf{k}|\mathbf{r}'\rangle = \left(\frac{1}{2\pi}\right)^3 \int \mathrm{d}\mathbf{k} e^{i\mathbf{k}(\mathbf{r}-\mathbf{r}')} \qquad (150)$$

and the same for the momentum space basis states,

$$\delta(\mathbf{k}-\mathbf{k}') = \langle \mathbf{k}|\mathbf{k}'\rangle = \langle \mathbf{k}|\mathbf{1}|\mathbf{k}'\rangle = \int \mathrm{d}\mathbf{r}\ \langle \mathbf{k}|\mathbf{r}\rangle\langle \mathbf{r}|\mathbf{k}'\rangle = \left(\frac{1}{2\pi}\right)^3 \int \mathrm{d}\mathbf{r} e^{i\mathbf{r}(\mathbf{k}-\mathbf{k}')} \qquad (151)$$

Mathematical Intermezzo, two-body Schrödinger in k-space

Projecting equation (146) on momentum states the momentum space Schrödinger equation is obtained,

$$\frac{\hbar^2}{2\mu}k^2\psi_n(\mathbf{k}) + \int d\mathbf{k}'\ V(\mathbf{k},\mathbf{k}')\psi_n(\mathbf{k}') = E_n\psi_n(\mathbf{k}) \tag{152}$$

Here the notation $\psi_n(\mathbf{k}) = \langle \mathbf{k}|\psi_n\rangle$ and $\langle \mathbf{k}\,|V|\mathbf{k}'\rangle = V(\mathbf{k},\mathbf{k}')$ has been introduced. The potential in momentum space is given by a double Fourier-transform of the potential in coordinate space, i.e.

$$V(\mathbf{k},\mathbf{k}') = \left(\frac{1}{2\pi}\right)^3 \int \mathrm{d}\mathbf{r} \int \mathrm{d}\mathbf{r}'\ e^{-i\mathbf{k}\mathbf{r}}\ V(\mathbf{r},\mathbf{r}')e^{i\mathbf{k}'\mathbf{r}'} \tag{153}$$

Mathematical Intermezzo, two-body Schrödinger in k-space

Here it is assumed that the potential interaction does not contain any spin dependence. Instead of a differential equation in coordinate space, the Schrödinger equation becomes an integral equation in momentum space. This has many tractable features. Firstly, most realistic nucleon-nucleon interactions derived from field-theory are given explicitly in momentum space. Secondly, the boundary conditions imposed on the differential equation in coordinate space are automatically built into the integral equation. And last, but not least, integral equations are easy to numerically implement, and convergence is obtained by just increasing the number of integration points. Instead of solving the three-dimensional integral equation given in equation (152), an infinite set of 1-dimensional equations can be obtained via a partial wave expansion.

Mathematical Intermezzo, two-body Schrödinger in k-space

The wave function $\psi_n(\mathbf{k})$ can be expanded in a complete set of spherical harmonics, i.e.

$$\psi_n(\mathbf{k}) = \sum_{lm} \psi_{nlm}(k) Y_{lm}(\hat{k}), \;\; \psi_{nlm}(k) = \int d\hat{k} \; Y^*_{lm}(\hat{k}) \psi_n(\mathbf{k}). \tag{154}$$

By inserting equation 154 in equation 152, and projecting from the left $Y_{lm}(\hat{k})$, the three-dimensional Schrödinger equation (152) is reduced to an infinite set of 1-dimensional angular momentum coupled integral equations,

$$\left(\frac{\hbar^2}{2\mu} k^2 - E_{nlm} \right) \psi_{nlm}(k) = - \sum_{l'm'} \int_0^\infty dk' k'^2 V_{lm,l'm'}(k,k') \psi_{nl'm'}(k') \tag{155}$$

where the angular momentum projected potential takes the form,

$$V_{lm,l'm'}(k,k') = \int \mathrm{d}\hat{k} \int \mathrm{d}\hat{k}' \; Y^*_{lm}(\hat{k}) V(\mathbf{k},\mathbf{k}') Y_{l'm'}(\hat{k}') \tag{156}$$

here $\mathrm{d}\hat{k} = \mathrm{d}\theta \sin\theta \, \mathrm{d}\varphi$. **Note that we discuss only the orbital momentum, we will include angular momentum and spin later**.

Mathematical Intermezzo, two-body Schrödinger in k-space

Often the potential is given in position space, so it is convenient to establish the connection between $V_{lm,l'm'}(k,k')$ and $V_{lm,l'm'}(r,r')$. Inserting position space completeness in equation (156) gives

$$\begin{aligned} V_{lm,l'm'}(k,k') &= \int \mathrm{d}\mathbf{r} \int \mathrm{d}\mathbf{r}' \int \mathrm{d}\hat{k} \int \mathrm{d}\hat{k}' \; Y^*_{lm}(\hat{k}) \langle \mathbf{k}|\mathbf{r}\rangle \langle \mathbf{r}|V|\mathbf{r}'\rangle \langle \mathbf{r}'|\mathbf{k}'\rangle Y_{lm}(\hat{k}') \\ &= \int \mathrm{d}\mathbf{r} \int \mathrm{d}\mathbf{r}' \left\{ \int \mathrm{d}\hat{k}\, Y^*_{lm}(\hat{k}) \langle \mathbf{k}|\mathbf{r}\rangle \right\} \\ &\quad \times \langle \mathbf{r}|V|\mathbf{r}'\rangle \left\{ \int \mathrm{d}\hat{k}' \; Y_{lm}(\hat{k}') \langle \mathbf{r}'|\mathbf{k}'\rangle \right\} \end{aligned} \tag{157}$$

