QM1 - Exam Question 8

February 11, 2015

1. The Hamiltonian:

$$\mathcal{H}=\sum_{i,j=1}^{\infty}\left\langle i\left|h\right|j\right\rangle a_i^{\dagger}a_j+\frac{V_0}{2}\left(\sum_{j=1}^{\infty}a_j^{\dagger}a_j-N_0\right)^2 \tag{1}$$

Consider for a second a general 2nd quantization Hamiltonian:

$$\mathcal{H}=\sum_{i,j}\left\langle i\left|h\right|j\right\rangle a_i^{\dagger}a_j+\frac{1}{2}\sum_{ijkl}\left\langle ij\left|V\right|kl\right\rangle a_i^{\dagger}a_j^{\dagger}a_la_k \tag{2}$$

We are describing electrons in a potential well with interactions. In position basis we will have:

$$\begin{cases}h=-\frac{\hbar^2}{2m}\nabla^2+U\left(\vec{r}\right)\\ V=V\left(\left|\vec{r}-\vec{r}'\right|\right)\end{cases} \tag{3}$$

There are two length scales in the problem. The first is the width of the potential well, and the second is the length scale on which the interaction changes. If we assume that the potential well is very narrow with respect to the interaction scale, i.e. the electrons are confined to a very short range on which the interaction doesn't change much, we can approximate the interaction as a constant:

$$V\left(\left|\vec{r}-\vec{r}'\right|\right)\approx V_0 \tag{4}$$

We have seen in class that for the 2nd quantization Hamiltonian in position space is:

$$\mathcal{H}=\int d^3r\psi^{\dagger}\left(\vec{r}\right)h\left(\vec{r}\right)\psi\left(\vec{r}\right)+\frac{1}{2}\int d^3rd^3r'\psi^{\dagger}\left(\vec{r}\right)\psi^{\dagger}\left(\vec{r}'\right)V\left(\vec{r},\vec{r}'\right)\psi\left(\vec{r}'\right)\psi\left(\vec{r}\right) \tag{5}$$

Using (4):

$$\mathcal{H}=\int d^3r\psi^{\dagger}\left(\vec{r}\right)h\left(\vec{r}\right)\psi\left(\vec{r}\right)+\frac{1}{2}V_0\int d^3r\psi^{\dagger}\left(\vec{r}\right)\hat{N}\psi\left(\vec{r}\right)=\int d^3r\psi^{\dagger}\left(\vec{r}\right)h\left(\vec{r}\right)\psi\left(\vec{r}\right)+\frac{1}{2}V_0\int d^3r\psi^{\dagger}\left(\vec{r}\right)\hat{N}\psi\left(\vec{r}\right)=$$

$$=\int d^3r\psi^{\dagger}\left(\vec{r}\right)h\left(\vec{r}\right)\psi\left(\vec{r}\right)+\frac{1}{2}V_0\int d^3r\psi^{\dagger}\left(\vec{r}\right)\left[\psi\left(\vec{r}\right)\hat{N}-\psi\left(\vec{r}\right)\right]=\int d^3r\psi^{\dagger}\left(\vec{r}\right)h\left(\vec{r}\right)\psi\left(\vec{r}\right)+\frac{1}{2}V_0\hat{N}^2-\frac{1}{2}V_0\hat{N}=$$

$$=\int d^3r\psi^{\dagger}\left(\vec{r}\right)h\left(\vec{r}\right)\psi\left(\vec{r}\right)+\frac{1}{2}V_0\left(\hat{N}^2-\hat{N}\right)=\int d^3r\psi^{\dagger}\left(\vec{r}\right)h\left(\vec{r}\right)\psi\left(\vec{r}\right)+\frac{1}{2}V_0\left(\hat{N}-\frac{1}{2}\right)^2-\frac{1}{8}V_0=$$

$$= \int d^3 r \psi^\dagger(\vec{r}) h(\vec{r}) \psi(\vec{r}) + \frac{1}{2} V_0 \left(\int d^3 r \psi^\dagger(\vec{r}) \psi(\vec{r}) - \frac{1}{2} \right)^2 - \frac{1}{8} V_0 \tag{6}$$

where we have used:

$$\left[\hat{N}, \psi(\vec{r})\right] = \int d^3 r' \left[\psi^\dagger(\vec{r}') \psi(\vec{r}'), \psi(\vec{r})\right] = -\int d^3 r' \left[\{\psi(\vec{r}), \psi^\dagger(\vec{r}')\} \psi(\vec{r}') - \psi^\dagger(\vec{r}') \{\psi(\vec{r}), \psi(\vec{r}')\}\right] = -\int d^3 r' \delta\left(\vec{r} - \vec{r'}\right) \psi(\vec{r}') = -\psi(\vec{r}) \tag{7}$$

