PHYSICS 320: Problem Set No. 1
Due: Wed. Sep. 1 2010

1. Consider a state

$$\Psi_m(\mathbf{r},\mathbf{R}) = \sum_n \phi_{mn}(\mathbf{R})\psi_n(\mathbf{r},\mathbf{R}),$$

of the system of ions and electrons. Here $\psi_n(\mathbf{r},\mathbf{R})$ is an eigenfunction of just the electronic part of the Hamiltonian. $\mathbf{R} = \{\mathbf{R}_i\}$ and $\mathbf{r} = \{\mathbf{r}_j\}$ are shorthand for the entire set of ionic and electronic coordinates respectively. The partial expectation value of the ionic kinetic energy in this state obtained by integrating only over the electronic coordinates has the following three terms:

$$T_m^{(1)}(\mathbf{R}) = -\frac{\hbar^2}{2M}\sum_n \left[\phi^*_{mn}(\mathbf{R})\sum_i \nabla^2_{\mathbf{R}_i}\phi_{mn}(\mathbf{R})\right],$$

$$T_m^{(2)}(\mathbf{R}) = -\frac{\hbar^2}{M}\sum_{n,p} \left[\phi^*_{mp}(\mathbf{R})\int d\mathbf{r}\ \psi^*_p(\mathbf{r},\mathbf{R})\sum_i \{\nabla_{\mathbf{R}_i}\phi_{mn}(\mathbf{R})\cdot\nabla_{\mathbf{R}_i}\psi_n(\mathbf{r},\mathbf{R})\}\right],$$

and

$$T_m^{(3)}(\mathbf{R}) = -\frac{\hbar^2}{2M}\sum_{n,p} \left[\phi^*_{mp}(\mathbf{R})\phi_{mn}(\mathbf{R})\int d\mathbf{r}\ \psi^*_p(\mathbf{r},\mathbf{R})\sum_i \nabla^2_{\mathbf{R}_i}\psi_n(\mathbf{r},\mathbf{R})\right].$$

$T_m^{(2)}(\mathbf{R})$ and $T_m^{(3)}(\mathbf{R})$ are the terms that are neglected in the Born-Oppenheimer approximation. Suppose $\psi_n(\mathbf{r},\mathbf{R}) \approx \psi_n(\mathbf{r}-\mathbf{R})$ is real.

(a) Show that sum of the diagonal terms in $\sum_{n,p}$ in the expression for $T_m^{(2)}(\mathbf{R})$ (i.e. terms with $n = p$) is zero.

(b) Show that the sum of the diagonal terms in $\sum_{n,p}$ in the expression for $T_m^{(3)}(\mathbf{R})$ gives a contribution that is proportional to m_e/M times the electronic kinetic energy. m_e is the mass of an electron.

The sum of the off-diagonal terms in $T_m^{(2)}(\mathbf{R})$ and $T_m^{(3)}(\mathbf{R})$ can also be argued to be smaller than $T_m^{(1)}(\mathbf{R})$ by powers of m_e/M but the arguments are more involved.

2. In this problem you will calculate the matrix element of a total single particle operator between bosonic occupation number states. As was shown 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. A total single particle 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) Show that $\langle B|F^{(1)}|A\rangle = 0$ for two occupation number states $|A\rangle$ and $|B\rangle$ if $|B\rangle$ is not the same state as $|A\rangle$ or cannot be obtained from it by moving one boson from single particle state k to state i.

(b) Now, consider $|A\rangle$ and $|B\rangle$ where the latter is obtained from the former by moving a boson from single particle state k to i. The two states are thus of the form

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

where N_A and N_B are the appropriate normalization factors and P_A and P_B, the appropriate sets of allowed values of the p_j's and p'_j's.
Consider a particular f_l and

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

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

(c) 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 $\langle B|F^{(1)}|A\rangle$?

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

3. Consider the Fock space of a single particle level of bosons.

(a) Show that the annihilation operator a in this space can have any complex eigenvalue α. What is the corresponding normalized eigenstate $|\alpha\rangle$ as a linear superposition of the occupation number states? What can be said about the eigenvalues and eigenstates of the creation operator $a^\dagger$?

(b) What is the probability $P_N(\alpha)$ of having N particles in the state $|\alpha\rangle$? What is the average number of particles in such a state and the uncertainty in the number of particles?