Mathematical Intermezzo, two-body Schrödinger in k-space

Since the plane waves depend only on the absolute values of position and momentum, $|\mathbf{k}|, |\mathbf{r}|$, and the angle between them, θ_{kr} , they may be expanded in terms of bipolar harmonics of zero rank, i.e.

$$e^{i\mathbf{k}\cdot\mathbf{r}} = 4\pi \sum_{l=0}^{\infty} i^l j_l(kr) \left(Y_l(\hat{k}) \cdot Y_l(\hat{r}) \right) = \sum_{l=0}^{\infty} (2l+1) i^l j_l(kr) P_l(\cos\theta_{kr}) \qquad (158)$$

where the addition theorem for spherical harmonics has been used in order to write the expansion in terms of Legendre polynomials. The spherical Bessel functions, $j_l(z)$, are given in terms of Bessel functions of the first kind with half integer orders,

$$j_l(z) = \sqrt{\frac{\pi}{2z}} J_{l+1/2}(z).$$

Mathematical Intermezzo, two-body Schrödinger in k-space

Inserting the plane-wave expansion into the brackets of equation (157) yields,

$$\int \mathrm{d}\hat{k}\, Y^*_{lm}(\hat{k})\langle \mathbf{k}|\mathbf{r}\rangle = \left(\frac{1}{2\pi}\right)^{3/2} 4\pi i^{-l} j_l(kr)\, Y^*_{lm}(\hat{r}),$$

$$\int \mathrm{d}\hat{k}'\; Y_{lm}(\hat{k}')\langle \mathbf{r}'|\mathbf{k}'\rangle = \left(\frac{1}{2\pi}\right)^{3/2} 4\pi i^{l'} j_{l'}(k'r')\, Y_{l'm'}(\hat{r}).$$

Mathematical Intermezzo, two-body Schrödinger in k-space

The connection between the momentum- and position space angular momentum projected potentials are then given,

$$V_{lm,l'm'}(k,k') = \frac{2}{\pi}\, i^{l'-l} \int_0^\infty dr\, r^2 \int_0^\infty dr'\, r'^2 j_l(kr) V_{lm,l'm'}(r,r') j_{l'}(k'r') \tag{159}$$

which is known as a double Fourier-Bessel transform. The position space angular momentum projected potential is given by

$$V_{lm,l'm'}(r,r') = \int \mathrm{d}\hat{r} \int \mathrm{d}\hat{r}'\; Y^*_{lm}(\hat{r}) V(\mathbf{r},\mathbf{r}') Y_{l'm'}(\hat{r}'). \tag{160}$$

Mathematical Intermezzo, two-body Schrödinger in k-space

No assumptions of locality/non-locality and deformation of the interaction has so far been made, and the result in equation (159) is general. In position space the Schrödinger equation takes form of an integro-differential equation in case of a non-local interaction, in momentum space the Schrödinger equation is an ordinary integral equation of the Fredholm type, see equation (155). This is a further advantage of the momentum space approach as compared to the standard position space approach. If we assume that the interaction is of local character, i.e.

$$\langle \mathbf{r}|\, V|\mathbf{r}'\rangle = V(\mathbf{r})\delta(\mathbf{r}-\mathbf{r}') = V(\mathbf{r})\frac{\delta(r-r')}{r^2}\,\delta(\cos\theta-\cos\theta')\delta(\varphi-\varphi'),$$

then equation (160) reduces to

$$V_{lm,l'm'}(r,r') = \frac{\delta(r-r')}{r^2}\int \mathrm{d}\hat{r}\; Y^*_{lm}(\hat{r})\,V(\mathbf{r})\,Y_{l'm'}(\hat{r}), \tag{161}$$

Mathematical Intermezzo, two-body Schrödinger in k-space

and equation (159) reduces to

$$V_{lm,l'm'}(k,k') = \frac{2}{\pi}\, i^{l'-l} \int_0^\infty dr\, r^2\, j_l(kr)\, V_{lm,l'm'}(r) j_{l'}(k'r) \tag{162}$$

where

$$V_{lm,l'm'}(r) = \int \mathrm{d}\hat{r}\; Y^*_{lm}(\hat{r})\, V(\mathbf{r})\, Y_{l'm'}(\hat{r}), \tag{163}$$

Mathematical Intermezzo, two-body Schrödinger in k-space

In the case that the interaction is central, $V(\mathbf{r}) = V(r)$, then

$$V_{lm,l'm'}(r) = V(r) \int \mathrm{d}\hat{r}\; Y^*_{lm}(\hat{r}) Y_{l'm'}(\hat{r}) = V(r)\delta_{l,l'}\delta_{m,m'}, \tag{164}$$

and

$$V_{lm,l'm'}(k,k') = \frac{2}{\pi} \int_0^\infty dr\, r^2\, j_l(kr) V(r) j_{l'}(k'r) \delta_{l,l'}\delta_{m,m'} = V_l(k,k')\delta_{l,l'}\delta_{m,m'} \tag{165}$$

where the momentum space representation of the interaction finally reads,

$$V_l(k,k') = \frac{2}{\pi} \int_0^\infty dr\, r^2\, j_l(kr) V(r) j_l(k'r). \tag{166}$$

Mathematical Intermezzo, two-body Schrödinger in k-space

For a local and spherical symmetric potential, the coupled momentum space Schrödinger equations given in equation (155) decouples in angular momentum, giving

$$\frac{\hbar^2}{2\mu}k^2\psi_{nl}(k) + \int_0^\infty dk' k'^2 V_l(k,k')\psi_{nl}(k') = E_{nl}\psi_{nl}(k) \tag{167}$$

