Quantum Mechanics I - Problem Set 6

Idan Tamir

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1.

I will use the next identities for the following calculation

$$Fermions \to aa^\dagger = -a^\dagger a + \underbrace{\left\{a, a^\dagger\right\}}_{=1}$$

$$Bosons \to aa^\dagger = a^\dagger a + \underbrace{\left[a, a^\dagger\right]}_{=1}$$

a. We first generally expand the norm

$$\left|\sum_{ij} C_{ij} a_i^\dagger a_j^\dagger \left|0\right\rangle\right|^2 = \left|\sum_{ij} C_{ij} \left(a_j a_i\right)^\dagger \left|0\right\rangle\right|^2 = \sum_{ijkl} C_{ij}^* C_{kl} \left\langle 0 \left| a_j a_i a_k^\dagger a_l^\dagger \right| 0 \right\rangle$$

Since $\left[a_i, a_j^\dagger\right] = \left\{a_i, a_j^\dagger\right\} = \delta_{ij}$, and $a_i \left|0\right\rangle = 0 \; \forall i$ all the terms that have three or four different indices are zero.

$$= \sum_{i \neq j} \left[\left|C_{ij}\right|^2 \underbrace{\left\langle 0 \left| a_j a_i a_i^\dagger a_j^\dagger \right| 0 \right\rangle}_{(1)} + C_{ij}^* C_{ji} \underbrace{\left\langle 0 \left| a_j a_i a_j^\dagger a_i^\dagger \right| 0 \right\rangle}_{(2)} \right] + \sum_i \left|C_{ii}\right|^2 \underbrace{\left\langle 0 \left| a_i a_i a_i^\dagger a_i^\dagger \right| 0 \right\rangle}_{(3)}$$

Define η to be (-1) for fermions and $(+1)$ for bosons

$$(1) = \eta \left\langle 0 \left| a_j a_i^\dagger a_i a_j^\dagger \right| 0 \right\rangle + \left\langle 0 \left| a_j a_j^\dagger \right| 0 \right\rangle = \left\langle 0 \left| a_j a_i^\dagger a_j^\dagger a_i \right| 0 \right\rangle + \eta \left\langle 0 \left| a_j^\dagger a_j \right| 0 \right\rangle + \left\langle 0 \left| 1 \right| 0 \right\rangle = 1$$

$$(2) = \eta \left\langle 0 \left| a_j a_j^\dagger a_i a_i^\dagger \right| 0 \right\rangle = \left\langle 0 \left| a_j a_j^\dagger a_i^\dagger a_i \right| 0 \right\rangle + \eta \left\langle 0 \left| a_j a_j^\dagger \right| 0 \right\rangle = \eta$$

For fermion $(3) = 0$ because $\left(a_i^\dagger\right)^2 \left|0\right\rangle = 0$, calculating for bosons

$$(3) = \left\langle 0 \left| a_i a_i^\dagger a_i a_i^\dagger \right| 0 \right\rangle + \left\langle 0 \left| a_i a_i^\dagger \right| 0 \right\rangle = \left\langle 0 \left| a_i a_i^\dagger a_i^\dagger a_i \right| 0 \right\rangle + 2 \left\langle 0 \left| a_i a_i^\dagger \right| 0 \right\rangle = 2$$

Now we can combine our calculation to get the final answer

$$\left|\sum_{ij} C_{ij} a_i^\dagger a_j^\dagger \left|0\right\rangle\right|^2 = \sum_{ij} \left(\left|C_{ij}\right|^2 + \eta C_{ij}^* C_{ji}\right)$$

b. For fermions we need to demand $i \neq j \neq k$ to get a state which is not zero. In this case

$$\left| a_i^\dagger a_j^\dagger a_k^\dagger \left|0\right\rangle \right|^2 = \left\langle 0 \left| a_k a_j a_i a_i^\dagger a_j^\dagger a_k^\dagger \right| 0 \right\rangle = \left\langle 0 \left| a_k a_j a_j^\dagger a_k^\dagger \right| 0 \right\rangle = \left\langle 0 \left| a_k a_k^\dagger \right| 0 \right\rangle = 1$$

For bosons

$$\left| a_i^\dagger a_j^\dagger a_k^\dagger \left|0\right\rangle \right|^2 = \left\langle 0 \left| a_k a_j a_i^\dagger a_i a_j^\dagger a_k^\dagger \right| 0 \right\rangle (\delta_{ij} + \delta_{ik}) + \left\langle 0 \left| a_k a_j a_j^\dagger a_k^\dagger \right| 0 \right\rangle$$

$$= \left\langle 0 \left| a_k a_j a_i^\dagger a_j^\dagger a_i a_k^\dagger \right| 0 \right\rangle \delta_{ij}\delta_{ik} + \left\langle 0 \left| a_k a_j a_i^\dagger a_k^\dagger \right| 0 \right\rangle \delta_{ij} + \left\langle 0 \left| a_k a_j a_i^\dagger a_j^\dagger \right| 0 \right\rangle \delta_{ik} + \left\langle 0 \left| a_k a_j^\dagger a_j a_k^\dagger \right| 0 \right\rangle \delta_{jk} + \left\langle 0 \left| a_k a_k^\dagger \right| 0 \right\rangle$$

$$= \left\langle 0 \left| a_k a_j a_i^\dagger a_j^\dagger \right| 0 \right\rangle \delta_{ij}\delta_{ik} + \left\langle 0 \left| a_k a_k^\dagger \right| 0 \right\rangle \delta_{ij} + \left\langle 0 \left| a_j a_j^\dagger \right| 0 \right\rangle \delta_{ik} + \left\langle 0 \left| a_k a_j^\dagger \right| 0 \right\rangle \delta_{jk} + 1$$

$$= \left(\left\langle 0 \left| a_k a_i^\dagger a_j a_j^\dagger \right| 0 \right\rangle + \left\langle 0 \left| a_k a_j^\dagger \right| 0 \right\rangle \right) \delta_{ij}\delta_{ik} + \delta_{ij} + \delta_{ik} + \delta_{jk} + 1 = \left(\left\langle 0 \left| a_k a_i^\dagger \right| 0 \right\rangle + 1 \right) \delta_{ij}\delta_{ik} + \delta_{ij} + \delta_{ik} + \delta_{jk} + 1$$

$$\Rightarrow \left| a_i^\dagger a_j^\dagger a_k^\dagger \left|0\right\rangle \right|^2 = 2\delta_{ij}\delta_{ik} + \delta_{ij} + \delta_{ik} + \delta_{jk} + 1$$