If we go back now to a general base, and omit the constant term, we get:

$$\boxed{\mathcal{H} = \sum_{ij} h_{ij} a_i^\dagger a_j + \frac{1}{2} V_0 \left(\sum_j a_j^\dagger a_j - \frac{1}{2} \right)^2} \tag{8}$$

Notice that this is very similar to our given Hamiltonian with $N_0 = \frac{1}{2}$! The given Hamiltonian is a similar approximation of electrons in a very narrow potential well with coulomb repulsion between them!
To find the ground state we need to diagonalize the Hamiltonian. Notice that changing bases to the base that diagonalizes h also diagonalizes the rest of $\mathcal{H}$:

$$\sum_{n,m=1}^{\infty} \sum_{i,j=1}^{\infty} \langle i|n\rangle \langle n|h|m\rangle \langle m|j\rangle a_i^\dagger a_j = \sum_{n,m=1}^{\infty} \epsilon_n \delta_{nm} \left[\sum_i \psi_n(i) a_i^\dagger\right] \left[\sum_j \psi_m^*(j) a_j\right] = \sum_n \epsilon_n b_n^\dagger b_n$$

$$\Rightarrow \begin{cases} b_n^\dagger = \sum_i \langle i|n\rangle a_i^\dagger = \sum_i \psi_n(i) a_i^\dagger \\ b_n = \sum_i \langle i|n\rangle^* a_i = \sum_i \psi_n^*(i) a_i \end{cases} \tag{9}$$

The reverse transformation is:

$$\Rightarrow \begin{cases} a_i^\dagger = \sum_n \langle i|n\rangle^* b_n^\dagger = \sum_n \psi_n^*(i) b_n^\dagger \\ a_i = \sum_n \langle i|n\rangle b_n = \sum_n \psi_n(i) b_n \end{cases} \tag{10}$$

In this base the Hamiltonian is:

$$\mathcal{H} = \sum_n \epsilon_n b_n^\dagger b_n + \frac{V_0}{2} \left(\sum_{n=1}^{\infty} b_n^\dagger b_n - N_0 \right)^2 = \sum_n \epsilon_n \hat{N}_n + \frac{V_0}{2} \left(\hat{N} - N_0\right)^2 \tag{11}$$

Consider the following M fermion state:

$$|\chi\rangle = \prod_{i=1}^{M} b_{n_i}^\dagger |0\rangle = b_{n_1}^\dagger b_{n_2}^\dagger \cdots b_{n_M}^\dagger |0\rangle \tag{12}$$

It's energy is given by:

$$\mathcal{H} |\chi\rangle = \left[\sum_{n_i} \epsilon_{n_i} + \frac{V_0}{2} (M - N_0)^2 \right] |\chi\rangle \tag{13}$$

$$\boxed{E_{\{n_i\}_{i=1}^M} = \sum_{n_i} \epsilon_{n_i} + \frac{V_0}{2} (M - N_0)^2} \tag{14}$$

The minimal $E_{\{n_i\}_{i=1}^{M}}$ is obtained when the M lowest energy single particle states are occupied. Assuming that $\epsilon_1 \leq \epsilon_2 \leq \cdots \leq \epsilon_n$, this will be:

$$\boxed{E_{gs} = \sum_{n=1}^{M} \epsilon_n + \frac{V_0}{2} \left(M - N_0\right)^2} \tag{15}$$

The ground state is therefore:

$$\boxed{|\chi\rangle = \prod_{i=1}^{M} b_i^\dagger |0\rangle = b_1^\dagger b_2^\dagger \cdots b_M^\dagger |0\rangle = \sum_{j_1, j_2, \cdots, j_M = 1}^{\infty} \psi_1^* (j_1) \, \psi_2^* (j_2) \, \psi_1^* \cdots \psi_M^* (j_M) \, a_{j_1}^\dagger a_{j_2}^\dagger \cdots a_{j_M}^\dagger |0\rangle} \tag{16}$$