Where we have written $\psi_{nl}(k) = \psi_{nlm}(k)$, since the equation becomes independent of the projection m for spherical symmetric interactions. The momentum space wave functions $\psi_{nl}(k)$ defines a complete orthogonal set of functions, which spans the space of functions with a positive finite Euclidean norm (also called l^2-norm), $\sqrt{\langle\psi_n|\psi_n\rangle}$, which is a Hilbert space. The corresponding normalized wave function in coordinate space is given by the Fourier-Bessel transform

$$\phi_{nl}(r) = \sqrt{\frac{2}{\pi}}\int dk\, k^2 j_l(kr)\psi_{nl}(k) \tag{168}$$

How to construct the force: Partial wave expansion of the nuclear force

We will thus assume that the interaction is spherically symmetric and use the partial wave expansion of the plane waves in terms of spherical harmonics. This means that we can separate the radial part of the wave function from its angular dependence. The wave function of the relative motion is described in terms of plane waves as

$$e^{i\mathbf{kr}} = \langle \mathbf{r}|\mathbf{k}\rangle = \mathbf{4}\pi \sum_{\mathbf{lm}} i^{\mathbf{l}} \mathbf{j_l}(\mathbf{kr}) \mathbf{Y^*_{lm}}(\hat{\mathbf{k}}) \mathbf{Y_{lm}}(\hat{\mathbf{r}}), \tag{169}$$

where j_l is a spherical Bessel function and Y_{lm} the spherical harmonics.

First Solution Step

In terms of the relative and center-of-mass momenta $\mathbf{k}$ and $\mathbf{K}$, the potential in momentum space is related to the nonlocal operator $V(\mathbf{r}, \mathbf{r}')$ by

$$\langle \mathbf{k}'\mathbf{K}'|V|\mathbf{k}\mathbf{K}\rangle = \int d\mathbf{r}d\mathbf{r}' e^{-\imath\mathbf{k}'\mathbf{r}'} V(\mathbf{r}', \mathbf{r}) e^{\imath\mathbf{k}\mathbf{r}} \delta(\mathbf{K}, \mathbf{K}').$$

We will assume that the interaction is spherically symmetric. Can separate the radial part of the wave function from its angular dependence. The wave function of the relative motion is described in terms of plane waves as

$$e^{\imath\mathbf{k}\mathbf{r}} = \langle \mathbf{r}|\mathbf{k}\rangle = \mathbf{4}\pi \sum_{\mathbf{lm}} \imath^{\mathbf{l}} \mathbf{j_l}(\mathbf{kr}) \mathbf{Y^*_{lm}}(\hat{\mathbf{k}}) \mathbf{Y_{lm}}(\hat{\mathbf{r}}),$$

where j_l is a spherical Bessel function and Y_{lm} the spherical harmonic.

How to construct the force: Partial wave expansion of the nuclear force

This partial wave basis is useful for defining the operator for the nucleon-nucleon interaction, which is symmetric with respect to rotations, parity and isospin transformations. These symmetries imply that the interaction is diagonal with respect to the quantum numbers of total relative angular momentum $\mathcal{J}$, spin S and isospin T (we skip isospin for the moment). Using the above plane wave expansion, and coupling to final $\mathcal{J}$ and S and T we get

$$\langle \mathbf{k}' | V | \mathbf{k} \rangle = (4\pi)^2 \sum_{STll' m_l m_{l'} \mathcal{J}} i^{l+l'} Y^*_{lm}(\hat{\mathbf{k}}) Y_{l'm'}(\hat{\mathbf{k}}')$$

$$\langle l m_l S m_S | \mathcal{J} M \rangle \langle l' m_{l'} S m_S | \mathcal{J} M \rangle \langle k' l' S \mathcal{J} M | V | k l S \mathcal{J} M \rangle,$$

where we have defined

$$\langle k' l' S \mathcal{J} M | V | k l S \mathcal{J} M \rangle = \int j_{l'}(k'r') \langle l' S \mathcal{J} M | V(r', r) | l S \mathcal{J} M \rangle j_l(kr) r'^2 dr' r^2 dr. \quad (170)$$

We have omitted the momentum of the center-of-mass motion **K** and the corresponding orbital momentum L, since the interaction is diagonal in these variables.

The Lippman-Schwinger equation in a partial wave expansion

We wrote the Lippman-Schwinger equation as

$$\langle \phi_m | \hat{T} | \phi_n \rangle = \langle \phi_m | \hat{V} | \phi_n \rangle + \sum_k \langle \phi_m | \hat{V} | \phi_k \rangle \frac{1}{(E_n - \omega_k)} \langle \phi_k | \hat{T} | \phi_n \rangle.$$

How do we rewrite it in a partial wave expansion with momenta k?

The general structure of the T-matrix in partial waves is

$$T^{\alpha}_{ll'}(kk'K\omega) = V^{\alpha}_{ll'}(kk')$$

$$+\frac{2}{\pi}\sum_{l''m_{l''}M_S}\int_0^{\infty} d\mathbf{q}(\langle l''m_{l''}Sm_S|\mathcal{J}M\rangle)^2\frac{Y^*_{l''m_{l''}}(\hat{\mathbf{q}})Y_{l''m_{l''}}(\hat{\mathbf{q}})V^{\alpha}_{ll''}(kq)T^{\alpha}_{l''l'}(qk'K\omega)}{\omega - H_0},$$

The shorthand notation

$$T^{\alpha}_{ll'}(kk'K\omega) = \langle kKlL\mathcal{J}S|T(\omega)|k'Kl'L\mathcal{J}S\rangle,$$

denotes the T-matrix with momenta k and k' and orbital momenta l and l' of the relative motion, and K is the corresponding momentum of the center-of-mass motion. Further, L, $\mathcal{J}$, S and T are the orbital momentum of the center-of-mass motion, the total angular momentum, spin and isospin, respectively. Due to the nuclear tensor force (to be discussed later), the interaction is not diagonal in ll'.