"Sanity check" for $i = j = k$. Expect to get norm equals 6, and indeed

$$\left(a^\dagger\right)^3 \left|0\right\rangle = \left(a^\dagger\right)^2 \left|1\right\rangle = \sqrt{2} a^\dagger \left|2\right\rangle = \sqrt{6} \left|3\right\rangle$$

$$\Rightarrow \left| \left(a^\dagger\right)^3 \left|0\right\rangle \right|^2 = \left\langle 0 \left| 6 \right| 0 \right\rangle = 6 \checkmark$$

2.

$$H = \sum_\alpha \epsilon_\alpha a_\alpha^\dagger a_\alpha + \frac{1}{2} \sum_{\alpha\beta} \left(V_{\alpha\beta\alpha\beta} a_\alpha^\dagger a_\beta^\dagger a_\alpha a_\beta + V_{\alpha\beta\beta\alpha} a_\alpha^\dagger a_\beta^\dagger a_\beta a_\alpha \right)$$

a. It is obvious that this Hamiltonian is invariant under $a_\alpha \to e^{i\theta_\alpha} a_\alpha \, \forall \alpha$.

Claim: the generators of this symmetry are the number operators $\hat{n}_\alpha = a_\alpha^\dagger a_\alpha$.

Proof: for an infinitesimal change $a \to e^{i\varepsilon} a \approx a (1 + \epsilon)$. Make an infinitesimal change using the generator

$$a \to e^{-i\varepsilon\hat{n}} a e^{i\varepsilon\hat{n}} \approx (1 - i\varepsilon\hat{n}) \, a \, (1 + i\varepsilon\hat{n}) = a + \varepsilon \left[a, \hat{n}\right] = a (1 + \epsilon)$$

So $\hat{n}$ is indeed the generator of the symmetry.

We can now use the fact that the generator is related to a conserved quanta, in this case number of particles per state α, to diagonalize H in Fock states $\left|\{n_\alpha\}\right\rangle$.

$$H \left|\{n_\alpha\}\right\rangle = \left[\sum_\alpha \epsilon_\alpha n_\alpha + \frac{1}{2} \sum_{\alpha \neq \beta} \left(\eta V_{\alpha\beta\alpha\beta} a_\alpha^\dagger a_\alpha a_\beta^\dagger a_\beta + V_{\alpha\beta\beta\alpha} a_\alpha^\dagger a_\alpha a_\beta^\dagger a_\beta \right) + \sum_\alpha V_{\alpha\alpha\alpha\alpha} a_\alpha^\dagger a_\alpha^\dagger a_\alpha a_\alpha \right] \left|\{n_\alpha\}\right\rangle$$

$$H \left|\{n_\alpha\}\right\rangle = \left[\sum_\alpha \epsilon_\alpha n_\alpha + \frac{1}{2} \sum_{\alpha \neq \beta} \left(\eta V_{\alpha\beta\alpha\beta} n_\alpha n_\beta + V_{\alpha\beta\beta\alpha} n_\alpha n_\beta \right) + \left\{ \begin{array}{c} \sum_\alpha V_{\alpha\alpha\alpha\alpha} n_\alpha (n_\alpha - 1) \;\; bosons \\ 0 \; fermions \end{array} \right. \right] \left|\{n_\alpha\}\right\rangle$$

With the same definition for η as in q.1.

b.

Fermions

$$H=\underbrace{\sum_{\alpha}\epsilon_{\alpha}a_{\alpha}^{\dagger}a_{\alpha}}_{H_0}+\frac{1}{2}\sum_{\alpha\beta}\left(V_{\alpha\beta\alpha\beta}a_{\alpha}^{\dagger}a_{\beta}^{\dagger}a_{\alpha}a_{\beta}+V_{\alpha\beta\beta\alpha}a_{\alpha}^{\dagger}a_{\beta}^{\dagger}a_{\beta}a_{\alpha}\right)$$

Assume a product state $|\psi\rangle=A\prod_{k=1}^{N}b_{i_k}^{\dagger}|0\rangle\,;\ b_{i_k}\equiv\sum_{\alpha}c_{i_k}(\alpha)\,a_{\alpha},\ \left\langle 0\left|b_i b_j^{\dagger}\right|0\right\rangle=\delta_{ij}$, A is an anti-symmetric combination. There exists $d_{\alpha}(i)$ s.t. $a_{\alpha}=\sum_i d_{\alpha}(i)\,b_i$, rewrite H using $b_i, b_i^{\dagger}$

$$H=\sum_{\alpha}\sum_{ij}\epsilon_{\alpha}d_{\alpha}^{*}(i)\,d_{\alpha}(j)\,b_i^{\dagger}b_j+\frac{1}{2}\sum_{\alpha\beta}\sum_{ijkl}\left(V_{\alpha\beta\beta\alpha}d_{\alpha}^{*}(i)\,d_{\beta}^{*}(j)\,d_{\beta}(k)\,d_{\alpha}(l)\,b_i^{\dagger}b_j^{\dagger}b_k b_l+V_{\alpha\beta\alpha\beta}d_{\alpha}^{*}(i)\,d_{\beta}^{*}(j)\,d_{\alpha}(k)\,d_{\beta}(l)\,b_i^{\dagger}b_j^{\dagger}b_k b_l\right)$$

