Slides from PHY981

Morten Hjorth-Jensen

Department of Physics and Center of Mathematics for Applications
University of Oslo, N-0316 Oslo, Norway and
National Superconducting Cyclotron Laboratory, Michigan State University, East
Lansing, MI 48824, USA

Spring 2013

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.

Topics for Week 3, January 14-18

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

- ► Tuesday:
- ► Hamiltonians and single-particle fields, continued from last week
- ► Thursday:
- ► Two-body wave functions and start discussion of Nuclear forces
- ► Exercises 1 and 2.

Suggested literature is AB chapters 9 and 10 and JS chapter 3

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

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 (Week of April 29 - May 3) you have to prepare five 20 minutes talks which cover the five main topics from the previous slide. At the exam, you will have to pick, randomly, one of the five topics. Duration of the examination is 40 minutes. The remaining 20 minutes are for questions from other topics as well.

I need your feedback by the end of this week. Also about the final dates for the exam.

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

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

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

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

and

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

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:

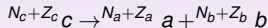$$BE(N, Z) = Z\Delta_H c^2 + N\Delta_n c^2 - \Delta(N, Z)c^2,$$

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*

$$^{N_a+Z_a}a + {}^{N_b+Z_b}b \rightarrow {}^{N_c+Z_c}c$$
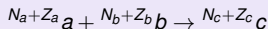
or the decay of nucleus *c* into two other nuclei *a* and *b*

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

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,

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

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:

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

where

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

where $R_{\mathrm{op}} = 0.875(7)$ fm is the rms radius of the proton, $R_{\mathrm{on}}^2 = 0.116(2)$ fm^2 is the mean-square radius of the neutron and $R_{\mathrm{rel}}^2 = 0.033$ 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

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

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

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

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

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

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

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

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 $u_i = u_{\text{ext}}(x_i)$ 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

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

with

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

The one-body part $u_{\text{ext}}(x_i)$ 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

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

with

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

In nuclear physics the one-body part $u_{\text{ext}}(x_i)$ 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

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

where ω is the oscillator frequency. This leads to

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

with

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

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

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

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

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

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

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

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

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

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

(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

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

with eigenvalues

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

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

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

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

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

Definitions and notations

Both $\hat{H}_0$ and $\hat{H}$ 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

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

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

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

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

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

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

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

and

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

Definitions and notations

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

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

or for a general matrix element

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

It has the symmetry property

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

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 (15) we obtain the energy functional

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

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