Lista 3 - Quântica B (2013)

1. Counting states

Consider a one-particle quantum mechanical system with a Hilbert space spanned by three orthonormal states $|n\rangle$, with $n = 1, 2, 3$. Three non-interacting particles occcupy these states. Determine how many distinct physical states there are if these particles are: (a) three identical fermions, (b) three identical bosons, (c) two identical fermions and one boson, (d) two identical bosons and one fermion, (e) three distinct fermions, and (f) three distinct bosons.

2. Exchange interaction

Consider a one-dimensional system of two spin-1/2 fermions. The two fermions move in the field of an anharmonic double-well oscillator and interact with each other through a repulsive pair interaction $V(|x|)$. The Hamiltonian for this two-particle system is

$$H = \frac{1}{2m}\left(p_1^2 + p_2^2\right) + U(x_1) + U(x_2) + V(|x_1 - x_2|),$$

where the double-well potential is $U(x) = \frac{U_0}{a^4}\left(x^2 - a^2\right)^2$. As for the pair potential $V(x)$, we will only need to assume that it is repulsive and that it decreases sufficiently fast so that all the integrals involved are convergent. Finally, let $\langle x|R\rangle = \psi_R(x)$ be the harmonic-oscillator ground-state wavefunction centered around $x = a$ and $\langle x|L\rangle = \psi_L(x)$ be the corresponding wave function centered around $x = -a$:

$$\psi_R = \left(\frac{1}{\pi\sigma^2}\right)^{1/4} e^{-\frac{(x-a)^2}{2\sigma^2}} \text{ and } \psi_L = \left(\frac{1}{\pi\sigma^2}\right)^{1/4} e^{-\frac{(x+a)^2}{2\sigma^2}}, \text{ with } \sigma^2 = \frac{\hbar a}{\sqrt{8mU_0}}.$$

(a) Give a justification for $\psi_{R,L}$. When are they expected to be a good approximation of the true ground-state wavefunctions? Compute the overlap $\ell = \langle L|R\rangle$.

(b) Find the expressions for the matrix elements of the one-particle Hamiltonian $H^{(1)} = \frac{1}{2m}p^2 + U(x)$ in the space spanned by the two single particle kets $|R\rangle$ and $|L\rangle$:

$$H_{\text{eff}}^{(1)} = \begin{pmatrix} \left\langle R\left|H^{(1)}\right|R\right\rangle & \left\langle R\left|H^{(1)}\right|L\right\rangle \\ \left\langle L\left|H^{(1)}\right|R\right\rangle & \left\langle L\left|H^{(1)}\right|L\right\rangle \end{pmatrix}.$$

Now, diagonalize $H_{\text{eff}}^{(1)}$ and find its two Eigenstates $|\pm\rangle$ and corresponding energies $E_\pm$.

(c) What is the maximum number of linearly independent, properly anti-symmetrized two-particle states (including spin)? Construct the two-particle basis using the single particle states $|+,\uparrow\rangle$, $|+,\downarrow\rangle$, $|-,\uparrow\rangle$, and $|-,\downarrow\rangle$.

(d) Calculate the matrix elements of the interaction term (V) of the two-particle Hamiltonian in the unsymmetrized (orbital) basis $|R,R\rangle$, $|R,L\rangle$, $|L,R\rangle$, and $|L,L\rangle$. Now, find an expression for the *appropriately defined* Direct (Coulomb) and Exchange integrals.

(e) Use these expressions (and the overlap ℓ) to compute the energy levels, their quantum numbers and their degeneracies for this two-particle system. Find an expression for the Exchange constant J. (*Hint*: Express your result in terms of $H_{\text{eff}} = \text{const} + J\mathbf{S}_1 \cdot \mathbf{S}_2$, with $\mathbf{S}_i$ being the spin operators.)

3. Free fermions

Consider a system of noninteracting N spin-1/2 particles which are free to move in a one-dimentional ring of length L. The one-particle wavefunctions are

$$\langle x, \sigma|\psi\rangle = \psi_{n,\sigma}(x),$$

with $\sigma = \uparrow, \downarrow$ representing the spin, and n a quantum number to be defined. Assume that $N/2$ is an odd integer.

(a) Write down the one-particle states wavefunctions $\psi_{\sigma,n}(x)$ which obey the boundary condition given above. What is the meaning of the quantum number n?

(b) Use the fermionic field operators $a_{n,\sigma}^\dagger(x)$ and $a_{n,\sigma}(x)$ in position space to write the Hamiltonian of this free fermion system in the Fock space. Do the same now for the operators in momentum space.

(c) Compute the anticommutators $\left\{\tilde{a}_\sigma(p), \tilde{a}_\tau^\dagger(p)\right\}$ and $\left\{\tilde{a}_\sigma(p), \tilde{a}_\tau(p)\right\}$.

(d) Construct the many-particle ground state $|G\rangle$ for this system in the Fock space. Compute the Fermi energy E_F, namely the energy of the topmost occupied state. How many single-particle states are present in $|G\rangle$?

(e) Show that the wavefunction of the ground state is an $N \times N$ Slater determinant. In addition, show this determinant can be factorized to the product of two $\frac{N}{2}\times\frac{N}{2}$ determinants. (*Hint*: Notice that $\langle x_{i,\sigma}|\psi_{n,\tau}\rangle = \delta_{\sigma,\tau}\psi_{n,\tau}(x_i)$, where $x_{i,\sigma}$ is the position of the i-th particle with spin σ.)