2. The time dependence of a_k is given by Heisenberg equation:

$$\frac{da_k}{dt} = \frac{i}{\hbar} \left[\mathcal{H}, a_k\right] = \frac{i}{\hbar} \left[\sum_{ij} h_{ij} a_i^\dagger a_j + \frac{1}{2} V_0 \left(\hat{N} - N_0\right)^2, a_k\right] =$$

$$= \frac{i}{\hbar} \sum_{ij} h_{ij} \left[a_i^\dagger a_j, a_k\right] + \frac{i}{\hbar} \frac{1}{2} V_0 \left[\hat{N}^2 - 2N_0 \hat{N} + N_0^2, a_k\right] =$$

$$= -\frac{i}{\hbar} \sum_{ij} h_{ij} \left[\left\{a_k, a_i^\dagger\right\} a_j - a_i^\dagger \left\{a_k, a_j\right\}\right] + \frac{i}{\hbar} \frac{1}{2} V_0 \left(\hat{N} \left[\hat{N}, a_k\right] + \left[\hat{N}, a_k\right] \hat{N}\right) - \frac{i}{\hbar} N_0 V_0 \left[\hat{N}, a_k\right] =$$

$$= -\frac{i}{\hbar} \sum_{ij} h_{ij} \delta_{ik} a_j - \frac{i}{\hbar} \frac{1}{2} V_0 \left(\hat{N} a_k + a_k \hat{N}\right) + \frac{i}{\hbar} N_0 V_0 a_k = -\frac{i}{\hbar} \sum_{ij} h_{ij} \delta_{ik} a_j - \frac{i}{\hbar} \frac{1}{2} V_0 \left(2\hat{N} a_k + a_k\right) + \frac{i}{\hbar} N_0 V_0 a_k =$$

$$= -\frac{i}{\hbar} \sum_{j} h_{kj} a_j - \frac{i}{\hbar} V_0 \left[\hat{N} - N_0 + \frac{1}{2}\right] a_k$$

$$\Rightarrow \boxed{\begin{cases} \frac{da_k}{dt} = -\frac{i}{\hbar} \sum_j h_{kj} a_j - \frac{i}{\hbar} V_0 \left[\hat{N} - N_0 + \frac{1}{2}\right] a_k \\ \frac{da_k^\dagger}{dt} = \frac{i}{\hbar} \sum_j a_j^\dagger h_{jk} + \frac{i}{\hbar} V_0 a_k^\dagger \left[\hat{N} - N_0 + \frac{1}{2}\right] \end{cases}} \tag{17}$$

These equations are coupled! In order to decouple and solve let's change bases to that of $b_n^\dagger, b_n$. Using (10) we obtain the following equations:

$$\sum_n \psi_n (k) \frac{db_n}{dt} = -\frac{i}{\hbar} \sum_j h_{kj} \sum_n \psi_n (j) \, b_n - \frac{i}{\hbar} V_0 \left[\hat{N} - N_0 + \frac{1}{2}\right] \sum_n \psi_n (k) \, b_n$$

Multiplying all equations by $\psi_l^* (k)$ and summing them (sum over k)

$$\Rightarrow \sum_k \sum_n \psi_n (k) \frac{db_n}{dt} \psi_l^* (k) = -\frac{i}{\hbar} \sum_k \sum_j h_{kj} \sum_n \psi_n (j) \, \psi_l^* (k) \, b_n - \frac{i}{\hbar} V_0 \left[\hat{N} - N_0 + \frac{1}{2}\right] \sum_k \sum_n \psi_n (k) \, \psi_l^* (k) \, b_n$$

$$\Rightarrow \sum_n \frac{db_n}{dt}\delta_{nl} = -\frac{i}{\hbar}\sum_k\sum_j\sum_n \langle l|k\rangle \langle k|h|j\rangle \langle j|n\rangle b_n - \frac{i}{\hbar}V_0\left[\hat{N} - N_0 + \frac{1}{2}\right]\sum_n \delta_{nl} b_n$$

$$\Rightarrow \frac{db_l}{dt} = -\frac{i}{\hbar}\sum_n \epsilon_n \delta_{nl} b_n - \frac{i}{\hbar}V_0\left[\hat{N} - N_0 + \frac{1}{2}\right] b_l \tag{18}$$

