Quantum Mechanics III
HW 8

Matthew Phelps

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6.7 Consider Bosons as an example. By studying the expression $\hat{n}(\mathbf{R})\psi^\dagger(\mathbf{r})\left|0\right\rangle$, argue that the effect of the field operator $\psi^\dagger(\mathbf{r})$ on the vacuum is to put a boson in the point $\mathbf{r}$ in space. Multiple operators $\psi^\dagger$ with different position arguments obviously work analogously, but how about $\psi^\dagger(\mathbf{r})\psi^\dagger(\mathbf{r})$?

Expanding out the operators in terms of creation/annihilation operators in terms of orthonormal basis $\{u_k\}$

$$\begin{aligned}
\hat{n}(\mathbf{R})\psi^\dagger(\mathbf{r})\left|0\right\rangle &= \sum_{k_1,k_2,k_3} u^*_{k_3}(\mathbf{R})u_{k_2}(\mathbf{R})u^*_{k_1}(\mathbf{r})b^\dagger_{k_3}b_{k_2}b^\dagger_{k_1}\left|0\right\rangle \\
&= \sum_{k_1,k_2,k_3} u^*_{k_3}(\mathbf{R})u_{k_2}(\mathbf{R})u^*_{k_1}(\mathbf{r})b^\dagger_{k_3}\delta_{k_1,k_2}\left|0\right\rangle \\
&= \sum_{k_2,k_3} u^*_{k_3}(\mathbf{R})\Big(u_{k_2}(\mathbf{R})u^*_{k_2}(\mathbf{r})\Big)b^\dagger_{k_3}\left|0\right\rangle \\
&= \sum_{k_3} u^*_{k_3}(\mathbf{R})\delta(\mathbf{R}-\mathbf{r})b^\dagger_{k_3}\left|0\right\rangle \\
&= \delta(\mathbf{R}-\mathbf{r})\sum_{k} u^*_{k}(\mathbf{R})b^\dagger_{k}\left|0\right\rangle \\
&= \delta(\mathbf{R}-\mathbf{r})\psi^\dagger(\mathbf{R})\left|0\right\rangle.
\end{aligned}$$

Hence $\psi(\mathbf{r})\left|0\right\rangle$ is a non-zero eigenstate of the particle density operator only at $\mathbf{R}=\mathbf{r}$. Moreover, note that $b^\dagger_k\left|0\right\rangle = \left|u_k\right\rangle$ (a single particle state with all other u_k unoccupied) and contract the expression with the position eigenstate $\left\langle\mathbf{r}'\right|$

$$\begin{aligned}
\left\langle\mathbf{r}'\right|\psi^\dagger(\mathbf{r})\left|0\right\rangle &= \left\langle\mathbf{r}'\right|\sum_k u^*_k(\mathbf{r})b^\dagger_k\left|0\right\rangle \\
&= \sum_k u^*_k(\mathbf{r})\left\langle\mathbf{r}'|u_k\right\rangle \\
&= \sum_k u^*_k(\mathbf{r})u_k(\mathbf{r}') \\
&= \delta(\mathbf{r}-\mathbf{r}') \\
&= \left\langle\mathbf{r}'|\mathbf{r}\right\rangle
\end{aligned}$$

Thus $\psi^\dagger(\mathbf{r})\left|0\right\rangle$ represents a single localized state at position $\mathbf{r}$. If we take our basis $\{u_k\}$ as the eigenstates of momentum $\{\left|\mathbf{k}\right\rangle\}$ (quantized in a cubic box with periodic b.c.'s for example), we identity $\psi^\dagger(\mathbf{r})\left|0\right\rangle = \sum_{\mathbf{k}}\left\langle\mathbf{k}|\mathbf{r}\right\rangle\left|\mathbf{k}\right\rangle$ as the familiar Fourier expansion of the position operator in terms of momentum, viz. a localized state is a linear superposition of all momentum states.