To calculate $\langle\psi|H|\psi\rangle$ first calculate

$$\left\langle\psi\left|b_i^{\dagger}b_j\right|\psi\right\rangle=\delta_{ij}n_i$$

$$\left\langle\psi\left|b_i^{\dagger}b_j^{\dagger}b_k b_l\right|\psi\right\rangle=n_k n_l\left(\delta_{jl}\delta_{ik}-\delta_{jk}\delta_{il}\right)$$

$$\Rightarrow\langle\psi|H|\psi\rangle=\sum_{\alpha}\sum_{i}\epsilon_{\alpha}\left|d_{\alpha}(i)\right|^2 n_i+\frac{1}{2}\sum_{\alpha\beta}\sum_{ij}\left[\begin{array}{c}V_{\alpha\beta\beta\alpha}\left(d_{\alpha}^{*}(i)\,d_{\beta}^{*}(j)\,d_{\beta}(i)\,d_{\alpha}(j)-\left|d_{\alpha}(i)\right|^2\left|d_{\beta}(j)\right|^2\right)\\+V_{\alpha\beta\alpha\beta}\left(\left|d_{\alpha}(i)\right|^2\left|d_{\beta}(j)\right|^2-d_{\alpha}^{*}(i)\,d_{\beta}^{*}(j)\,d_{\alpha}(j)\,d_{\beta}(i)\right)\end{array}\right]n_i n_j$$

Need to solve $\delta\left|\langle\psi|H|\psi\rangle-E|\psi|^2\right|=0$ for each $d_{\alpha}(i)$ with $n_i\neq 0$. Note that $E|\psi|^2=\sum E_i\left|d_{\alpha}(i)\right|^2 n_i$.

$$H.F.\rightarrow\ \epsilon_{\alpha}d_{\alpha}(i)+\sum_{\beta}\sum_{j}\left(V_{\alpha\beta\beta\alpha}-V_{\alpha\beta\alpha\beta}\right)\left(d_{\beta}^{*}(j)\,d_{\beta}(i)\,d_{\alpha}(j)-d_{\alpha}(i)\left|d_{\beta}(j)\right|^2\right)n_j=E_i d_{\alpha}(i)$$

We want a state $|\psi\rangle$ s.t. $\langle\psi|H_0|\psi\rangle=\sum_{i=1}^{N}\epsilon_i$. A good guess will be $b_i^{\dagger}=a_i^{\dagger}\Rightarrow d_{\alpha}(i)=\delta_{i\alpha}$. Using our guess in H.F. equation

$$\epsilon_i+\sum_{j}\left(V_{ijji}-V_{ijij}\right)n_j=E_i$$

Our guess solved H.F. equation with one particle energy E_i. So the „optimal" solution in this case is

$$|\psi\rangle=A\prod_{i=1}^{N}a_i^{\dagger}|0\rangle\,,\ E_{\psi}=\sum_{i=1}^{N}\left[\epsilon_i+\frac{1}{2}\sum_{j}\left(V_{ijji}-V_{ijij}\right)n_j\right]$$

I used the fact that the energy of a product state is the sum of energies of each state in the product. The $\frac{1}{2}$ before the second sum is to avoid double summing.

In this case we found that H.F. solved the problem exactly.

Bosons

Assume a product state $|\psi\rangle=\left(b_k^{\dagger}\right)^N|0\rangle\,;\ b_i\equiv\sum_{\alpha}c_i(\alpha)\,a_{\alpha}$. There exists $d_{\alpha}(i)$ s.t. $a_{\alpha}=\sum_i d_{\alpha}(i)\,b_i$, rewrite H using $b_i, b_i^{\dagger}$

$$H=\sum_{\alpha}\sum_{ij}\epsilon_{\alpha}d_{\alpha}^{*}\left(i\right)d_{\alpha}\left(j\right)b_{i}^{\dagger}b_{j}+\frac{1}{2}\sum_{\alpha\beta}\sum_{ijkl}\left(V_{\alpha\beta\beta\alpha}d_{\alpha}^{*}\left(i\right)d_{\beta}^{*}\left(j\right)d_{\beta}\left(k\right)d_{\alpha}\left(l\right)b_{i}^{\dagger}b_{j}^{\dagger}b_{k}b_{l}+V_{\alpha\beta\alpha\beta}d_{\alpha}^{*}\left(i\right)d_{\beta}^{*}\left(j\right)d_{\alpha}\left(k\right)d_{\beta}\left(l\right)b_{i}^{\dagger}b_{j}^{\dagger}b_{k}b_{l}\right)$$

To calculate $\langle\psi\left|H\right|\psi\rangle$ first calculate

$$\left\langle\psi\left|b_{i}^{\dagger}b_{j}\right|\psi\right\rangle=\delta_{ij}n_{i}=N\delta_{ij}\delta_{ik}$$

$$\left\langle\psi\left|b_{i}^{\dagger}b_{j}^{\dagger}b_{n}b_{l}\right|\psi\right\rangle=\left(N^{2}-N\right)\delta_{ij}\delta_{in}\delta_{il}\delta_{ik}$$

$$\Rightarrow\langle\psi\left|H\right|\psi\rangle=\sum_{\alpha}\epsilon_{\alpha}\left|d_{\alpha}\left(k\right)\right|^{2}N+\frac{1}{2}\sum_{\alpha\beta}\left[\begin{array}{c}V_{\alpha\beta\beta\alpha}\left(d_{\alpha}^{*}\left(k\right)d_{\beta}^{*}\left(k\right)d_{\beta}\left(k\right)d_{\alpha}\left(k\right)+\left|d_{\alpha}\left(k\right)\right|^{2}\left|d_{\beta}\left(k\right)\right|^{2}\right)\\+V_{\alpha\beta\alpha\beta}\left(\left|d_{\alpha}\left(k\right)\right|^{2}\left|d_{\beta}\left(k\right)\right|^{2}+d_{\alpha}^{*}\left(k\right)d_{\beta}^{*}\left(k\right)d_{\alpha}\left(k\right)d_{\beta}\left(k\right)\right)\end{array}\right]\left(N^{2}-N\right)$$