We finally obtain the following equations:

$$\Rightarrow \begin{cases} \frac{db_l}{dt} = -\frac{i}{\hbar}\left[\epsilon_l + V_0\left(\hat{N} - N_0 + \frac{1}{2}\right)\right] b_l \\ \frac{db_l^\dagger}{dt} = \frac{i}{\hbar} b_l^\dagger \left[\epsilon_l + V_0\left(\hat{N} - N_0 + \frac{1}{2}\right)\right] \end{cases} \tag{19}$$

Their solutions are:

$$\boxed{\begin{cases} b_l(t) = exp\left[-\frac{i}{\hbar}\left(\epsilon_l + V_0\left(\hat{N} - N_0 + \frac{1}{2}\right)\right)t\right] b_l(0) \\ b_l^\dagger(t) = b_l^\dagger(0)\, exp\left[\frac{i}{\hbar}\left(\epsilon_l + V_0\left(\hat{N} - N_0 + \frac{1}{2}\right)\right)t\right] \end{cases}} \tag{20}$$

And we can return to the original ladder operator using (10):

$$\boxed{\begin{cases} a_i^\dagger(t) = \sum_n \psi_n^*(i)\, b_n^\dagger(0)\, exp\left[\frac{i}{\hbar}\left(\epsilon_n + V_0\left(\hat{N} - N_0 + \frac{1}{2}\right)\right)t\right] \\ a_i(t) = \sum_n \psi_n(i)\, exp\left[-\frac{i}{\hbar}\left(\epsilon_n + V_0\left(\hat{N} - N_0 + \frac{1}{2}\right)\right)t\right] b_n(0) \end{cases}} \tag{21}$$

Consider the following $|M\rangle$ with M particle state. In order to find the energy of $M+1$ particles we act with $b_n^\dagger$:

$$\mathcal{H} b_n^\dagger |M\rangle = \left(b_n^\dagger \mathcal{H} + \left[\mathcal{H}, b_n^\dagger\right]\right)|M\rangle = \left[b_n^\dagger E_M + b_n^\dagger\left(\epsilon_l + V_0\left(\hat{N} - N_0 + \frac{1}{2}\right)\right)\right]|M\rangle =$$

$$= b_n^\dagger\left(E_M + \epsilon_l + V_0\left(M - N_0 + \frac{1}{2}\right)\right)|M\rangle = b_n^\dagger\left[E_M + \epsilon_n + V_0 M - V_0 N_0 + \frac{1}{2}V_0\right]|M\rangle \tag{22}$$

Notice that we have assumed that there was no occupancy at the mode n (otherwise this will be zero). We find that the state $b_n^\dagger|M\rangle$ is an eigenstate of $\mathcal{H}$ with energy:

$$\boxed{E_{M+1} = E_M + \epsilon_n + V_0 M - V_0 N_0 + \frac{1}{2}V_0 \Rightarrow E_{M+1} - E_M = \epsilon_n + V_0 M - V_0 N_0 + \frac{1}{2}V_0} \tag{23}$$

In the same way:

$$b_l(t)|M\rangle = exp\left[-\frac{i}{\hbar}\left(\epsilon_l + V_0\left(\hat{N} - N_0 + \frac{1}{2}\right)\right)t\right] b_l(0)|M\rangle = exp\left[-\frac{i}{\hbar}\left(\epsilon_l + V_0\left(M - 1 - N_0 + \frac{1}{2}\right)\right)t\right]|M-1\rangle$$

$$\mathcal{H} b_n|M\rangle = \left(b_n\mathcal{H} + [\mathcal{H}, b_n]\right)|M\rangle = \left[b_n E_M - \left[\epsilon_l + V_0\left(\hat{N} - N_0 + \frac{1}{2}\right)\right]b_n\right]|M\rangle == \left[b_n E_M - \epsilon_n - V_0\left(b_n\hat{N} - b_n\right) + b_n N_0 V_0 - \frac{1}{2}V_0 b_n\right]|M\rangle =$$