Using the orthogonality properties of the Clebsch-Gordan coefficients and the spherical harmonics, we obtain the well-known one-dimensional angle independent integral equation

$$T^{\alpha}_{ll'}(kk'K\omega) = V^{\alpha}_{ll'}(kk') + \frac{2}{\pi}\sum_{l''}\int_0^{\infty} dqq^2 \frac{V^{\alpha}_{ll''}(kq)T^{\alpha}_{l''l'}(qk'K\omega)}{\omega - H_0}.$$

Inserting the denominator we arrive at

$$\hat{T}^{\alpha}_{ll'}(kk'K) = \hat{V}^{\alpha}_{ll'}(kk') + \frac{2}{\pi}\sum_{l''}\int_0^{\infty} dqq^2 \hat{V}^{\alpha}_{ll''}(kq)\frac{1}{k^2 - q^2 + i\epsilon}\hat{T}^{\alpha}_{l''l'}(qk'K).$$

How do we construct the interaction: Lippman-Schwinger Equation

To parameterize the nucleon-nucleon interaction we solve the Lippman-Scwhinger equation

$$T^{\alpha}_{ll'}(kk'K) = V^{\alpha}_{ll'}(kk') + \frac{2}{\pi}\sum_{l''}\int_0^{\infty} dqq^2 V^{\alpha}_{ll''}(kq)\frac{1}{k^2 - q^2 + i\epsilon}T^{\alpha}_{l''l'}(qk'K).$$

The shorthand notation

$$T(\hat{V})^{\alpha}_{ll'}(kk'K\omega) = \langle kKlL\mathcal{J}S|T(\omega)|k'Kl'L\mathcal{J}S\rangle,$$

denotes the $T(V)$-matrix with momenta k and k' and orbital momenta l and l' of the relative motion, and K is the corresponding momentum of the center-of-mass motion. Further, L, $\mathcal{J}$, and S are the orbital momentum of the center-of-mass motion, the total angular momentum and spin, respectively. We skip for the moment isospin.

Numerical Solution

For scattering states, the energy is positive, $E > 0$. The Lippman-Schwinger equation (a rewrite of the Schrödinger equation) is an integral equation where we have to deal with the amplitude $R(k, k')$ (reaction matrix, which is the real part of the full complex T-matrix) defined through the integral equation for one partial wave (no coupled-channels)

$$R_l(k, k') = V_l(k, k') + \frac{2}{\pi}\mathcal{P}\int_0^\infty dq q^2 V_l(k, q)\frac{1}{E - q^2/m}R_l(q, k').$$

For negative energies (bound states) and intermediate states scattering states blocked by occupied states below the Fermi level.

Relation to data

The symbol $\mathcal{P}$ in the previous slide indicates that Cauchy's principal-value prescription is used in order to avoid the singularity arising from the zero of the denominator.
The total kinetic energy of the two incoming particles in the center-of-mass system is

$$E = \frac{k_0^2}{m_n}.$$

The matrix $R_l(k, k')$ relates to the the phase shifts through its diagonal elements as

$$R_l(k_0, k_0) = -\frac{tan\delta_l}{mk_0}.$$

Recipe I, possible topic for project 2

This material is optional, but could define a possible project 2.
From now on we will drop the subscript l in all equations. In order to solve the Lippman-Schwinger equation in momentum space, we need first to write a function which sets up the mesh points. We need to do that since we are going to approximate an integral through

$$\int_a^b f(x)dx \approx \sum_{i=1}^{N} w_i f(x_i),$$

where we have fixed N lattice points through the corresponding weights w_i and points x_i. Typically obtained via methods like Gaussian quadrature.

Recipe II

If you use Gauss-Legendre the points are determined for the interval $x_i \in [-1, 1]$ You map these points over to the limits in your integral. You can then use the following mapping

$$k_i = const \times tan\left\{\frac{\pi}{4}(1 + x_i)\right\},$$

and

$$\omega_i = const\frac{\pi}{4}\frac{w_i}{cos^2\left(\frac{\pi}{4}(1 + x_i)\right)}.$$

If you choose units fm^{-1} for k, set $const = 1$. If you choose to work with MeV, set $const \sim 200$ ($\hbar c = 197$ MeVfm).

Recipe III

The principal value integral is rather tricky to evaluate numerically, mainly since computers have limited precision. We will here use a subtraction trick often used when dealing with singular integrals in numerical calculations. We introduce first the calculus relation

$$\int_{-\infty}^{\infty} \frac{dk}{k-k_0} = 0.$$

It means that the curve $1/(k-k_0)$ has equal and opposite areas on both sides of the singular point k_0. If we break the integral into one over positive k and one over negative k, a change of variable $k \rightarrow -k$ allows us to rewrite the last equation as

$$\int_{0}^{\infty} \frac{dk}{k^2-k_0^2} = 0.$$

Recipe IV

We can then express a principal values integral as

$$\mathcal{P}\int_0^\infty \frac{f(k)dk}{k^2-k_0^2} = \int_0^\infty \frac{(f(k)-f(k_0))dk}{k^2-k_0^2},$$

where the right-hand side is no longer singular at $k = k_0$, it is proportional to the derivative df/dk, and can be evaluated numerically as any other integral.

Recipe V

We can then use this trick to obtain

$$R(k,k') = V(k,k') + \frac{2}{\pi}\int_0^\infty dq \frac{q^2 V(k,q)R(q,k') - k_0^2 V(k,k_0)R(k_0,k')}{(k_0^2 - q^2)/m}.$$

This is the equation to solve numerically in order to calculate the phase shifts. We are interested in obtaining $R(k_0, k_0)$.