Need to solve $\delta\left|\langle\psi\left|H\right|\psi\rangle-E\left|\psi\right|^{2}\right|=0$ for each $d_{\alpha}\left(i\right)$ with $n_{i}\neq0$ (only $i=k$ in this case). Note that $E\left|\psi\right|^{2}=E_{k}\left|d_{\alpha}\left(k\right)\right|^{2}n_{k}$.

$$G.P.\rightarrow\ \epsilon_{k}d_{\alpha}\left(k\right)+\sum_{\beta}\left(V_{\alpha\beta\beta\alpha}+V_{\alpha\beta\alpha\beta}\right)d_{\alpha}\left(k\right)\left|d_{\beta}\left(k\right)\right|^{2}\left(N-1\right)=E_{k}d_{\alpha}\left(k\right)$$

Again guess $b_{k}^{\dagger}=a_{k}^{\dagger}\Rightarrow d_{\alpha}\left(k\right)=\delta_{k\alpha}$. Using our guess in G.P. equation

$$\epsilon_{k}+V_{kkkk}\left(N-1\right)=E_{k}$$

Our guess solved H.F. equation with one particle energy E_{k}. So the „optimal" solution in this case is

$$\left|\psi\right\rangle=\prod_{i=1}^{N}a_{k}^{\dagger}\left|0\right\rangle,\ E_{\psi}=N\left[\epsilon_{k}+\left(N-1\right)V_{kkkk}\right]$$

In this case we found that G.P. didn't solve the problem exactly, it neglected all the options with different particles.

c. Using Heisenberg equations of motion $\dot{A}=\frac{i}{\hbar}\left[H,A\right]$ for the creation and annihilation operators we get

$$\dot{a}_{k}=\frac{i}{\hbar}\sum_{\alpha}\epsilon_{\alpha}\left[a_{\alpha}^{\dagger}a_{\alpha},a_{k}\right]+\frac{i}{2\hbar}\sum_{\alpha\neq\beta}\left(V_{\alpha\beta\alpha\beta}\left[a_{\alpha}^{\dagger}a_{\beta}^{\dagger}a_{\alpha}a_{\beta},a_{k}\right]+V_{\alpha\beta\beta\alpha}\left[a_{\alpha}^{\dagger}a_{\beta}^{\dagger}a_{\beta}a_{\alpha},a_{k}\right]\right)$$

$$\dot{a}_{k}=\frac{i}{\hbar}\sum_{\alpha}\epsilon_{\alpha}\left[\hat{n}_{\alpha},a_{k}\right]+\frac{i}{2\hbar}\sum_{\alpha\neq\beta}\left(V_{\alpha\beta\beta\alpha}-V_{\alpha\beta\alpha\beta}\right)\left[\hat{n}_{\alpha}\hat{n}_{\beta},a_{k}\right]$$

Using $\left[AB,C\right]=A\left\{B,C\right\}-\left\{A,C\right\}B\Rightarrow\left[\hat{n}_{\alpha},a_{k}\right]=a_{\alpha}^{\dagger}\left\{a_{\alpha},a_{k}\right\}-\left\{a_{\alpha}^{\dagger},a_{k}\right\}a_{\alpha}=-\delta_{\alpha k}a_{\alpha}$

$$\dot{a}_{k}=-\frac{i}{\hbar}\epsilon_{k}a_{k}+\frac{i}{2\hbar}\sum_{\alpha\neq\beta}\left(V_{\alpha\beta\beta\alpha}-V_{\alpha\beta\alpha\beta}\right)\left(\hat{n}_{\alpha}\left[\hat{n}_{\beta},a_{k}\right]+\left[\hat{n}_{\alpha},a_{k}\right]\hat{n}_{\beta}\right)$$

$$\dot{a}_{k}=-\frac{i}{\hbar}\epsilon_{k}a_{k}+\frac{i}{2\hbar}\sum_{\alpha\neq\beta}\left(V_{\alpha\beta\alpha\beta}-V_{\alpha\beta\beta\alpha}\right)\left(\delta_{\alpha k}a_{\alpha}\hat{n}_{\beta}+\hat{n}_{\alpha}\delta_{\beta k}a_{\beta}\right)=\frac{i}{\hbar}\left[-\epsilon_{k}+\frac{1}{2}\sum_{\alpha\neq k}\underbrace{\left(V_{k\alpha k\alpha}-V_{k\alpha\alpha k}+V_{\alpha k\alpha k}-V_{\alpha kk\alpha}\right)}_{\equiv-U_{\alpha k}}\hat{n}_{\alpha}\right]a_{k}$$

$$a_k(t) = a_k exp\left\{-\frac{i}{\hbar}\left[\epsilon_k + \frac{1}{2}\sum_{\alpha\neq k} U_{\alpha k}\hat{n}_\alpha\right]\right\}$$

And in the same way (or simply by taking h.c. remembering that $\hat{n}_i^\dagger = \hat{n}_i$, $H^\dagger = H$) we get

$$a_k^\dagger(t) = a_k^\dagger exp\left\{\frac{i}{\hbar}\left[\epsilon_k + \frac{1}{2}\sum_{\alpha\neq k} U_{\alpha k}\hat{n}_\alpha\right]\right\}$$

If we rewrite H using $a_i(t), a_i^\dagger(t)$ we get the same H, so we can use the same wave functions and energy spectrum we found in a. Now let us calculate the energy difference of adding one particle to a given M particles Fock state $|\{n_k\}\rangle$

$$H = \sum_\alpha \epsilon_\alpha \hat{n}_\alpha + \frac{1}{2}\sum_{\alpha\neq\beta}\left(-V_{\alpha\beta\alpha\beta}\hat{n}_\alpha\hat{n}_\beta + V_{\alpha\beta\beta\alpha}\hat{n}_\alpha\hat{n}_\beta\right)$$

$$Ha_l^\dagger(t)|\{n_k\}\rangle = Ha_k^\dagger exp\left\{\frac{i}{\hbar}\left[\epsilon_k + \frac{1}{2}\sum_{\alpha\neq k} U_{\alpha k}\hat{n}_\alpha\right]\right\}|\{n_k\}\rangle$$