$$= b_n\left(E_M - \epsilon_n - V_0\left(\hat{N} - 1 - N_0 + \frac{1}{2}\right)\right)|M\rangle = b_n\left[E_M - \epsilon_n - V_0\left(M - 1 - N_0 + \frac{1}{2}\right)\right]|M\rangle \tag{24}$$

$$\Rightarrow \boxed{E_{M-1} = E_M - \epsilon_n - V_0\left(M-1\right) + V_0 N_0 - \frac{1}{2}V_0 \Rightarrow E_M - E_{M-1} = \epsilon_n + V_0\left(M-1\right) - V_0 N_0 + \frac{1}{2}V_0} \tag{25}$$

As for the energies of states with M particles given by excitations of $a_i^\dagger$:

$$|\psi\rangle = \prod_{j=1}^{\infty} a_{i_j}^\dagger |0\rangle \tag{26}$$

These state do not have defined energies, as they are not eigenstates of the 2nd quantization Hamiltonian! However, using their form in the base of $b_n^\dagger$ and b_n we can find the energy distribution, expectation values etc.

3. Again the Heisenberg equation is:

$$\frac{da_k^\dagger a_i}{dt} = \frac{i}{\hbar}\left[\mathcal{H}, a_k^\dagger a_i\right] = \frac{i}{\hbar}\left(a_k^\dagger\left[\mathcal{H}, a_i\right] + \left[\mathcal{H}, a_k^\dagger\right]a_i\right) = \frac{i}{\hbar}\left[a_k^\dagger\left(-i\hbar\dot{a}_i\right) + \left(-i\hbar\dot{a}_k^\dagger\right)a_i\right] =$$

$$= a_k^\dagger\dot{a}_i + \dot{a}_k^\dagger a_i = a_k^\dagger\left(-\frac{i}{\hbar}\sum_j h_{ij}a_j - \frac{i}{\hbar}V_0\left[\hat{N} - N_0 + \frac{1}{2}\right]a_i\right) + \left(\frac{i}{\hbar}\sum_j a_j^\dagger h_{kj} + \frac{i}{\hbar}V_0 a_k^\dagger\left[\hat{N} - N_0 + \frac{1}{2}\right]\right)a_i \tag{27}$$

Again we want to change bases, and find the time evolution of $b_m^\dagger b_n$ etc. (perhaps if this is in the test we should do all this work, however...). We can also just look at this:

$$\mathcal{H}b_m^\dagger b_n|M\rangle = \left(b_m^\dagger b_n\mathcal{H} + \left[\mathcal{H}, b_m^\dagger b_n\right]\right)|M\rangle = \left(b_m^\dagger b_n E_M + b_m^\dagger\left[\mathcal{H}, b_n\right] + \left[\mathcal{H}, b_m^\dagger\right]b_n\right) =$$

$$= \left(b_m^\dagger b_n E_M - b_m^\dagger\left(\left[\epsilon_n + V_0\left(\hat{N} - N_0 + \frac{1}{2}\right)\right]b_n\right) + \left(b_m^\dagger\left[\epsilon_m + V_0\left(\hat{N} - N_0 + \frac{1}{2}\right)\right]\right)b_n\right)|M\rangle =$$

$$= \left[b_m^\dagger b_n E_M - b_m^\dagger b_n\left(\epsilon_n - \epsilon_m\right)\right]|M\rangle = \left[E_M - \left(\epsilon_n - \epsilon_m\right)\right]b_m^\dagger b_n|M\rangle \tag{28}$$

4. The Hamiltonian in some general single particle base:

$$\mathcal{H} = \sum_{i,j=1}^{\infty}\langle i|h|j\rangle d_i^\dagger d_j + \frac{V_0}{2}\left(\sum_{j=1}^{\infty} d_j^\dagger d_j - N_0\right)^2$$