(f) Show that

$$\Psi\left(x_{1,\uparrow}, x_{1,\downarrow}, \ldots, x_{\frac{N}{2},\uparrow}, x_{\frac{N}{2},\downarrow}\right) = \prod_{i<j=1}^{\frac{N}{2}} \left(z_{i,\uparrow} - z_{j,\uparrow}\right)\left(z_{i,\downarrow} - z_{j,\downarrow}\right), \text{ where } z_{i,\sigma} = e^{i\frac{2\pi}{L}x_{i,\sigma}}.$$

(*Hint*: Recall the Vandermonde matrix.)

4. Two coupled bosons

Consider a system of two distinct bosonic particle (type A and B) in which only one mode is present:

$$H = \epsilon_{\mathrm{A}} a^\dagger a + \epsilon_{\mathrm{B}} b^\dagger b + V a^\dagger b + V^* b^\dagger a.$$

(a) Show that $c \equiv ua - vb$ and $d \equiv v^* a + u^* b$, with $|u|^2 + |v|^2 = 1$ are bosonic operators.

(b) Show that when $\epsilon_{\mathrm{A}} = \epsilon_{\mathrm{B}}$ and $V = V^*$, the choice $u = v = 1/\sqrt{2}$ decouples the system of bosonic particles C and D.

(c) Determine u and v that diagonalizes the system in the general case. Find the Eigenenergies and Eigenvectors of the system.

5. Two coupled fermions

Consider a system of two spin-1/2 identical fermionic particles that can occupy three different states of energies E_i, $i = 1, 2, 3$. The matrix elements allowing the transitions between these states are M_{ij}.

(a) Write down the system Hamiltonian in terms of the criation and annihilation operators.

(b) Determine the equation that gives the Eigenenergies of the sytem.

(c) Diagonalize the system for the particular case $E_i = E$ and $M_{ij} = M$, and the spins of the particles are the same.

6. Grand-canonical ensamble

The Grand partition function is given by the trace

$$Z_{\mathrm{G}} = \operatorname{tr} e^{-\beta(H-\mu N)}, \text{ where } H = \sum_i \epsilon_i a_i^\dagger a_i \text{ and } N = \sum_i a_i^\dagger a_i,$$

and the constants β and μ are the inverse of temperature and the chemical potential, respectively. In the following compute the required quantities for both cases of identical bosonic and fermionic particles.

(a) Compute Z_{G}. (*Hint*: Use the trace in the Fock space: $\operatorname{tr} O = \langle n_1 \ldots n_\infty | O | n_1 \ldots n_\infty\rangle$, and recall that in the Grand-canonical ensamble the number of particles if not fixed.)

(b) Compute the average occupation number $\langle n_i\rangle$, such that $N = \sum_i \langle n_i\rangle$. (*Hint*: Recall the thermodynamic Grand-potential $\Omega(T, V, \mu) = \beta^{-1} \ln Z_{\mathrm{G}}$, and that $N = -\left(\frac{\partial\Omega}{\partial\mu}\right)_{T,V}$.)

(c) Show that the fractional deviation from the mean occupation number

$$\frac{\left\langle \left(n_i - \langle n_i\rangle\right)^2\right\rangle}{\langle n_i\rangle^2} = e^{\beta(\epsilon_i - \mu)} = \frac{1}{\langle n_i\rangle} + \zeta,$$

with the $\zeta = \pm 1$ for bosons and fermions, respectively.

7. Holes in a magnetic moment closed shell as an antiparticle (Merzbacher, chap. 22)

Let $a_{j,m}^\dagger$ be a criation operator of fermionic particle with angular momentum j and projection in the z-direction m.

(a) Construct the closed-shell state: a state in which all one-particle states $m = -j$ to $= +j$ are occupied.

(b) Prove that the this state has zero total angular momentum.

(c) If a fermion with a certain magnetic quantum number $m = k$ is missing from this closed-shell state of particles, show that, for angular momentum purposes, this hole state can be treated as the state of a single particle with quantum number $-k$, and effective creation operator $(-1)^{j-k} a_{j,k}$.

8. (Optional) More on exchange (Merzbacher, chap. 22)

Consider the unperturbed states of n spin-1/2 particles, $a^\dagger_{n,\sigma_n} \dots a^\dagger_{k,\sigma_k} \dots a^\dagger_{1,\sigma_1} |0\rangle$, each occupying one of the n equivalent, degenerate orthogonal orbitals labeled by the quantum number k, with $\sigma_k = \pm 1/2$ denoting the spin quantum number associate with the orbital k. Show that in the space of the 2^n unperturbed states a spin-independent two-body interaction may, in first-order perturbation theory, be replaced by the effective exchange (Heisenberg) Hamiltonian

$$H_{\text{eff}} = -\frac{1}{\hbar^2} \sum_{k,\ell} \langle k, \ell\, |V|\, \ell, k\rangle\, \mathbf{S}_k \cdot \mathbf{S}_\ell + \text{const}, \;\text{ where } \mathbf{S}_k = \frac{\hbar}{2} \sum_{\sigma_k, \tau_k} a^\dagger_{k,\sigma_k} a_{k,\tau_k} \,\langle \sigma_k\, |\boldsymbol{\sigma}|\, \tau_k\rangle$$

is the localized spin operator, and $\boldsymbol{\sigma} = (\sigma^x, \sigma^y, \sigma^z)$ are the Pauli matrices.