Using the fact that $[H, \hat{n}_\alpha] = 0$, $\forall\alpha$

$$= exp\left\{\frac{i}{\hbar}\left[\epsilon_l + \frac{1}{2}\sum_{\alpha\neq l} U_{\alpha l}\hat{n}_\alpha\right]\right\} Ha_l^\dagger|\{n_k\}\rangle = exp\left\{\frac{i}{\hbar}\left[\epsilon_l + \frac{1}{2}\sum_{\alpha\neq l} U_{\alpha l}\hat{n}_\alpha\right]\right\}\left(a_l^\dagger H + \left[H, a_l^\dagger\right]\right)|\{n_k\}\rangle$$

$$= a_l^\dagger(t)\left[E_{\{n_k\}} + \left(\epsilon_l + \frac{1}{2}\sum_{\alpha\neq l} U_{\alpha l}\hat{n}_\alpha\right)\right]|\{n_k\}\rangle = E\left(a_l^\dagger(t)|\{n_k\}\rangle\right)$$

So the energy of adding one particle is $\Delta E = \epsilon_l + \frac{1}{2}\sum_{\alpha\neq l}\left(V_{\alpha kk\alpha} - V_{k\alpha k\alpha} + V_{k\alpha\alpha k} - V_{\alpha k\alpha k}\right)n_\alpha$.

From H.F. we know that the energy of one particle state is $\Delta E = \epsilon_i + \sum_j\left(V_{ijji} - V_{ijij}\right)n_j$. So if V is real (so also symmetric due to the Hamiltonian hermiticity) the energy due to adding one particle is the same as a one particle state energy calculated using the H.F. approximation.

In the same way, the energy difference of taking out a particle will be

$$Ha_l(t)|\{n_k\}\rangle = exp\left\{-\frac{i}{\hbar}\left[\epsilon_l + \frac{1}{2}\sum_{\alpha\neq l} U_{\alpha l}\hat{n}_\alpha\right]\right\}\left(a_l H + [H, a_l]\right)|\{n_k\}\rangle$$

$$= a_l(t)\left[E_{\{n_k\}} - \left(\epsilon_l + \frac{1}{2}\sum_{\alpha\neq l} U_{\alpha l}\hat{n}_\alpha\right)\right]|\{n_k\}\rangle \Rightarrow \Delta E = -\left(\epsilon_l + \frac{1}{2}\sum_{\alpha\neq l} U_{\alpha l} n_\alpha\right)$$

The same (but the sign) as for adding a particle.

3.

The Schrodinger equation for a single particle $\psi(r,t)$ in an external potential $U(r)$ is

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

Insert $\psi = \sqrt{\rho}e^{i\chi}$, $\chi, \rho \in \mathbb{R}$

$$i\hbar\left(\frac{1}{2\sqrt{\rho}}\frac{\partial\rho}{\partial t} + i\sqrt{\rho}\frac{\partial\chi}{\partial t}\right)e^{i\chi} = \left[-\frac{\hbar^2}{2m}\left(\frac{1}{2\sqrt{\rho}}\nabla^2\rho - \frac{1}{4\rho^{3/2}}\left(\nabla\rho\right)^2 + \sqrt{\rho}\left(i\nabla^2\chi - \left(\nabla\chi\right)^2\right) + \frac{i}{\sqrt{\rho}}\nabla\rho\nabla\chi\right) + U\left(r\right)\sqrt{\rho}\right]e^{i\chi}$$

Multiplying both sides by $e^{i\chi}\rho^{-1/2}$ to get

$$i\hbar\left(\frac{1}{2\rho}\frac{\partial\rho}{\partial t} + i\frac{\partial\chi}{\partial t}\right) = -\frac{\hbar^2}{2m}\left(\frac{1}{2\rho}\nabla^2\rho - \frac{1}{4\rho^2}\left(\nabla\rho\right)^2 + i\nabla^2\chi - \left(\nabla\chi\right)^2 + \frac{i}{\rho}\nabla\rho\cdot\nabla\chi\right) + U\left(r\right)$$

Demanding equality on both real and imaginary parts gives two equations

$$(1)\ \ \frac{1}{\rho}\frac{\partial\rho}{\partial t} = -\frac{\hbar}{m}\left(\nabla^2\chi + \frac{1}{\rho}\nabla\rho\cdot\nabla\chi\right)$$

$$(2)\ \ \hbar\frac{\partial\chi}{\partial t} = \frac{\hbar^2}{2m}\left(\frac{1}{2\rho}\nabla^2\rho - \frac{1}{4\rho^2}\left(\nabla\rho\right)^2 - \left(\nabla\chi\right)^2\right) - U\left(r\right)$$

Introduce the „velocity field" $v = \nabla\chi$ into (2)

$$\frac{\partial\rho}{\partial t} = -\frac{\hbar}{m}\left(\rho\nabla\cdot v + \nabla\rho\cdot v\right) = -\frac{\hbar}{m}\nabla\cdot\left(\rho v\right)$$

So if we define (naturally) $\frac{\hbar}{m}\rho v = j$ we got

$$\frac{\partial\rho}{\partial t} = -\nabla\cdot j$$

Now by taking $\nabla\left(1\right)$ we can write

$$(3)\ \ \hbar\frac{\partial v}{\partial t} = \nabla\left[\frac{\hbar^2}{4m}\left(\frac{1}{\rho}\nabla^2\rho - \frac{1}{2\rho^2}\left(\nabla\rho\right)^2 - v^2\right) - U\left(r\right)\right]$$

We can rewrite (3) as

$$\frac{\partial v}{\partial t} + \underbrace{\frac{\hbar}{m}v}_{\equiv u}\cdot\nabla v = \nabla\left[\frac{\hbar}{4m\sqrt{\rho}}\nabla\left(\frac{1}{\sqrt{\rho}}\nabla\rho\right) - \frac{1}{\hbar}U\left(r\right)\right]$$