Let's use the following trial-ket of HF:

$$|\xi\rangle = \prod_{i=1}^{M} d_{n_i}^\dagger|0\rangle \tag{29}$$

Namely we are guessing that the solution is multiplication state. The expectation value of the Hamiltonian is:

$$\langle\xi|\mathcal{H}|\xi\rangle = \langle\xi|\sum_{i,j=1}^{\infty}\langle i|h|j\rangle\delta_{ij}n_j + \frac{V_0}{2}\left(\sum_{i,j=1}^{\infty} d_j^\dagger d_j d_i^\dagger d_i - 2N_0\sum_{j=1}^{\infty} d_j^\dagger d_j + N_0^2\right)|\xi\rangle =$$

$$= \sum_i\langle i|h|i\rangle n_i + \frac{V_0}{2}\left(\langle\xi|\sum_{i,j=1}^{\infty} d_j^\dagger\left(\delta_{ij} - d_i^\dagger d_j\right)a_i|\xi\rangle - 2N_0 M + N_0^2\right) =$$

$$= \sum_{i}^{\infty} \langle i | h | i \rangle n_i + \frac{V_0}{2} \left(- \langle \xi | \sum_{i,j=1}^{\infty} d_j^\dagger d_i^\dagger d_j d_i | \xi \rangle - (2N_0 - 1) M + N_0^2 \right) =$$

$$= \sum_{i}^{\infty} \langle i | h | i \rangle n_i + \frac{V_0}{2} \left(M^2 - 2N_0 M + N_0^2 \right) \tag{30}$$

Let us now write this using the single particle base given by a_k:

$$\langle \xi | \mathcal{H} | \xi \rangle = \sum_{i,k,l} \phi_i (k) \langle k | h | l \rangle \phi_i^* (l) n_i + \frac{V_0}{2} \left(M^2 - 2N_0 M + N_0^2 \right)$$

$$\frac{\delta}{\delta \phi_n^* (m)} \left\{ \sum_{i,k,l} \phi_i (k) \langle k | h | l \rangle \phi_i^* (l) n_i + \frac{V_0}{2} \left(M^2 - 2N_0 M + N_0^2 \right) - \sum_{i,k} n_i \epsilon_i \phi_i (k) \phi_i^* (k) \right\} = 0$$

$$\Rightarrow \sum_{i,k,l} \phi_i (k) \langle k | h | l \rangle \delta_{in} \delta_{lm} n_i - \sum_{i,k} n_i \epsilon_i \phi_i (k) \delta_{ni} \delta_{mk} = 0$$

$$n_n \sum_{k} \phi_n (k) \langle k | h | m \rangle - n_n \epsilon_n \phi_i (m) = 0$$

$$\sum_{i} \phi_n (i) \langle i | h | j \rangle = \epsilon_n \phi_i (j) \tag{31}$$

This is the eigenvalue equation that we know that the single particle states that $b_n^\dagger$ and b_n create! Therefore, HF found the actual accrutate diagonalizing base of the entire Hamiltonian! This is to be expected since the accurate solution is of the form of the guessed trial function (i.e. also a multiplication state).

$$E_{HF} = \sum_{i} \epsilon_i n_i + \frac{V_0}{2} \left(M^2 - 2N_0 M + N_0^2 \right) \tag{32}$$

Notice that for $N_0 = \frac{1}{2}$

$$E_{HF} = \sum_{\mathrm{i}=1}^{M} \epsilon_{n_i} + \frac{V_0}{2} M (M-1) + \frac{1}{8} V_0 \tag{33}$$

$$E_M - E_{M-1} = \epsilon_n + V_0 (M-1)$$

$$\Rightarrow E_M = E_{M-1} + \epsilon_{n_1} + V_0 (M-1) = E_{M-2} + \epsilon_{n_2} + V_0 (M-2) + \epsilon_{n_1} + V_0 (M-1) = \sum_{\mathrm{i}=1}^{M} \epsilon_{n_i} + V_0 \sum_{\mathrm{i}=1}^{M-2} (M-i) =$$

$$= \sum_{\mathrm{i}=1}^{M} \epsilon_{n_i} + V_0 M (M-1) - V_0 M \left(\frac{M-1}{2} \right) + E_0 = \sum_{\mathrm{i}=1}^{M} \epsilon_{n_i} + \frac{V_0}{2} M (M-1) + E_0 \tag{34}$$

For $E_0 = \frac{1}{8} V_0$ they fully coincide!! notice that the sum is up to $M-2$ since when $M - M + 1 = 1$ we have one particle and it does not interact with itself.