As for the next part,

$$\hat{n}(\mathbf{r}')\psi^\dagger(\mathbf{r})\psi^\dagger(\mathbf{r})\left|0\right\rangle = \sum_{k_1,k_2,k_3,k_4} u^*_{k_4}(\mathbf{r}')u_{k_3}(\mathbf{r}')u^*_{k_2}(\mathbf{r})u^*_{k_1}(\mathbf{r})b^\dagger_{k_4}b_{k_3}b^\dagger_{k_2}b^\dagger_{k_1}\left|0\right\rangle$$

$$
\begin{aligned}
&= \sum_{k_1,k_2,k_3,k_4} u^*_{k_4}(\mathbf{r}')u_{k_3}(\mathbf{r}')u^*_{k_2}(\mathbf{r})u^*_{k_1}(\mathbf{r})b^\dagger_{k_4}(\delta_{k_2,k_3} + b^\dagger_{k_2}b_{k_3})b^\dagger_{k_1}\left|0\right\rangle \\
&= \sum_{k_1,k_2,k_3,k_4} u^*_{k_4}(\mathbf{r}')u_{k_3}(\mathbf{r}')u^*_{k_2}(\mathbf{r})u^*_{k_1}(\mathbf{r})b^\dagger_{k_4}\left(\delta_{k_2,k_3}b^\dagger_{k_1}\left|0\right\rangle + b^\dagger_{k_2}b_{k_3}b^\dagger_{k_1}\left|0\right\rangle\right) \\
&= \sum_{k_1,k_2,k_4} u^*_{k_4}(\mathbf{r}')u_{k_2}(\mathbf{r}')u^*_{k_2}(\mathbf{r})u^*_{k_1}(\mathbf{r})b^\dagger_{k_4}b^\dagger_{k_1}\left|0\right\rangle \\
&\quad + \sum_{k_1,k_2,k_4} u^*_{k_4}(\mathbf{r}')u_{k_1}(\mathbf{r}')u^*_{k_2}(\mathbf{r})u^*_{k_1}(\mathbf{r})b^\dagger_{k_4}b^\dagger_{k_2}\left|0\right\rangle \\
&= \delta(\mathbf{r}'-\mathbf{r})\sum_{k_1,k_4} u^*_{k_4}(\mathbf{r}')u^*_{k_1}(\mathbf{r})b^\dagger_{k_4}b^\dagger_{k_1}\left|0\right\rangle \\
&\quad + \delta(\mathbf{r}'-\mathbf{r})\sum_{k_2,k_4} u^*_{k_4}(\mathbf{r}')u^*_{k_2}(\mathbf{r})b^\dagger_{k_4}b^\dagger_{k_2}\left|0\right\rangle \\
&= 2\delta(\mathbf{r}'-\mathbf{r})\sum_{k_1,k_2} u^*_{k_2}(\mathbf{r}')u^*_{k_1}(\mathbf{r})b^\dagger_{k_2}b^\dagger_{k_1}\left|0\right\rangle \\
&= 2\delta(\mathbf{r}'-\mathbf{r})\psi^\dagger(\mathbf{r}')\psi^\dagger(\mathbf{r})\left|0\right\rangle
\end{aligned}
$$

We have formed an eigenstate of the particle density operator with eigenvalue 2 if and only if $\mathbf{r}' = \mathbf{r}$. This creates precisely two particles at position $\mathbf{r}$.

6.8 Consider a spin-0 Bose gas; for a multicomponent gas there are analogous results, but we do not go into this. Just as one may write the Heisenberg equation of motion for the field operator, one can do it also for the particle density operator $\hat{n}(\mathbf{r})$. Now, if it is possible to identify a many-body operator $\hat{\mathbf{j}}(\mathbf{r})$ in such a way that the equation of continuity $\frac{\partial}{\partial t}\hat{n}(\mathbf{r}) + \nabla\cdot\hat{\mathbf{j}}(\mathbf{r}) = 0$ is valid, $\hat{\mathbf{j}}(\mathbf{r})$ is evidently the quantum operator for the particle current density. Find it!