Recipe VI

How do we proceed?
Using the mesh points k_j and the weights ω_j, we reach

$$R(k,k') = V(k,k') + \frac{2}{\pi}\sum_{j=1}^{N}\frac{\omega_j k_j^2 V(k,k_j)R(k_j,k')}{(k_0^2-k_j^2)/m} - \frac{2}{\pi}k_0^2 V(k,k_0)R(k_0,k')\sum_{n=1}^{N}\frac{\omega_n}{(k_0^2-k_n^2)/m}.$$

Recipe VII

This equation contains now the unknowns $R(k_i, k_j)$ (with dimension $N \times N$) and $R(k_0, k_0)$.
We can turn it into an equation with dimension $(N+1) \times (N+1)$ with a mesh which contains the original mesh points k_j for $j = 1, N$ and the point which corresponds to the energy k_0. Consider the latter as the 'observable' point. The mesh points become then k_j for $j = 1, n$ and $k_{N+1} = k_0$.
With these new mesh points we define the matrix

$$A_{i,j} = \delta_{i,j} - V(k_i, k_j)u_j,$$

Recipe VIII

where δ is the Kronecker δ and

$$u_j = \frac{2}{\pi} \frac{\omega_j k_j^2}{(k_0^2 - k_j^2)/m} \qquad j = 1, N$$

and

$$u_{N+1} = -\frac{2}{\pi} \sum_{j=1}^{N} \frac{k_0^2 \omega_j}{(k_0^2 - k_j^2)/m}.$$

Recipe IX

The first task is then to set up the matrix A for a given k_0. This is an $(N+1) \times (N+1)$ matrix. It can be convenient to have an outer loop which runs over the chosen observable values for the energy k_0^2/m. *Note that all mesh points k_j for $j = 1, N$ must be different from k_0. Note also that $V(k_i, k_j)$ is an $(N+1) \times (N+1)$ matrix.*
With the matrix A we can rewrite the problem as a matrix problem of dimension $(N+1) \times (N+1)$. All matrices R, A and V have this dimension and we get

$$A_{i,l} R_{l,j} = V_{i,j},$$

or just

$$AR = V.$$

Recipe X

Since you already have defined A and V (these are stored as $(N+1) \times (N+1)$ matrices) The final equation involves only the unknown R. We obtain it by matrix inversion, i.e.,

$$R = A^{-1} V.$$

Thus, to obtain R, you will need to set up the matrices A and V and invert the matrix A. With the inverse A^{-1}, perform a matrix multiplication with V results in R.
With R you can then evaluate the phase shifts by noting that

$$R(k_{N+1}, k_{N+1}) = R(k_0, k_0) = -\frac{tan\delta}{mk_0},$$

where δ are the phase shifts.

Phase shifts

For elastic scattering, the scattering potential can only change the outgoing spherical wave function up to a phase. In the asymptotic limit, far away from the scattering potential, we get for the spherical bessel function

$$j_l(kr) \xrightarrow{r\gg 1} \frac{\sin(kr - l\pi/2)}{kr} = \frac{1}{2ik}\left(\frac{e^{i(kr-l\pi/2)}}{r} - \frac{e^{-i(kr-l\pi/2)}}{r}\right)$$

The outgoing wave will change by a phase shift δ_l, from which we can define the S-matrix $S_l(k) = e^{2i\delta_l(k)}$. Thus, we have

$$\frac{e^{i(kr-l\pi/2)}}{r} \xrightarrow{\text{phase change}} \frac{S_l(k)e^{i(kr-l\pi/2)}}{r}$$

Cross section

The solution to the Schrodinger equation for a spherically symmetric potential, will have the form

$$\psi_k(r) = e^{ikr} + f(\theta)\frac{e^{ikr}}{r}$$

where $f(\theta)$ is the scattering amplitude, and related to the differential cross section as

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2$$

Using the expansion of a plane wave in spherical waves, we can relate the scattering amplitude $f(\theta)$ with the partial wave phase shifts δ_l by identifying the outgoing wave

$$\psi_k(r) = e^{ikr} + \left[\frac{1}{2ik}\sum_l i^l(2l+1)(S_l(k)-1)P_l(\cos(\theta))e^{-il\pi/2}\right]\frac{e^{ikr}}{r}$$