Define $\nabla P = \rho\nabla\left[\frac{-\hbar^2}{4m^2\sqrt{\rho}}\nabla\left(\frac{1}{\sqrt{\rho}}\nabla\rho\right) + \frac{1}{m}U\left(r\right)\right]$ to get Euler equation

$$\rho\left(\frac{\partial}{\partial t} + u\cdot\nabla\right)u + \nabla P = 0$$

Need to verify that P as defined is well defined, will do so by integrating over all space

$$P = \int\rho\nabla\left[\frac{-\hbar^2}{4m^2}\nabla\left(\frac{1}{\rho}\nabla^2\rho - \frac{1}{2\rho^2}\left(\nabla\rho\right)^2\right) + \frac{1}{m}U\left(r\right)\right]dV$$

Using integration by parts to get

$$P = \int\frac{\hbar^2}{4m^2}\left(\frac{1}{\rho}\nabla^2\rho - \frac{1}{2\rho^2}\left(\nabla\rho\right)^2\right)\nabla\rho + \frac{1}{m}\int\rho\nabla U\left(r\right)dV = \int\frac{\hbar^2}{8m^2}\nabla\left(\frac{1}{\rho}\left(\nabla\rho\right)^2\right) + \frac{1}{m}\int\rho\nabla U\left(r\right)dV$$

$$\Rightarrow P = \frac{\hbar^2}{8m^2\rho}\left(\nabla\rho\right)^2 + \int\frac{\rho}{m}\nabla U\left(r\right)dV$$

So P we defined was OK. Defining $F \equiv -\nabla U$ the second term of the pressure looks like „regular" pressure and the $\hbar$ dependent part can be though as „quantum" pressure.

We saw that $\rho \,\&\, \nabla\chi$ can be though of as classical density and velocity that obey Euler equation of fluid mechanics by adding another „quantum" term to the pressure.

4.

a. The time dependent Gross-Pitaevskii equation without external potential and short range two body interaction is

$$i\hbar\frac{\partial}{\partial t}\psi(\mathbf{r},t) = -\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r},t) + V_0\left|\psi(\mathbf{r},t)\right|^2\psi(\mathbf{r},t)$$

Inserting $\psi(\mathbf{r},t) = \sqrt{\rho(\mathbf{r},t)}e^{i\chi(\mathbf{r},t)}$ to GP and using the results from q.3

$$i\hbar\left(\frac{1}{2\rho}\frac{\partial\rho}{\partial t} + i\frac{\partial\chi}{\partial t}\right) = -\frac{\hbar^2}{2m}\left(\frac{1}{2\rho}\nabla^2\rho - \frac{1}{4\rho^2}(\nabla\rho)^2 + i\nabla^2\chi - (\nabla\chi)^2 + \frac{i}{\rho}\nabla\rho\cdot\nabla\chi\right) + V_0\rho$$

$$(1)\quad \frac{\partial\rho}{\partial t} = -\frac{\hbar}{m}\left(\rho\nabla^2\chi + \nabla\rho\cdot\nabla\chi\right)$$

$$(2)\quad \frac{\partial\chi}{\partial t} = \frac{\hbar}{2m}\left(\frac{1}{2\rho}\nabla^2\rho - \frac{1}{4\rho^2}(\nabla\rho)^2 - (\nabla\chi)^2\right) - \frac{V_0}{\hbar}\rho$$

To show that ρ,χ are canonical variables we need to write the Hamiltonian explicitly

$$H = \int d^3x\psi^*\left(-\frac{\hbar^2}{2m}\nabla^2 + V_0|\psi|^2\right)\psi = \int d^3x\left[\psi^*\frac{-\hbar^2}{2m}\nabla^2\psi + \frac{V_0}{2}|\psi|^4\right]$$

Integration by part yields

$$H = \int d^3x\left[\frac{\hbar^2}{2m}\nabla\psi^*\nabla\psi + \frac{V_0}{2}|\psi|^4\right]$$

$$\nabla\psi = \left(\frac{1}{2\sqrt{\rho}}\nabla\rho + \sqrt{\rho}i\nabla\chi\right)e^{i\chi} \Rightarrow \nabla\psi^*\nabla\psi = \left(\frac{1}{4\rho}(\nabla\rho)^2 + \rho(\nabla\chi)^2\right)$$

So we can write H for ρ,χ

$$H = \int d^3x\left[\frac{\hbar^2}{2m}\left(\frac{1}{4\rho}(\nabla\rho)^2 + \rho(\nabla\chi)^2\right) + \frac{V_0}{2}\rho^2\right]$$

Taking the variation of H

$$\delta H = \int d^3x\left[\frac{\hbar^2}{2m}\left(\frac{1}{4(\rho+\delta\rho)}(\nabla(\rho+\delta\rho))^2 + (\rho+\delta\rho)(\nabla(\chi+\delta\chi))^2\right) + \frac{V_0}{2}(\rho+\delta\rho)^2\right] - H(\rho,\chi)$$

$$\delta H = \int d^3x\left[\frac{\hbar^2}{2m}\left\{\frac{1}{4\rho}\left(1-\frac{\delta\rho}{\rho}\right)\left((\nabla\rho)^2 + 2\nabla\rho\nabla(\delta\rho)\right) + (\rho+\delta\rho)\left((\nabla\chi)^2 + 2\nabla\chi\nabla(\delta\chi)\right)\right\} + \frac{V_0}{2}\left(\rho^2 + 2\rho\delta\rho\right)\right] - H(\rho,\chi)$$

Using integration by parts

$$\int\frac{1}{2\rho}\nabla\rho\nabla(\delta\rho) = -\int\nabla\left(\frac{1}{2\rho}\nabla\rho\right)\delta\rho = \int\left(\frac{1}{2\rho^2}(\nabla\rho)^2 - \frac{1}{2\rho}\nabla^2\rho\right)\delta\rho$$

$$\int 2\rho\nabla\chi\nabla\left(\delta\chi\right)=-\int 2\left(\nabla\rho\nabla\chi+\rho\nabla^{2}\chi\right)\delta\chi$$

