Physics 581: Quantum Mechanics II
Department of Physics, UIUC
Spring Semester 2007
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Problem Set No. 4:
Identical Particles and Second Quantization
Due Date: Monday April 9, 2007

1 Counting States of Particles with Different Statistics

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 system of two fermions with spin $\frac{1}{2}$ in one dimension. 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 with coordinates x_1, x_2 and momenta p_1 and p_2 is

$$H = \frac{p_1^2}{2M} + \frac{p_2^2}{2M} + U(x_1) + U(x_2) + V(|x_1 - x_2|) \tag{1}$$

The double-well potential is

$$U(x) = \frac{U_0}{a^4} \left(x^2 - a^2\right)^2 \tag{2}$$

where U_0 has units of energy and $\pm a$ are the two minima of the potential. As for the pair potential we will only need to assume that it is repulsive and that it decreases sufficiently fast so that the various integrals that you will need are convergent. Let $\langle x|R\rangle_0 = \psi_R(x)$ be the *harmonic oscillator* ground state wave function centered around $x = a$ and $\langle x|L\rangle_0 = \psi_L(x)$ be the corresponding wave function centered arpund $x = -a$,

$$\psi_{R,L}(x) = \frac{1}{\sqrt{2\pi\xi^2}} e^{-\frac{(x\pm a)^2}{4\xi^2}} \tag{3}$$

where $\xi = \left(\frac{\hbar^2 a^2}{32 M U_0}\right)^{\frac{1}{4}}$.

1. Find an expression for the matrix elements of the one-particle Hamiltonian $H^{(1)} = \frac{p^2}{2M} + U(x)$ in the space spanned by the two single particle kets $|R\rangle$ and $|L\rangle$
$$H^{(1)}_{\text{eff}} = \begin{pmatrix} \langle R|H^{(1)}|R\rangle & \langle R|H^{(1)}|L\rangle \\ \langle L|H^{(1)}|R\rangle & \langle L|H^{(1)}|L\rangle \end{pmatrix} \tag{4}$$

2. Diagonalize this 2×2 effective one-electron Hamiltonian. Determine its two eigenstates $|+\rangle$ and $|-\rangle$ and their energies $E_{\pm}$. Calculate the overlap $\ell = \langle L|R\rangle$.

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

4. Calculate the matrix elements of the interaction term of the two-particle Hamiltonian in the unsymmetrized (orbital) basis $|RR\rangle, |RL\rangle|LR\rangle, |LL\rangle$. Find an expression for the appropriately defined Coulomb and Exchange integrals V and U.

5. 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.

3 Spin-$\frac{1}{2}$ Ferromagnet

Consider a system with N spin-$\frac{1}{2}$ degrees of freedom each sitting on a fixed site of a one-dimensional chain. We will label the sites with an integer index $j = 1, \ldots, N$. To simplify matters we will consider a closed chain, namely site $N+1$ coincides with site 1. The spacial degrees of freedom of these particles are frozen out and inly the quantum mechanical degrees of freedom associated with their spins survive. At each site there is a spin-$\frac{1}{2}$ Hilbert space. Let $\vec{\sigma}_j$ be a vector at each site whose components are the three Pauli matrices. Let us denote the two states that span the Hilbert space at site j by $|s_j\rangle$ with $s_j = \pm$. For the rest of this problem we will use units in which $\hbar = 1$ and the lattice spacing $a = 1$. Thus the length of the system is $L = Na = N$ in these units.

The dynamics of this system of N spins is governed by the Heisenberg exchange Hamiltonian
$$H = -J \sum_{j=1}^{N} \vec{\sigma}(j) \cdot \vec{\sigma}(j+1) \tag{5}$$
where $J > 0$ is the (positive) exchange constant.

1. What is the size of the Hilbert space at each site and for the entire system?

2. Show that the state $|+_1, \ldots, +_N\rangle$ is an eigenstate of H and compute its eigenvalue.

3. Show that there is a manifold of degenerate ground states. Enumerate and construct explicitly the set of ground states. How many of them there are? Calculate the ground state energy.
   Hint: Show first that the operators $\sigma_a^{\text{total}} = \sum_{j=1}^{N} \sigma_a(j)$ with $a = 1, 2, 3$ commute with H and with $\vec{\sigma}^{\text{total}} \cdot \vec{\sigma}^{\text{total}}$.