If we can find $\frac{d}{dt}\hat{n}$ then hopefully we can express this as a divergence of some vector quantity, thus finding the current density. Under second quantization, we may express our Hamiltonian

$$
H = \int d^3r\ \psi^\dagger(\mathbf{r})\left[-\frac{\hbar^2}{2m}\nabla^2 + U(\mathbf{r})\right]\psi(\mathbf{r}) + \frac{2\pi\hbar^2 a}{m}\int d^3r\ \psi^\dagger(\mathbf{r})\psi^\dagger(\mathbf{r})\psi(\mathbf{r})\psi(\mathbf{r}).
$$

We include the two body operator of the contact interaction model for added generality, though we will find it is independent of $\frac{d}{dt}\hat{n}$. Using the result derived in the script for $\frac{\partial}{\partial t}\psi(\mathbf{r})$ along with its conjugate

$$
\begin{aligned}
i\hbar\frac{\partial}{\partial t}(\psi^\dagger(\mathbf{r})\psi(\mathbf{r})) &= i\hbar\left(\frac{\partial}{\partial t}\psi^\dagger(\mathbf{r})\psi(\mathbf{r}) + \psi^\dagger(\mathbf{r})\frac{\partial}{\partial t}\psi(\mathbf{r})\right) \\
&= -\left[\frac{-\hbar^2}{2m}\nabla^2 + U(\mathbf{r})\right]\psi^\dagger(\mathbf{r})\psi(\mathbf{r}) - \frac{4\pi\hbar^2 a}{m}\psi^\dagger(\mathbf{r})\hat{n}^\dagger(\mathbf{r})\psi(\mathbf{r}) \\
&\quad + \psi^\dagger(\mathbf{r})\left[\frac{-\hbar^2}{2m}\nabla^2 + U(\mathbf{r})\right]\psi(\mathbf{r}) + \frac{4\pi\hbar^2 a}{m}\psi^\dagger(\mathbf{r})\hat{n}(\mathbf{r})\psi(\mathbf{r})
\end{aligned}
$$

†Since $U(\mathbf{r})$ commutes with the $\psi, \psi^\dagger$ operators and $\hat{n} = \hat{n}^\dagger$, this leaves us with

$$
i\hbar\frac{d}{dt}\hat{n} = -\frac{\hbar^2}{2m}\left[\psi^\dagger(\mathbf{r})\nabla^2\psi(\mathbf{r}) - (\nabla^2\psi^\dagger(\mathbf{r}))\psi(\mathbf{r})\right].
$$

This can be more symmetrically arranged by noting that ψ and $\psi^\dagger$ are both evaluated at $\mathbf{r}$, so their commutator vanishes

$$
i\hbar\frac{d}{dt}\hat{n} = -\frac{\hbar^2}{2m}\left[\psi^\dagger(\mathbf{r})\nabla^2\psi(\mathbf{r}) - \psi(\mathbf{r})\nabla^2\psi^\dagger(\mathbf{r})\right].
$$

We can express the right hand side in terms of a divergence

$$\nabla \cdot \left(\psi^\dagger(\mathbf{r})\nabla\psi(\mathbf{r}) - \psi(\mathbf{r})\nabla\psi^\dagger(\mathbf{r})\right) = \psi^\dagger(\mathbf{r})\nabla^2\psi(\mathbf{r}) - \psi(\mathbf{r})\nabla^2\psi^\dagger(\mathbf{r}).$$

Cross terms from the derivative cancel from again $[\psi(\mathbf{r}), \psi^\dagger(\mathbf{r})] = 0$. Thus the particle current density is

$$\hat{\mathbf{j}} = -\frac{i\hbar}{2m}\left(\psi^\dagger(\mathbf{r})\nabla\psi(\mathbf{r}) - \psi(\mathbf{r})\nabla\psi^\dagger(\mathbf{r})\right).$$

$^\dagger U(\mathbf{r})$ is actually just a scalar as a function of position. It originated in the integrand of the Hamiltonian and the actual operators reside in the fields $\psi \sim a_{\mathbf{k}}$ and $\psi^\dagger \sim a_{\mathbf{k}}^\dagger$.

6.10 In terms of plane-wave states labeled by the wave number $\mathbf{k}$, the Hamiltonian of a single-component Bose gas under the contact interaction model with scattering length a reads

$$H = \sum_k \epsilon_k b_{\mathbf{k}}^\dagger b_{\mathbf{k}} + \frac{2\pi\hbar^2 a}{mV} \sum_{\substack{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4 \\ \mathbf{k}_1+\mathbf{k}_2=\mathbf{k}_3+\mathbf{k}_4}} b_{\mathbf{k}_1}^\dagger b_{\mathbf{k}_2}^\dagger b_{\mathbf{k}_3} b_{\mathbf{k}_4}$$

In a noninteracting zero-temperature Bose-Einstein condensate all $N \gg 1$ atoms are in the state with $\mathbf{k} = 0$.

