Physics 560A lecture 9

Second quantization for bosons (general case).

Phonons:

$$H = \sum_\nu \hbar\omega_\nu \left(a_\nu^\dagger a_\nu + \frac{1}{2}\right)$$

$$[a_\mu, a_\nu^\dagger] = \delta_{\mu\nu}$$

$$[a_\mu, a_\nu] = 0$$

$$[a_\mu^\dagger, a_\nu^\dagger] = 0$$

General bosons:
(neglecting interparticle interactions)

$$H = \sum_\nu \varepsilon_\nu a_\nu^\dagger a_\nu ,$$

where

$$H\,\psi_\nu(\vec{x}) = \left[-\frac{\hbar^2}{2m}\nabla^2 + U(\vec{x})\right]\psi_\nu(\vec{x}) = \varepsilon_\nu \psi_\nu$$

The creation and annihilation operators can be expressed in terms of field operators $\hat{\psi}$ and $\hat{\psi}^\dagger$:

$$a_\nu = \int d^3x\ \psi_\nu^*(\vec{x})\ \hat{\psi}(\vec{x})$$

$$a_\nu^\dagger = \int d^3x\ \psi_\nu(\vec{x})\ \hat{\psi}^\dagger(\vec{x})$$

$$\left[\ a_\nu^\dagger(t) = \int d^3x\ \psi_\nu(x)\ \hat{\psi}^\dagger(\vec{x},t)\ \right]$$

$$\hat{\psi}(\vec{x}) = \sum_\nu \psi_\nu(\vec{x})\ a_\nu$$

$$\hat{\psi}^\dagger(\vec{x}) = \sum_\nu \psi_\nu^*(\vec{x})\ a_\nu^\dagger$$

Check:

$$a_\nu^\dagger = \int d^3x \; \psi_\nu(\vec{x}) \sum_\mu \psi_\mu^*(\vec{x})\, a_\mu^\dagger$$

$$= \sum_\mu a_\mu^\dagger \underbrace{\int d^3x \; \psi_\mu^*(\vec{x})\, \psi_\nu(\vec{x})}_{\delta_{\mu\nu}}$$

$$= a_\nu^\dagger \quad \checkmark$$

What are the commutation relations for the field operators?

$$\boxed{[\hat{\psi}(\vec{x}), \hat{\psi}(\vec{y})] = 0 \qquad [\hat{\psi}^\dagger(\vec{x}), \hat{\psi}^\dagger(\vec{y})] = 0}$$

$$[\hat{\psi}(\vec{x}), \hat{\psi}^\dagger(\vec{y})] = \sum_\mu \sum_\nu \psi_\mu(\vec{x})\, \psi_\nu^*(\vec{y}) \times \underbrace{[a_\mu, a_\nu^\dagger]}_{\delta_{\mu\nu}}$$

$$[\hat{\psi}(\vec{x}), \hat{\psi}^{+}(\vec{y})] = \sum_{\mu} \psi_\mu(\vec{x}) \psi_\mu^{*}(\vec{y})$$

$$= \sum_{\mu} \langle \vec{x} | \mu \rangle \langle \mu | \vec{y} \rangle$$

$$= \langle \vec{x} | \vec{y} \rangle = \delta^{(3)}(\vec{x} - \vec{y})$$

(or simply $\delta(\vec{x} - \vec{y})$

$$\boxed{[\hat{\psi}(\vec{x}), \hat{\psi}^{+}(\vec{y})] = \delta(\vec{x} - \vec{y})}$$

Just as for phonons, the energy eigenstate $| \{n_\nu\} \rangle$ is

$$| \{n_\nu\} \rangle = \prod_{\nu} \frac{(a_\nu^{+})^{n_\nu}}{\sqrt{n_\nu!}} | 0 \rangle ,$$

where $|0\rangle$ = state with no bosons.

However $\langle \hat{n}_\nu \rangle = \dfrac{1}{e^{\beta(\varepsilon_\nu - \mu)} + 1}$.

