

Questions for self studies in Quantum Mechanics II, in the spring of 2002 (FYS 251).

1. Angular momenta

The angular momentum \mathbf{J} for a particular system is the sum of two dynamically independent parts, \mathbf{J}_1 and \mathbf{J}_2 :

$$\mathbf{J} = \mathbf{J}_1 + \mathbf{J}_2, \quad [\mathbf{J}_1, \mathbf{J}_2] = 0$$

The operators \mathbf{J}_1 and \mathbf{J}_2 are assumed to fulfill the angular momentum commutation relations.

- Show that the components of \mathbf{J} commute as angular momentum
- Show that $\mathbf{J}_1^2, J_{1z}, \mathbf{J}_2^2, J_{2z}$ is one set of complete commuting observables, and that
- $\mathbf{J}_1^2, \mathbf{J}_2^2, \mathbf{J}^2, J_z$ is another set.

Do all operators in the two sets commute with one another?

The eigenvectors to the set (ii) above span a subspace of dimension $(2j_1 + 1)(2j_2 + 1)$.

- What are the values of \mathbf{J}, J_z in this subspace?
- Show that the number of independent common eigenvectors of the two sets (ii) and (iii) is the same, namely $(2j_1 + 1)(2j_2 + 1)$.
- From these results, define the Clebsch-Gordan coefficient $\langle jm | j_1 m_1; j_2 m_2 \rangle$.

Consider the addition of two spins, $\mathbf{S} = \mathbf{S}_1 + \mathbf{S}_2$. Determine the eigenstates to \mathbf{S}, S_z , i.e. the coefficients $\langle Sm | \frac{1}{2} m_1; \frac{1}{2} m_2 \rangle$. Do also the corresponding construction for addition of two angular momenta $l_1 = l_2 = 1$.

Show that the components of $\mathbf{V} = (V_x, V_y, V_z)$ transform as a vector provided they fulfill the vector commutation law

$$[V_k, J_l] = i\hbar \sum_m \epsilon_{klm} V_m$$

What is a tensor operator? Show that $Y_{lm}(\hat{r})$, considered as a multiplicative operator, is a tensor operator of rank l .

How are vector operators and tensor operators of rank 1 related?

Let us consider product states $|j_1 m_1 \rangle |j_2 m_2 \rangle$ and states obtained by acting with a tensor operator, $T_{j_1 m_1} |j_2 m_2 \rangle$. Show that the two set of states transform in the same way under infinitesimal rotations.

Formulate the Wigner-Eckart theorem. Prove the m selection rule

$$\langle j_1 m_1 | T_{j_2 m_2} | j_3 m_3 \rangle = \delta_{m_1, m_2 + m_3}$$

directly without using the theorem.

Use the Wigner-Eckart theorem to determine selection rule in optical absorption of atoms. Limit your discussion to the dipole approximation.

Use the Wigner-Eckart theorem to prove the ‘projection’ theorem

$$\langle jm | \mathbf{V} | jm' \rangle = C \langle jm | \mathbf{J} | jm' \rangle$$

Also show that $C = \langle jm | \mathbf{V} \cdot \mathbf{J} | jm \rangle / j(j+1)$ (which is independent of m).

2. Identical particles

Why do we need a symmetrization postulate in order to describe identical particles?

Discuss the connection between spin and statistics. How is the Pauli principle reflected in shell structure of atoms and nuclei?

Describe how one can build basis functions for symmetric and antisymmetric states from a complete set of functions (‘orbitals’) for one particle, $\phi_n(\mathbf{r})$.

Assume that Φ is an (anti-)symmetric basis function for N particles in which the orbital ϕ_k occurs n_k times:

$$|\Psi\rangle = |n_1, n_2, \dots\rangle \quad \sum_k n_k = N$$

Express the expectation value of a one-body operator such as

$$H_1 = \sum_k \frac{p_k^2}{2m} + w(\mathbf{r}_k)$$

and a two-body operator such as

$$H_2 = \sum_{k < l \leq N} v(|\mathbf{r}_k - \mathbf{r}_l|)$$

in terms of one- and two-particle matrix elements and the occupation numbers n_k .

Verify the above results for the case of two identical fermions.

Specialize to the He atom

$$H = \frac{1}{2} \mathbf{p}_1^2 + \frac{1}{2} \mathbf{p}_2^2 - \frac{Z}{r_1} - \frac{Z}{r_2} + \frac{1}{r_{12}}$$

and an antisymmetric wave function representing the configuration $|ns n's\rangle$

$$(\phi_{ns}(r_1) \phi_{n's}(r_2) |\sigma, \sigma'\rangle - (\phi_{n's}(r_1) \phi_{ns}(r_2) |\sigma', \sigma\rangle) / \sqrt{2}$$

Obtain an approximations to the triplet and singlet energies of He in the configuration $|nsn's\rangle$ in terms of one-body expectation values $\langle ns|\mathbf{p}^2/2 - Z/r|ns\rangle$ and two-body direct (I) and exchange (J) integrals,

$$I = \langle nsn's | \frac{1}{r_{12}} | nsns' \rangle, \quad J = \langle nsn's | \frac{1}{r_{12}} | n'sns \rangle.$$

Explain the idea behind the Hartree-Fock (HF) approximation. Derive the HF equation for He in the ground state $|1s^2\rangle$ and show that orbital ϕ_{1s} obeys

$$\left[\frac{1}{2} \mathbf{p}^2 - \frac{Z}{r} + V_H(r) \right] \phi_{1s}(r) = \epsilon_{1s} \phi_{1s}(r)$$

Write down the HF equations for N fermions in a one-body potential $w(\mathbf{r})$. The particles interact via a two-body potential $v(|\mathbf{r}_1 - \mathbf{r}_2|)$.