which can be simplified further by cancelling i^l with $e^{-il\pi/2}$

Cross section

From the previous slide we have

$$\psi_k(r) = e^{ikr} + f(\theta)\frac{e^{ikr}}{r}$$

with

$$f(\theta) = \sum_l (2l+1) f_l(\theta) P_l(\cos(\theta))$$

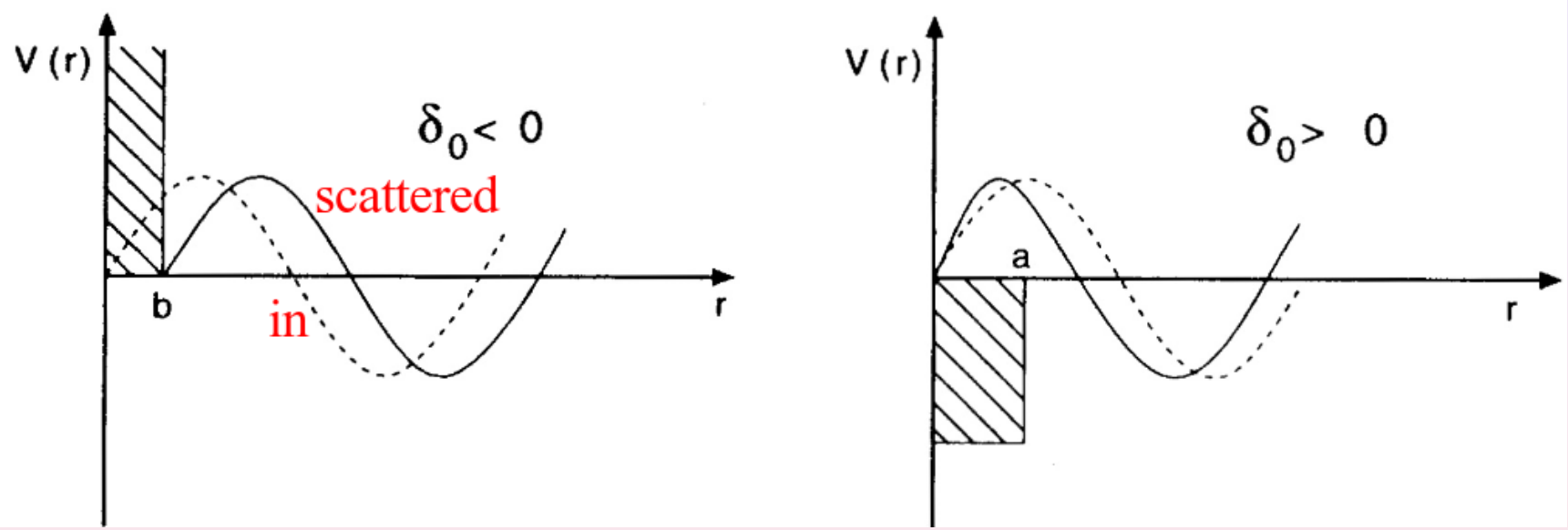
where the partial wave scattering amplitude is given by

$$f_l(\theta) = \frac{1}{k}\frac{(S_l(k)-1)}{2i} = \frac{1}{k}\sin\delta_l(k)e^{i\delta_l(k)}$$

With Eulers formula for the cotanget, this can also be written as

$$f_l(\theta) = \frac{1}{k}\frac{1}{\cot\delta_l(k) - i}$$

Meaning of the phase shift



Cross Section

The integrated cross section is given by

$$\begin{aligned}\sigma &= 2\pi \int_0^\pi |f(\theta)|^2 \sin\theta \, \mathrm{d}\theta = \\ &= 2\pi \sum_l |\frac{(2l+1)}{k} \sin\delta_l|^2 \int_0^\pi (P_l(\cos\theta))^2 \sin\theta \, \mathrm{d}\theta = \\ &= \frac{4\pi}{k^2} \sum_l (2l+1) \sin^2\delta_l(k) = 4\pi \sum_l (2l+1)|f_l(\theta)|^2\end{aligned} \tag{171}$$

Where the orthogonality of the Legendre polynomials was used to evaluate the last integral

$$\int_0^\pi P_l(\cos\theta)^2 \sin\theta \, \mathrm{d}\theta = \frac{2}{2l+1}$$

Thus, the *total* cross section is the sum of the partial-wave cross sections. Note that the differential cross section contains cross-terms from different partial waves. The integral over the full sphere enables the use of the legendre orthogonality, and this kills the cross-terms.

Low energy scattering: the scattering length

At low energy, $k \to 0$, S-waves are most important. In this region we can define the scattering length a and the effective range r. The $S-$wave scattering amplitude is given by

$$f_l(\theta) = \frac{1}{k} \frac{1}{\cot \delta_l(k) - i}$$

Taking the limit $k \to 0$, gives us the expansion

$$k \cot \delta_0 = -\frac{1}{a} + \frac{1}{2} r_0 k^2 + \dots$$

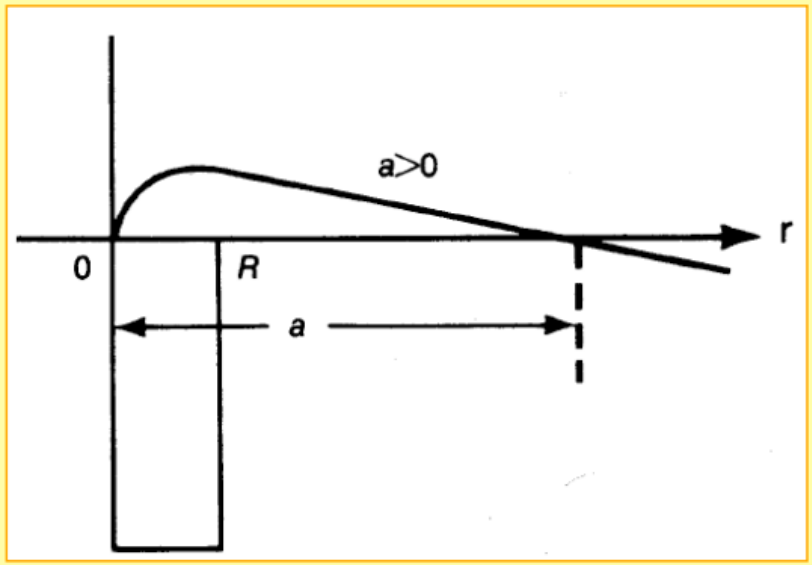
Thus the low energy cross section is given by