We find

$$\delta H=\int d^{3}x\frac{\hbar^{2}}{2m}\left[\left(\frac{1}{4\rho^{2}}\left(\nabla\rho\right)^{2}-\frac{1}{2\rho}\nabla^{2}\rho+\left(\nabla\chi\right)^{2}+\frac{2mV_{0}}{\hbar^{2}}\rho\right)\delta\rho-2\left(\nabla\rho\nabla\chi+\rho\nabla^{2}\chi\right)\delta\chi\right]$$

Recall Hamilton equation of motion $\dot{q}=\frac{\delta H}{\delta p}$, $\dot{p}=-\frac{\delta H}{\delta q}$, so for $q\to\rho$, $q\to\chi$ we get

$$\frac{1}{\hbar}\frac{\delta H}{\delta\chi}=-\frac{\hbar}{m}\left(\nabla\rho\nabla\chi+\rho\nabla^{2}\chi\right)\underbrace{=}_{(1)}\dot{\rho}$$

$$-\frac{\delta H}{\delta\rho}=\hbar\left[\frac{\hbar}{2m}\left(\frac{1}{2\rho}\nabla^{2}\rho-\frac{1}{4\rho^{2}}\left(\nabla\rho\right)^{2}-\left(\nabla\chi\right)^{2}\right)-\frac{V_{0}}{\hbar}\rho\right]\underbrace{=}_{(2)}\hbar\dot{\chi}$$

Defining $\chi'=\hbar\chi\Rightarrow$

$$\dot{\rho}=\frac{\delta H}{\delta\chi'},\ \dot{\chi}'=-\frac{\delta H}{\delta\rho}$$

Looking for uniform stationary solution $(\nabla\chi'=\nabla\rho=0)$

$$\frac{\partial\rho}{\partial t}=0\Rightarrow\rho=\rho_{0};\ \frac{\partial\chi'}{\partial t}=-V_{0}\rho_{0}\Rightarrow\chi'=-V_{0}\rho_{0}t+\chi_{0}'$$

Using the time independent Hamiltonian

$$\underbrace{-\frac{\hbar^{2}}{2m}\nabla^{2}\psi\left(t\right)}_{=0}+V_{0}\left|\psi\left(t\right)\right|^{2}\psi\left(t\right)=E\psi\Rightarrow V_{0}\rho_{0}^{3/2}=E\rho_{0}^{1/2}$$

$$\rho=\rho_{0}=\frac{E}{V_{0}};\ \chi=-\frac{E}{\hbar}t+\chi_{0}$$

For small oscillations $\rho=\rho_{0}+\delta\rho$ $\chi=-\frac{E}{\hbar}t+\chi_{0}+\delta\chi$ the equations of motion (up to first order in $\delta\chi,\delta\rho$) take the form of

$$\frac{\partial\left(\delta\rho\right)}{\partial t}=-\frac{\hbar}{m}\left(\left(\rho_{0}+\delta\rho\right)\nabla^{2}\left(-\frac{E}{\hbar}t+\chi_{0}+\delta\chi\right)+\nabla\left(\left(\rho_{0}+\delta\rho\right)\right)\cdot\nabla\left(-\frac{E}{\hbar}t+\chi_{0}+\delta\chi\right)\right)$$

$$\Rightarrow\frac{\partial\left(\delta\rho\right)}{\partial t}=-\frac{\hbar E}{mV_{0}}\nabla^{2}\left(\delta\chi\right)$$

$$-\frac{E}{\hbar}+\frac{\partial\left(\delta\chi\right)}{\partial t}=\frac{\hbar}{2m}\left(\frac{1}{2\rho}\nabla^{2}\left(\delta\rho\right)\right)-\frac{V_{0}}{\hbar}\left(\rho_{0}+\delta\rho\right)$$

$$\Rightarrow\frac{\partial\left(\delta\chi\right)}{\partial t}=\frac{\hbar V_{0}}{4mE}\nabla^{2}\left(\delta\rho\right)-\frac{V_{0}}{\hbar}\delta\rho$$

We can decouple the equations by taking time derivatives

$$\frac{\partial^{2}\left(\delta\rho\right)}{\partial t^{2}}=-\frac{\hbar^{2}}{4m^{2}}\nabla^{2}\left(\nabla^{2}\left(\delta\rho\right)\right)+\frac{E}{m}\nabla^{2}\left(\delta\rho\right)$$

$$\frac{\partial^2(\delta\chi)}{\partial t^2} = -\frac{\hbar^2}{4m^2}\nabla^2\left(\nabla^2(\delta\chi)\right) + \frac{E}{m}\nabla^2(\delta\chi)$$

We found (the same) wave equation for $\delta\chi, \delta\rho$ with dispersion relation (calculated by solving using a plain wave)

$$\omega^2 = \frac{\hbar^2 k^4}{4m^2} + \frac{E}{m}k^2$$

Solving with waves $\delta\rho = acos(\mathbf{k}\cdot\mathbf{r} - \omega t)$, $\delta\chi = bsin(\mathbf{k}\cdot\mathbf{r} - \omega t)$ the original equations we find the relation between a and b.

$$\omega asin(\mathbf{k}\cdot\mathbf{r} - \omega t) = \frac{\hbar E k^2}{mV_0} bsin(\mathbf{k}\cdot\mathbf{r} - \omega t) \Rightarrow a = \frac{\hbar E k^2}{\omega m V_0} b$$

