PHYSICS 320: Problem Set No. 2
Due: Friday Aug. 28 2009

1. In this problem you will calculate the matrix element of a single particle operator between bosonic occupation number states. As we showed in class, an occupation number state of N bosons has the following form

$$|n_1, n_2, \ldots, n_M\rangle = \left(\frac{\prod_{i=1}^{M} n_i!}{N!}\right)^{1/2} \sum_{P(\{p_j\})} |p_1\rangle_1 |p_2\rangle_2 \ldots |p_N\rangle_N.$$

Here, M is the total number of single particle states and n_i is the occupancy of the i^{th} single particle state. $|p_j\rangle_j$ is the single particle state the j^{th} particle is in. Thus, the possible range of values of p_j is 1 to M. $P(\{p_j\})$ is the set of all possible p_j's such that n_1 of them are equal to 1, n_2 equal to 2 and so on.

Now, consider two states where one is obtained from the other by moving a boson from the k^{th} single particle state to the i^{th} state. The two states are thus of the form

$$\begin{aligned} |A\rangle = |n_1, n_2, \ldots, n_i, \ldots, n_k, \ldots, n_M\rangle &= N_A \sum_{P_A(\{p_j\})} |p_1\rangle_1 \; |p_2\rangle_2 \ldots \; |p_N\rangle_N, \\ |B\rangle = |n_1, n_2, \ldots, n_i + 1, \ldots, n_k - 1, \ldots, n_M\rangle &= N_B \sum_{P_B(\{p'_j\})} |p'_1\rangle_1 \; |p'_2\rangle_2 \ldots \; |p'_N\rangle_N. \end{aligned}$$

Here N_A and N_B are the appropriate normalization factors for the two states and P_A and P_B, the appropriate sets of allowed values of the p_j's and p'_j's. A single body operator can be written as

$$F^{(1)} = \sum_{l=1}^{N} f_l,$$

where f_l acts only on the l^{th} particle and all the f_l's act in the same way on the corresponding particles (since we are describing a system of identical particles).

   (a) Consider a particular f_l and

$$\langle B|f_l|A\rangle = N_A N_B \sum_{P_A(\{p_j\}), P_B(\{p'_j\})} \left({}_1\langle p'_1| \; {}_2\langle p'_2| \ldots \; {}_N\langle p'_N|\right) f_l \left(|p_1\rangle_1 \; |p_2\rangle_2 \ldots \; |p_N\rangle_N\right).$$

   How many terms in the sum are non-zero? What are their values?

   (b) Using the above information and the actual values of N_A and N_B, calculate $\langle B|f_l|A\rangle$. What is thus, the value of $\langle B|F^{(1)}|A\rangle$?

   (c) Repeat the above procedure to calculate the diagonal matrix element $\langle A|F^{(1)}|A\rangle$.

2. Consider the tight binding Hamiltonian on a 1D lattice

$$H = -t \sum_i a_i^\dagger a_{i+1} + \text{h.c.},$$

where h.c. denotes the Hermitian conjugate and i labels the lattice sites and $\{a_i\}$ and $\{a_i^\dagger\}$ are either bosonic or fermionic operators. In class we obtained the single particle energy band for this model. Now, assume that every alternate particle is moved a little to its left so that the hopping parameter is alternately $t + \epsilon$ and $t - \epsilon$.

   (a) What is the unit cell of the new lattice? What is the first Brillouin zone? How many bands of single particle states are there?

   (b) Calculate the band structure and show that you recover the original band structure for uniform hopping by taking the appropriate limit.

3. Define bosons whose creation and annihilation operators $\{a_i\}$ and $\{a_i^\dagger\}$ on a lattice (of sites labelled by i) obey the usual commutation relations

$$[a_i, a_j] = [a_i, a_j^\dagger] = 0, \; \forall i \neq j,$$

but whose occupancy at each site is restricted to a maximum of 1. Such bosons are called hard core bosons.

(a) Show that this implies that $[a_i, a_i^\dagger] \neq 1$ but $\{a_i, a_i^\dagger\} = 1$ in the allowed Fock space. Also, show that $a_i^2 = \left(a_i^\dagger\right)^2 = 0$.

(b) Thus, the operators defined are bosonic as far as the relation between pairs on different sites is concerned but fermionic for pairs on the same site. In 1D, it is possible to define a new set of operators $\{c_i\}$ in terms of $\{a_i\}$ and $\{a_i^\dagger\}$,

$$c_i = (-1)^{\phi_i} a_i,$$

where $\phi_i = \sum_{j<i} a_j^\dagger a_j$. Show that the operators $\{c_i\}$ and $\{c_i^\dagger\}$ satisfy the regular fermionic anticommutation relations.