4. Show that the states $|p\rangle$ (where $p = 2\pi \frac{n}{N}$ and $1 \leq n \leq N$) defined by

$$|p\rangle = \frac{1}{\sqrt{N}} \sum_{j=1}^{N} e^{ipj} \sigma^{-}(j) \; |G\rangle \tag{6}$$

   are eigenstates of H, where $\sigma^{-}(j)$ is the spin raising operator, and $|G\rangle$ is a ground state of H. Compute the energy of the state $|p\rangle$. Give a physical interpretation of what this excited state looks like.

4 A free fermion system

Consider a system of particles of mass M and spin spin-$\frac{1}{2}$. The particles are restricted to move on a line of length L and do not interact with each other. we will assume that the one-particle wave functions $\langle x, \sigma|\psi\rangle = \psi_\sigma(x)$ (with $\sigma = \uparrow, \downarrow$) obey periodic boundary conditions,

$$\psi(x) = \psi(x + L) \tag{7}$$

Consider the problem in general, without specifying the number of particles at first.

1. Write down the one-particle states $\psi_\sigma(x)$ which obey the boundary conditions given above.

2. Use fermion creation and anihilation operators $a^\dagger(x)$ and $a(x)$ in position space to write an expression for the Hamiltonian of this free fermion system in Fock space. Write the same Hamiltonian in momentum space.

3. Compute the following anticommutators $\{a(p), a(p')\}$, $\{a^\dagger(p), a^\dagger(p')\}$ and $\{a(p), a^\dagger(p')\}$.

4. Construct the ground state $|gnd\rangle$ for a system of N fermions with spin spin-$\frac{1}{2}$. Assume that N is an even number and that $N/2$ is odd. Compute the Fermi energy E_F, namely the energy of the topmost occupied state. How many single particle states with this energy are present?.

5. Show that the wave function of the N-particle ground state (with N an even number) is an $N \times N$ Slater determinant, $\Psi(x_{1,\uparrow}, x_{1,\downarrow}, \ldots, x_{\frac{N}{2},\uparrow}, x_{\frac{N}{2},\downarrow})$.

6. Let $x_{j,\uparrow}$ and $x_{j,\downarrow}$ be the coordinates of the j-th particle with spin $\uparrow$ or $\downarrow$. Show that

$$\Psi(x_{1,\uparrow}, x_{1,\downarrow}, \ldots, x_{\frac{N}{2},\uparrow}, x_{\frac{N}{2},\downarrow}) = \prod_{i<j=1}^{\frac{N}{2}} \left(e^{i\frac{2\pi}{L}x_{i,\uparrow}} - e^{i\frac{2\pi}{L}x_{j,\uparrow}}\right)\left(e^{i\frac{2\pi}{L}x_{i,\downarrow}} - e^{i\frac{2\pi}{L}x_{j,\downarrow}}\right) \tag{8}$$

Hint: you may use the identity (Vandermonde determinant)

$$\det a_{ij} = \begin{vmatrix} 1 & 1 & \ldots & 1 \\ z_1 & z_2 & \ldots & z_N \\ \ldots & \ldots & \ldots & \ldots \\ z_1^{N-1} & z_2^{N-1} & \ldots & z_N^{N-1} \end{vmatrix} = \prod_{i<j=1}^{N} (z_i - z_j) \tag{9}$$

for a matrix $a_{ij} = z_i^{j-1}$, $i, j = 1, \ldots, N$; $z_1, \ldots, z_N$ are complex numbers.

7. Define a new set of creation and anihilation operators that anihilate the ground state $|gnd\rangle$. Write the Hamiltonian in terms of these new operators. Construct the spectrum of excitations in terms of particle and hole states with a given spin. Compute the excitation energies as a function of momentum p determine and the degeneracies of the single particle and single hole states with arbitrary spin.

8. Construct excited states with two particles, two holes and one particle and one hole. In each case assume that the excitations have momenta p and p' and arbitary spin. Compute the energy and the total number of fermions for each state.