(c) Calculate $\langle\alpha'|\alpha\rangle$ for two states $|\alpha\rangle$ and $|\alpha'\rangle$. Why is this quantity not zero?

(d) Show that

$$\int \frac{d\alpha d\alpha^*}{2\pi i} e^{-|\alpha|^2} |\alpha\rangle\langle\alpha| = I,$$

where I is the identity operator of the Fock space and the integration is over the entire complex plane.

4. The Hamiltonian

$$H = \sum_i -t\left(c_i^\dagger c_{i+1} + \text{h.c.}\right) + \epsilon_i n_i,$$

describes fermions on a 1D lattice where n_i and ϵ_i are respectively the number of fermions and on-site energy at site i. Assume a lattice spacing a and periodic boundary conditions.

(a) Assume $\epsilon_i = \epsilon$, $\forall i$. What is the band structure? What is the first Brillouin zone? For which value(s) of the density of fermions is the system an insulator?

(b) Now, assume that $\epsilon_i = \epsilon_1$ for odd i and $\epsilon_i = \epsilon_2$ for even i. Calculate the band structure. What is the first Brillouin zone? In this case, for which value(s) of the density of fermions is the system an insulator?

(c) Set $\epsilon_1 = \epsilon_2$ in (b) and show that you recover the results of (a).

5. 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 $\langle\ldots\rangle$ 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?

6. Suppose there is a system of bosons such that two or more of them cannot occupy a single particle state. Such bosons are called hardcore bosons. Let the the creation and annihilation operators for hardcore bosons in single particle levels labelled by i be $\{b_i^\dagger\}$ and $\{b_i\}$ respectively. The bosonic nature of these particles is reflected by the fact that $[b_i, b_j] = [b_i, b_j^\dagger] = 0$, when $i \neq j$. They are also like fermions in the sense that no single particle state can have two or more of them.

   (a) Show that the complete algebra of $\{b_i^\dagger\}$ and $\{b_i\}$ is different from that of regular bosons or fermions by calculating $[b_i, b_i^\dagger]$, $\{b_i, b_j\}$ and $\{b_i, b_j^\dagger\}$.

   (b) Now, consider the following 1D tight binding model on a lattice with N sites.

$$H_b = -t \sum_i b_i^\dagger b_{i+1} + \text{h.c.}$$

   and

$$H_f = -t \sum_i c_i^\dagger c_{i+1} + \text{h.c.},$$

   where $\{b_i^\dagger\}$ and $\{b_i\}$ are hardcore bosonic operators and $\{c_i^\dagger\}$ and $\{c_i\}$ are fermionic operators. Assume periodic boundary conditions for both cases. Numerically diagonalize both Hamiltonians to obtain their energy spectra for $N = 4$ and number of particles $M = 1, 2$ and 3. It might help to use occupation numbers states for each site as basis states to write down the Hamiltonians as matrices that can then be diagonalized numerically.

   Even though for both hardcore bosons and fermions every site can have at most one particle, you should find a difference in the energy spectra for the two for some value(s) of M (which one(s)?). This is due to the difference in the algebra of creation and annihilation operators between the two cases.

   (c) Show that if we define new operators

$$\tilde{c}_i = (-1)^{\phi_i}\, b_i,$$

   $\{\tilde{c}_i^\dagger\}$ and $\{\tilde{c}_i\}$ obey the algebra for fermions, when $\phi_1 = 0$ and $\phi_i = \sum_{j<i} b_j^\dagger b_j$ for all other i.

   (d) Now, use the mapping from (c) to convert H_b into a Hamiltonian in terms of the operators $\{\tilde{c}_i^\dagger\}$ and $\{\tilde{c}_i\}$ for a general N. Show that the spectrum of eigenvalues of H_b is the same or different compared to H_f depending on whether the number of particles M is odd or even. *(Hint: Show that the boundary conditions on the fermions defined by $\{\tilde{c}_i^\dagger\}$ and $\{\tilde{c}_i\}$ are periodic or antiperiodic depending on whether M is odd or even.)*

   (e) Calculate the energy spectrum analytically for H_b and H_f for general N and M (you may leave the energy in terms of single particle energy eigenvalues and the occupation numbers of single particle levels). Show that the expressions that you get agree with the numerical answers for $N = 4$ and $M = 1, 2$ and 3 from (b).