(c) Now, consider the tight binding model for hard core bosons,

$$H = -t \sum_i a_i^\dagger a_{i+1} + \text{h.c.}$$

on an infinite 1D chain. Certain systems of bosons in optical lattices can be described by Hamiltonians similar to this. What is the ground state energy when the density of bosons is n? (*Hint: Express the operators* $\{a_i\}$ *and* $\{a_i^\dagger\}$ *in terms of* $\{c_i\}$ *and* $\{c_i^\dagger\}$. *What is* ϕ_i *in terms of* $\{c_i\}$ *and* $\{c_i^\dagger\}$*?*)

4. Consider the ground state of a non-interacting 3D gas of electrons with Fermi momentum k_F.

(a) The density operator

$$n_s(\mathbf{r}) = \Psi_s^\dagger(\mathbf{r})\Psi_s(\mathbf{r}),$$

where s is the spin and $\Psi_s^\dagger(\mathbf{r})$ and $\Psi_s(\mathbf{r})$ are the field operators defined in class. Calculate the following quantities: $\langle n_\uparrow(\mathbf{r})\rangle$, $\langle n_\downarrow(\mathbf{r})\rangle$, $\langle n_\uparrow(\mathbf{r})n_\uparrow(\mathbf{r'})\rangle$, $\langle n_\downarrow(\mathbf{r})n_\downarrow(\mathbf{r'})\rangle$ and $\langle n_\uparrow(\mathbf{r})n_\downarrow(\mathbf{r'})\rangle$, where $\langle \dots \rangle$ denotes the expectation value in the ground state. Why is $\langle n_\uparrow(\mathbf{r})n_\downarrow(\mathbf{r'})\rangle$ different from $\langle n_\uparrow(\mathbf{r})n_\uparrow(\mathbf{r'})\rangle$ and $\langle n_\downarrow(\mathbf{r})n_\downarrow(\mathbf{r'})\rangle$?

(b) With Coulomb interactions, the exact ground state is no longer like that of a non-interacting gas of electrons. Qualitatively, how do you expect the quantity $\langle n_\uparrow(\mathbf{r})n_\downarrow(\mathbf{r'})\rangle$ to be different in this case from what you calculated for the non-interacting system?

5. The density matrix in the grand canonical ensemble can be written as an operator in the occupation number formalism as

$$\rho = \frac{1}{\text{Tr}\left[e^{-\beta(H-\mu N)}\right]} e^{-\beta(H-\mu N)}.$$

Here N is the operator that counts the total number of particles in the system (the number operator), $\beta = 1/k_B T$, where T is the temperature and μ is the chemical potential.

(a) If the Hamiltonian

$$H = \sum_\alpha \epsilon_\alpha a_\alpha^\dagger a_\alpha,$$

where ϵ_α is the energy of a single particle state α, calculate the occupation $\langle n_\alpha \rangle$ when the particles are (i) bosons and (ii) fermions.

(b) Now suppose that the particles are spin 1/2 fermions and the Hamiltonian is

$$H = \sum_{\alpha,s} \epsilon_\alpha a_{\alpha,s}^\dagger a_{\alpha,s},$$

where s is the spin and can take on the values $\uparrow$ and $\downarrow$. Further, suppose that a given state α cannot simultaneously have an $\uparrow$ and $\downarrow$ electron. What is $\langle n_\alpha \rangle = \langle n_{\alpha,\uparrow} \rangle + \langle n_{\alpha,\downarrow} \rangle$? This sort of situation occurs for dopant levels of n type semiconductors.

Remember that for any operator A, $\langle A \rangle = \text{Tr}(\rho A)$.

6. It was shown in class that a general Hamiltonian with one and two body terms can be written as

$$H = \int d\mathbf{r}\Psi^\dagger(\mathbf{r})\left[-\frac{\hbar^2}{2m}\nabla^2 + U^{(1)}(\mathbf{r})\right]\Psi(\mathbf{r}) + \int d\mathbf{r}d\mathbf{r}'\Psi^\dagger(\mathbf{r})\Psi^\dagger(\mathbf{r}')U^{(2)}(\mathbf{r},\mathbf{r}')\Psi(\mathbf{r}')\Psi(\mathbf{r}),$$

where $\Psi^\dagger$ and Ψ are the field operators. We can define a time dependent version of $\Psi(\mathbf{r})$ as

$$\Psi(\mathbf{r},t) = e^{-iHt/\hbar}\Psi(\mathbf{r})e^{iHt/\hbar}.$$

(a) Derive the equation of motion for $\Psi(\mathbf{r},t)$ (i.e. calculate $\partial\Psi(\mathbf{r},t)/\partial t$) when the field operators are bosonic and fermionic. (*Hint: You will need to calculate commutators of the sort* $[AB,C]$ *and* $[ABCD,E]$ *where* A*,* B*,* C*,* D *and* E *are field operators. Express these commutators as sums of products of terms containing only commutators (in the bosonic case) or anticommutators (in the fermionic case) of two field operators.*)

(b) When there is only one particle, show that the equation of motion just gives you the regular Schrödinger equation

$$i\hbar\frac{\partial\psi(\mathbf{r},t)}{\partial t} = \left[\frac{-\hbar^2}{2m}\nabla^2 + U^{(1)}(\mathbf{r})\right]\psi(\mathbf{r},t),$$

where $\psi(\mathbf{r},t)$ is the wavefunction.