3. Approximations for time-dependent problems

In order to obtain approximate solutions to the time-dependent Schrödinger equation

$$i\hbar \dot{\Psi}(t) = [H_0 + V] \Psi(t)$$

one may expand in eigenstates to H_0

$$\Psi(t) = \sum_n c_n(t) e^{-iE_n t/\hbar} |n\rangle.$$

In this way one can obtain perturbation expansions in increasing powers of V .

- a) Derive the equation of motion for the coefficient c_n .
- b) Show that these equations conserve the total probability, i.e.

$$\sum_n |c_n(t)|^2 = 1$$

A particular system is initially in a discrete (sharp) state "0". We assume that the system also has continuum levels "n" which are degenerate with "0". Add now a perturbation V that couples "0" and the continuum states "n". The initial state can e.g. model an excited atomic state, and the the continuum states a ground-state atom plus an emitted photon $\mathbf{k}\lambda$.

- a) Show using perturbation theory that the transition probabilities per unit time are given approximately by the "Golden Rule":

$$\frac{d}{dt} |c_n(t)|^2 \approx \frac{2\pi}{\hbar} |\langle n|V|0\rangle|^2 \delta(E_n - E_0) \quad (6)$$

- b) Discuss the validity of the above approximation and explain why it does not hold for very long times.
- c) Explain qualitatively how one can modify the expression so as to conserve the total probability and remain valid also for long times.

How is 'Golden Rule' modified when the perturbation has a sinusoidal time dependence?

Calculate the optical absorption

$$\sigma(\omega) = \frac{\text{absorbed power}}{\text{incident energy flux}}$$

for a hydrogen-like ion expressed in e.g the dipole matrix element $\langle f|z|i \rangle$.

Explain what the ‘adiabatic approximation’ means. Give some example when it applies.

What is the ‘sudden approximation’?

4. Scattering theory

In what follows we consider scattering of two particles in the center-of-mass frame. We assume that the particles interact via a centrally symmetric and short-ranged potential $V(r)$.

Under the conditions stated above we can find continuum solutions to the Schrödinger equation of the form

$$\psi(\mathbf{r}) = e^{ikz} + \phi_{scatt}(\mathbf{r}), \quad (2a)$$

where

$$\phi_{scatt}(\mathbf{r}) \approx f(\hat{r}) \frac{e^{ikr}}{kr} \quad (2b)$$

at far distances.

- Calculate the current from the two terms separately at far distances.
- In addition to the contribution above there is in principle also interference between the two terms in the wave function. Explain qualitatively why these interference terms do not contribute to the observed scattering.
- Using the results above, explain the physical meaning of the angle-dependent factor $f(\hat{r})$.

Let us specialize to spherically symmetric potentials $V(r)$. Explain how ψ may be expanded in spherical waves and how the the problem of finding the scattering cross section is reduced to a simpler problem of solving one-dimensional Schrödinger equations, one for each angular momentum l .

Find the spherically symmetric ingoing/outgoing solutions to

$$[\nabla^2 + k^2]\psi = 0$$

- Use the above result to show that

$$\left[E - \frac{\mathbf{p}^2}{2m}\right]G(E, |\mathbf{r} - \mathbf{r}'|) = 0 \text{ if } \mathbf{r} \neq \mathbf{r}'$$

where

$$G(E, r) = -\frac{m}{2\pi\hbar^2} \frac{e^{ikr}}{kr}$$

b) When $r \rightarrow 0$, $G(E, r)$ is approximately the same as the potential from a point charge $-m/(2\pi\hbar^2)$. Make use of this observation to obtain the full result

$$\left[E - \frac{\mathbf{p}^2}{2m}\right]G(E, |\mathbf{r} - \mathbf{r}'|) = \delta(\mathbf{r} - \mathbf{r}')$$

Use the result of the previous question to obtain the Lippmann-Schwinger equation

$$\psi(\mathbf{r}) = e^{ikz} + \int d\mathbf{r}'^3 G(E, |\mathbf{r} - \mathbf{r}'|) V(\mathbf{r}') \psi(\mathbf{r}') \quad (3a)$$

or, in symbolic form,

$$\psi = e^{ikz} + G(E) V \psi$$

Explain qualitatively how one can verify the asymptotic form at far distances of the scattering states in Eq. (2). Also derive the (implicit) equation for the scattering amplitude:

$$f_{\mathbf{k}}(\hat{r}) = -\frac{m}{2\pi\hbar^2} \langle \mathbf{k}_f | V | \psi_{\mathbf{k}} \rangle \quad (4)$$

Derive the Born approximation from Eq. (4). When is it valid?

How are the results discussed here modified when two identical particles are scattered against one another?