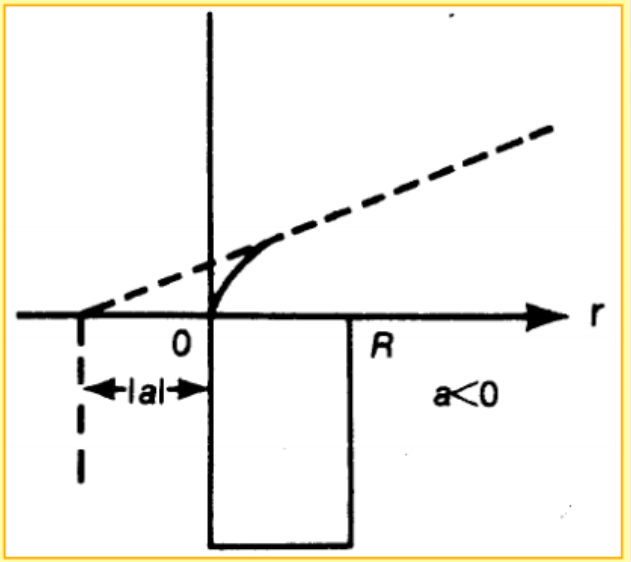
$$\sigma = 4\pi a^2$$

If the system contains a bound state, the scattering length will become positive (np $^3S_1$). For the $^1S_0$ wave, the scattering length is negative and large. This indicates that the wave function of the system is at the verge of turning over to get a node, but cant create a bound state in this wave.

(`http://people.ccmr.cornell.edu/~emueller/well.html`)

Low energy scattering: the scattering length





How to extract phase shifts

It is important to realize that the phase shifts themselves aren't observables. The measurable scattering quantity is the cross section, or the differential cross section. The partial wave phase shifts can be thought of as a parameterization of the (experimental) cross sections. The phase shifts provide insights into the physics of partial wave projected nuclear interactions, and are thus important quantities to know.

The nucleon-nucleon differential cross section have been measured at almost all energies up to the pion production threshold (290 MeV in the Lab frame), and this experimental data base is what provides us with the constraints on our nuclear interaction models. In order to pin down the unknown coupling constants of the theory, a statistical optimization with respect to cross sections need to be carried out. This is how we constraint the nucleon-nucleon interaction in practice!

Nijmegen multi-energy *pp* PWA phase shifts

TABLE IV. *pp* isovector phase shifts and their multienergy error in degrees as obtained in the multienergy *pp* analysis. Errors smaller than 0.0005° are not shown. The lower part lists the phase shifts as obtained in the combined $pp + np$ analysis.

T_{lab}	$^1S_0$	$^1D_2$	$^1G_4$	$^3P_0$	$^3P_1$	$^3F_3$	$^3P_2$	ϵ_2	$^3F_2$	$^3F_4$	ϵ_4	$^3H_4$
1	32.684	0.001	0.000	0.134	−0.081	−0.000	0.014	−0.001	0.000	0.000	−0.000	0.000
	±0.005											
5	54.832	0.043	0.000	1.582	−0.902	−0.005	0.214	−0.052	0.002	0.000	−0.000	0.000
	±0.017			±0.006	±0.001		±0.001					
10	55.219	0.165	0.003	3.729	−2.060	−0.032	0.651	−0.200	0.013	0.001	−0.004	0.000
	±0.025			±0.017	±0.002		±0.002					
25	48.672	0.696	0.040	8.575	−4.932	−0.231	2.491	−0.810	0.105	0.020	−0.049	0.004
	±0.039	±0.001		±0.053	±0.008		±0.008	±0.001				
50	38.899	1.711	0.152	11.47	−8.317	−0.690	5.855	−1.712	0.338	0.108	−0.195	0.026
	±0.049	±0.004		±0.09	±0.017		±0.016	±0.004		±0.001		
100	24.97	3.790	0.418	9.45	−13.258	−1.517	11.013	−2.659	0.817	0.478	−0.539	0.108
	±0.08	±0.018	±0.001	±0.11	±0.032	±0.003	±0.025	±0.017	±0.004	±0.007		
150	14.75	5.606	0.700	4.74	−17.434	−2.100	13.982	−2.873	1.197	1.032	−0.849	0.211
	±0.13	±0.033	±0.003	±0.14	±0.045	±0.010	±0.039	±0.029	±0.014	±0.022		
200	6.55	7.058	0.993	−0.37	−21.25	−2.487	15.63	−2.759	1.424	1.678	−1.108	0.321
	±0.16	±0.045	±0.010	±0.17	±0.07	±0.025	±0.052	±0.037	±0.034	±0.039		
250	−0.31	8.27	1.272	−5.43	−24.77	−2.724	16.59	−2.542	1.47	2.325	−1.314	0.428
	±0.18	±0.06	±0.024	±0.21	±0.12	±0.049	±0.07	±0.046	±0.06	±0.051		
300	−6.15	9.42	1.503	−10.39	−27.99	−2.84	17.17	−2.34	1.34	2.89	−1.47	0.526
	±0.25	±0.08	±0.048	±0.33	±0.19	±0.11	±0.10	±0.09	±0.11	±0.06		
350	−11.13	10.69	1.64	−15.30	−30.89	−2.87	17.54	−2.21	1.04	3.30	−1.588	0.608
	±0.46	±0.14	±0.08	±0.57	±0.27	±0.13	±0.15	±0.11	±0.16	±0.11	±0.001	
100	24.97	3.782	0.418	9.55	−13.245	−1.518	11.013	−2.654	0.816	0.471	−0.539	0.108
	±0.08	±0.017		±0.09	±0.030	±0.002	±0.021	±0.016	±0.003	±0.006		
200	6.55	7.039	0.993	−0.27	−21.18	−2.499	15.65	−2.731	1.414	1.656	−1.107	0.321
	±0.16	±0.043	±0.008	±0.17	±0.06	±0.021	±0.05	±0.035	±0.029	±0.034		
300	−6.22	9.42	1.501	−10.44	−27.80	−2.89	17.15	−2.27	1.30	2.95	−1.473	0.526
	±0.23	±0.08	±0.040	±0.29	±0.16	±0.07	±0.09	±0.06	±0.09	±0.05		