The ket $|\mu\nu\gamma\ldots\rangle$ is completely symmetric under particle interchange:

$$|\mu\nu\gamma\ldots\rangle = a_\mu^\dagger a_\nu^\dagger a_\gamma^\dagger \cdots |0\rangle$$

$$|\nu\mu\gamma\cdots\rangle = a_\nu^\dagger a_\mu^\dagger a_\gamma^\dagger \cdots |0\rangle = |\mu\nu\gamma\ldots\rangle$$

In terms of wavefunctions,

$$\langle \vec{x}_1, \vec{x}_2 | \mu\nu\rangle = \frac{1}{\sqrt{2}}\left[\psi_\mu(\vec{x}_1)\psi_\nu(\vec{x}_2) + \psi_\mu(\vec{x}_2)\psi_\nu(\vec{x}_1)\right]$$

$$\begin{aligned}\langle \vec{x}_1, \vec{x}_2, \vec{x}_3 | \mu\nu\gamma\rangle = \frac{1}{\sqrt{3!}}\Big(&\psi_\mu(\vec{x}_1)\psi_\nu(\vec{x}_2)\psi_\gamma(\vec{x}_3) + \psi_\mu(\vec{x}_1)\psi_\nu(\vec{x}_3)\psi_\gamma(\vec{x}_2)\\ &+ \psi_\mu(\vec{x}_2)\psi_\nu(\vec{x}_1)\psi_\gamma(\vec{x}_3) + \psi_\mu(\vec{x}_3)\psi_\nu(\vec{x}_2)\psi_\gamma(\vec{x}_1)\\ &+ \psi_\mu(\vec{x}_3)\psi_\nu(\vec{x}_1)\psi_\gamma(\vec{x}_2) + \psi_\mu(\vec{x}_2)\psi_\nu(\vec{x}_3)\psi_\gamma(\vec{x}_1)\Big)\end{aligned}$$

In general, for N particles

$$\psi(\vec{x}_1, \vec{x}_2, \ldots, \vec{x}_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \psi_{\mu_1}(\vec{x}_1) & \psi_{\mu_1}(\vec{x}_2) & \cdots & \psi_{\mu_1}(\vec{x}_N) \\ \psi_{\mu_2}(\vec{x}_1) & \psi_{\mu_2}(\vec{x}_2) & \cdots & \\ & & & \\ \psi_{\mu_N}(\vec{x}_1) & \cdots & & \psi_{\mu_N}(\vec{x}_N) \end{vmatrix}_+$$

where $| \;\; |_+$ is the "permanent", like a determinant, but symmetric under interchange of rows & columns.

Writing out the wavefunction quickly becomes intractable, since for N particles, there are N! different permutations!

The corresponding Hamiltonian for N particles is

$$H = \sum_{i=1}^{N} \left[\frac{\vec{P}_i^{\,2}}{2m} + U(\vec{x}_i) \right].$$

This has the disadvantage that N must be known in advance.

What is H in terms of $\hat{\varphi}$ and $\hat{\varphi}^+$?

$$H = \sum_{\nu} \varepsilon_\nu a_\nu^+ a_\nu$$

Now $\langle \mu | -\frac{\hbar^2}{2m}\nabla^2 + U | \nu \rangle = \varepsilon_\mu \delta_{\mu\nu}$

so

$$H = \sum_{\mu,\nu} a_\mu^+ \langle \mu | -\frac{\hbar^2}{2m}\nabla^2 + U | \nu \rangle a_\nu$$

$$H = \int d^3x \int d^3y \sum_{\mu,\nu} \hat{\psi}^{+}(\vec{x})\, \psi_\mu(\vec{x}) \langle \mu | -\frac{\hbar^2}{2m}\nabla^2 + U | \nu \rangle \times \psi_\nu^*(\vec{y})\, \hat{\psi}(\vec{y})$$

$$= \int d^3x \int d^3y \; \hat{\psi}^{+}(\vec{x}) \langle \vec{x} | -\frac{\hbar^2}{2m}\nabla^2 + U | \vec{y} \rangle \hat{\psi}(\vec{y})$$

But $\langle \vec{x} | -\frac{\hbar^2}{2m}\nabla^2 + U | \vec{y} \rangle = \left[-\frac{\hbar^2}{2m}\nabla^2 + U(\vec{x}) \right] \delta(\vec{x}-\vec{y})$