(a) Use perturbation theory to calculate the energy of the condensate to first order in the atom-atom interaction strength.

At $T = 0$, all N particles lie in the $\mathbf{k} = 0$ state, which can be expressed as the Fock state $|\psi\rangle$

$$|\psi\rangle = |N, 0, 0, ...\rangle.$$

Treating the gas nonrelativistically (appropriate for a finite number of N atoms with large masses), the dispersion relation is

$$\epsilon_k = \frac{\hbar^2 k^2}{2m}$$

and, consequently, the noninteracting contribution from the Hamiltonian is zero

$$H^0 |\psi\rangle = \epsilon_0 \hat{n}_0 |\psi\rangle = 0 \Rightarrow E^0 = 0.$$

However, taking the contact interaction as a perturbation, we have the first order correction to the energy

$$E^1 = \frac{2\pi\hbar^2 a}{mV} \sum_{\substack{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4 \\ \mathbf{k}_1+\mathbf{k}_2=\mathbf{k}_3+\mathbf{k}_4}} \langle\psi| b_{\mathbf{k}_1}^\dagger b_{\mathbf{k}_2}^\dagger b_{\mathbf{k}_3} b_{\mathbf{k}_4} |\psi\rangle = \sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4} \delta_{\mathbf{k}_1+\mathbf{k}_2,\mathbf{k}_3+\mathbf{k}_4} \langle\psi| b_{\mathbf{k}_1}^\dagger b_{\mathbf{k}_2}^\dagger b_{\mathbf{k}_3} b_{\mathbf{k}_4} |\psi\rangle$$

The expectation term

$$\langle\psi| b_{\mathbf{k}_1}^\dagger b_{\mathbf{k}_2}^\dagger b_{\mathbf{k}_3} b_{\mathbf{k}_4} |\psi\rangle = \langle ..., 0, 0, N || b_{\mathbf{k}_1}^\dagger b_{\mathbf{k}_2}^\dagger b_{\mathbf{k}_3} b_{\mathbf{k}_4} | N, 0, 0, ...\rangle$$

can only be nonzero given that

$$b_{\mathbf{k}_1}^\dagger b_{\mathbf{k}_2}^\dagger b_{\mathbf{k}_3} b_{\mathbf{k}_4} |\psi\rangle \to \delta_{\mathbf{k}_1,0}\delta_{\mathbf{k}_2,0}\delta_{\mathbf{k}_3,0}\delta_{\mathbf{k}_4,0} b_{\mathbf{k}_1}^\dagger b_{\mathbf{k}_2}^\dagger b_{\mathbf{k}_3} b_{\mathbf{k}_4} |\psi\rangle.$$

This still preserves the relation $\mathbf{k}_1 + \mathbf{k}_2 = \mathbf{k}_3 + \mathbf{k}_4$. Now our sum reduces to

$$\begin{aligned} E^1 &= \frac{2\pi\hbar^2 a}{mV} \langle ..., 0, 0, N | b_0^\dagger b_0^\dagger b_0 b_0 | N, 0, 0, ...\rangle \\ &= \frac{2\pi\hbar^2 a}{mV} \sqrt{N}\sqrt{N-1}\sqrt{N-1}\sqrt{N} \langle ..., 0, 0, N | N, 0, 0, ...\rangle \\ &= \frac{2\pi\hbar^2 a}{mV} N(N-1) \end{aligned}$$

(b) What is the pressure of this weakly interacting condensate?

Although the usual thermodynamic quantities like entropy and pressure do not exist in a BEC condensate (in the thermodynamic limit), when we add in interactions, they may. Proceeding on the assumption they do, we have the Helmholtz free energy $F(T, V)$,

$$F = U - TS$$

and its relation to pressure

$$p = -\left(\frac{\partial F}{\partial V}\right)_T.$$

At $T = 0$ then, $F = U$ and $p = -\frac{\partial U}{\partial V}$. Thus

$$p = \frac{2\pi\hbar^2 a}{mV^2}(N^2 - N).$$

For $N \gg 1$ this may be approximated as

$$p = \frac{2\pi\hbar^2 a}{mV^2}N^2 = \frac{2\pi\hbar^2 a}{m}n^2.$$