The *pp*-data is more accurate than the *np*-data, and for *nn* there is no data. The quality of a potential is gauged by the χ^2/datum with respect to the scattering data base

np-χ^2/datum for some potentials

T_{lab} bin (MeV)	N3LO[1]	NNLO[2]	NLO[2]	AV18[3]
0-100	1.05	1.7	4.5	0.95
100-190	1.08	22	100	1.10
190-290	1.15	47	180	1.11
0-290	**1.10**	**20**	**86**	**1.04**

[1] R. Machleidt et al., Phys. Rev. C68, 041001(R) (2003)
[2] E. Epelbaum et al., Eur. Phys. J. A19, 401 (2004)

[3] R. B. Wiringa et al., Phys. Rev. C5, 38 (1995)

An example: chiral twobody interactions

Chiral effective Lagrangian.

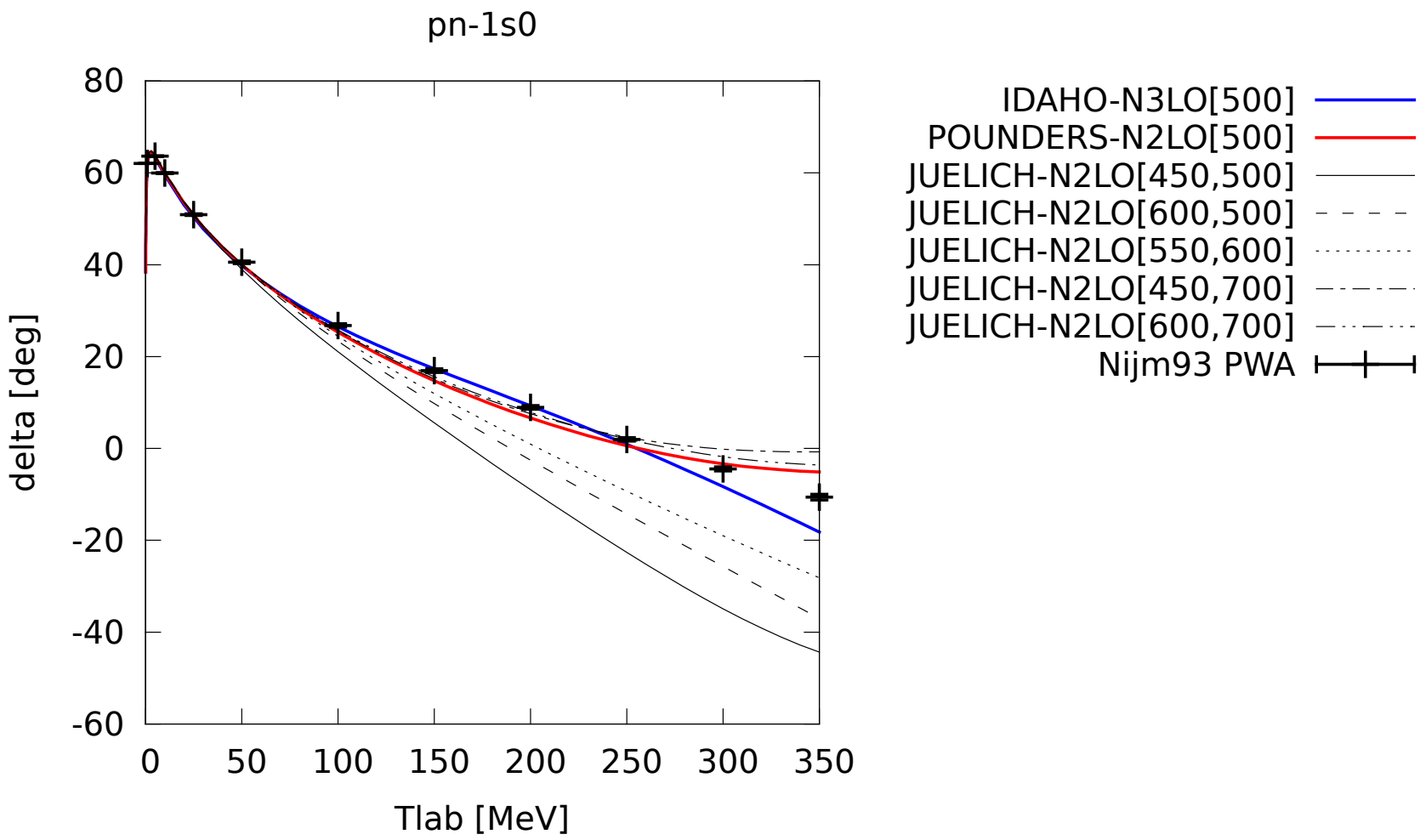
$$\mathcal{L}_{\text{eff}} = \mathcal{L}_{\pi\pi}(f_\pi, m_\pi) + \mathcal{L}_{\pi N}(f_\pi, M_N, g_A, c_i, d_i, ...) + \mathcal{L}_{NN}(C_i, \tilde{C}_i, D_i, ...) + \ldots$$

R. Machleidt, D. R. Entem, Phys. Rep. 503, 1 (2011)

E. Epelbaum, H.-W. Hammer, Ulf-G. Meißner, Rev. Mod. Phys. 81, 1773 (2009)

Phase shift

pn-$^1S_0$ phase shift. Note that the Nijm93 PWA phase shift becomes negative at $T_{lab} > 250$MeV. This indicates that the nucleon-nucleon potential is repulsive at short distances



Differential cross section