Taking the limit $k \to 0$ we find the dispersion relation is $\omega^2 \approx \frac{E}{m}k^2 \Rightarrow \omega \approx \sqrt{\frac{E}{m}}k$. In this approximation

$$\rho = \rho_0 + \delta\rho \approx \frac{E}{V_0} + acos\left(k\left(\hat{k}\cdot\mathbf{r} - \sqrt{\frac{E}{m}}t\right)\right) \approx \frac{E}{V_0} + a$$

$$\chi \approx -\frac{E}{\hbar}t + \chi_0 + bsin\left(k\left(\hat{k}\cdot\mathbf{r} - \sqrt{\frac{E}{m}}t\right)\right) \approx -\frac{E}{\hbar}t + \chi_0 + b\left(\mathbf{k}\cdot\mathbf{r} - \sqrt{\frac{E}{m}}kt\right)$$

$$\Rightarrow \psi(\mathbf{r}, t) = \sqrt{\frac{E}{V_0} + a}exp\left\{b\left(\mathbf{k}\cdot\mathbf{r} - \left(\sqrt{\frac{E}{m}}k - \frac{E}{\hbar}\right)t\right) + \chi_0\right\}$$

Since $k \to 0 \Rightarrow \lambda \to \infty$ so we see a long wave length oscillations in the phase.

From this we see that the uniform stationary solution was changed due to a small change of χ, i.e. the global gauge symmetry $\left(\psi \to e^{i\theta}\psi\right)$ is broken by the uniform solution.

In the non-interacting case ($V_0 = 0$) we will find that the wave equations for χ, ρ has a dispersion relation of the form $\omega = \frac{\hbar k^2}{2m}$. There will be no first order correction term to the phase which means that the global symmetry will be kept (at least for small changes of phase).

b. Adding a Coulomb interaction to the GP equation we get

$$i\hbar\frac{\partial}{\partial t}\psi(\mathbf{r}, t) = -\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r}, t) + V_0|\psi(\mathbf{r}, t)|^2\psi(\mathbf{r}, t) + \int d^3r'\left(\frac{q^2|\psi(\mathbf{r}', t)|^2}{|\mathbf{r} - \mathbf{r}'|} - \rho_N\right)\psi(\mathbf{r}, t)$$

I defined ρ_N such that the total charge of the system is zero i.e.

$$\int d^3r'\frac{q^2|\psi(\mathbf{r}', t)|^2}{|\mathbf{r} - \mathbf{r}'|} = \int d^3r'\rho_N$$

We can rewrite the equations for ρ, χ for this new case

$$(3)\quad \frac{\partial\rho}{\partial t} = -\frac{\hbar}{m}\left(\rho\nabla^2\chi + \nabla\rho\cdot\nabla\chi\right)$$

$$(4)\quad \frac{\partial\chi}{\partial t} = \frac{\hbar}{2m}\left(\frac{1}{2\rho}\nabla^2\rho - \frac{1}{4\rho^2}(\nabla\rho)^2 - (\nabla\chi)^2\right) - \frac{V_0}{\hbar}\rho - \frac{1}{\hbar}\int d^3r'\left(\frac{q^2\rho(\mathbf{r}', t)}{|\mathbf{r} - \mathbf{r}'|} - \rho_N\right)$$

Looking for uniform stationary solution ($\nabla\chi = \nabla\rho = 0$)

$$\rho = \rho_0,\, \chi = -\frac{V_0}{\hbar}\rho t - \underbrace{\frac{1}{\hbar}\int d^3r' \left(\frac{q^2\rho_0}{|\mathbf{r}-\mathbf{r}'|} - \rho_N\right)}_{=0} + \chi_0$$

The same as we found in a.

For small oscillations $\rho = \rho_0 + \delta\rho$ $\chi = -\frac{E}{\hbar}t + \chi_0 + \delta\chi$ the equations of motion (up to first order in $\delta\chi, \delta\rho$) take the form of

$$\frac{\partial\left(\delta\rho\right)}{\partial t} = -\frac{\hbar E}{mV_0}\nabla^2\left(\delta\chi\right)$$

$$\frac{\partial\left(\delta\chi\right)}{\partial t} = \frac{\hbar V_0}{4mE}\nabla^2\left(\delta\rho\right) - \frac{V_0}{\hbar}\delta\rho - \frac{q^2}{\hbar}\int d^3r'\frac{\delta\rho\left(\mathbf{r}'\right)}{|\mathbf{r}-\mathbf{r}'|}$$

Again we can decouple the equations by taking time derivatives

$$\frac{\partial^2\left(\delta\rho\right)}{\partial t^2} = -\frac{\hbar^2}{4m^2}\nabla^2\left(\nabla^2\left(\delta\rho\right)\right) + \frac{E}{m}\nabla^2\left(\delta\rho\right) - \frac{q^2E}{mV_0}\int d^3r'\underbrace{\nabla_r^2\left(\frac{1}{|\mathbf{r}-\mathbf{r}'|}\right)}_{=-4\pi\delta(r-r')}\delta\rho\left(\mathbf{r}'\right)$$

$$\frac{\partial^2\left(\delta\rho\right)}{\partial t^2} = -\frac{\hbar^2}{4m^2}\nabla^2\left(\nabla^2\left(\delta\rho\right)\right) + \frac{E}{m}\nabla^2\left(\delta\rho\right) + \frac{4\pi q^2E}{mV_0}\delta\rho$$

The new dispersion relation is then

$$\omega^2 = \frac{\hbar^2k^4}{4m^2} + \frac{E}{m}k^2 + \frac{4\pi q^2E}{mV_0}$$

For large enough k's the dispersion relation will be the same as the one in a. but for $k \to 0$ we get a constant frequency $\omega \approx \sqrt{\frac{4\pi E}{mV_0}}q \neq 0$. If we relate the frequency to energy using special relativity equation

$$\left(\hbar\omega\right)^2 = \left(\hbar kc\right)^2 + \left(m^*c^2\right)^2 \Rightarrow \omega\left(k=0\right) = \frac{c^2}{\hbar}m^* \Rightarrow m^* = \sqrt{\frac{4\pi E}{mV_0}}\frac{\hbar q}{c^2}$$

we can say that the interaction with the field added a mass term (m^*) to the field.