So $\boxed{H = \int d^3x \; \hat{\psi}^{+}(\vec{x}) \left[-\frac{\hbar^2}{2m}\nabla^2 + U(\vec{x}) \right] \hat{\psi}(\vec{x})}$

<u>Density operator</u> $\quad \hat{\rho}(\vec{x}) = \hat{\psi}^{+}(\vec{x})\, \hat{\psi}(\vec{x})$

$$\hat{\rho}(\vec{x}) = \sum_\mu \sum_\nu \psi_\mu^*(\vec{x})\, \psi_\nu(\vec{x})\, a_\mu^{+} a_\nu$$

$$\langle \hat{\rho}(\vec{x}) \rangle = \sum_\mu |\psi_\mu(\vec{x})|^2 \langle \hat{n}_\mu \rangle$$

$= $ density of particles at $\vec{x}$

Two-body interaction

In "first quantization," the two-body interaction is

$$H^{(2)} = \frac{1}{2} \sum_{i \neq j} V(\vec{x}_i - \vec{x}_j)$$

Since the 1-body interaction

$$\sum_{i=1}^{N} U(\vec{x}_i) \longrightarrow \int d^3x \; U(\vec{x}) \, \hat{\psi}^\dagger(\vec{x}) \, \hat{\psi}(x)$$

$$= \int d^3x \; U(\vec{x}) \, \hat{\rho}(\vec{x}),$$

we expect the two-body term to be

$$H^{(2)} \overset{?}{=} \frac{1}{2} \int d^3x \int d^3y \; \hat{\rho}(\vec{x}) \, V(\vec{x}-\vec{y}) \, \hat{\rho}(\vec{y})$$

This term, however, includes an unphysical self-interaction. Consider a state with just one particle:

$$|\mu\rangle = a_\mu^\dagger |0\rangle.$$

$$\langle\mu| H^{(2)} |\mu\rangle = ?$$

$$\langle\mu| \hat{\rho}(\vec{x})\, \hat{\rho}(\vec{y}) |\mu\rangle$$

$$= |\psi_\mu(\vec{x})|^2\, \delta(\vec{x}-\vec{y})$$ (after some algebra)

$$\Rightarrow \langle\mu| H^{(2)} |\mu\rangle = \frac{1}{2}\int d^3x\, V(0)\, |\psi_\mu(\vec{x})|^2$$

$$= \frac{1}{2} V(0)$$

$\Rightarrow$ self-interaction (not physical)

The correct form of the two-body interaction is

$$H^{(2)} = \frac{1}{2}\int d^3x \int d^3y \; \hat{\psi}^{\dagger}(\vec{x})\hat{\psi}^{\dagger}(\vec{y})\, V(\vec{x}-\vec{y})$$

$$\times \; \hat{\psi}(\vec{y})\,\hat{\psi}(\vec{x})$$

It is easy to see that

$\langle H^{(2)} \rangle \equiv 0$ in any state with just one particle.

Ordering the creation and annihilation operators in this way is refered to as "normal ordering."

We can also write the various terms in the Hamiltonian using creation and annihilation operators for any complete set of states:

$$\hat{\Psi}(\vec{x}) = \sum_{\ell} \psi_{\ell}(\vec{x})\, a_{\ell}$$

$$\hat{\Psi}^{\dagger}(\vec{x}) = \sum_{\ell} \psi_{\ell}^{*}(\vec{x})\, a_{\ell}^{\dagger}$$

$$H = \sum_{\ell,m} H^{(1)}_{\ell m}\, a_{\ell}^{\dagger} a_{m} + \frac{1}{2} \sum_{\substack{\ell,m\\ i,j}} V_{\ell m i j}\, a_{j}^{\dagger} a_{m}^{\dagger} a_{\ell} a_{i},$$

where $$H^{(1)}_{\ell m} = \langle \ell | -\frac{\hbar^2}{2m}\nabla^2 + U\, | m \rangle$$

and

$$V_{\ell m i j} = \int d^3x \int d^3y\, \psi_m^{*}(\vec{x})\, \psi_{\ell}(\vec{x})\, V(\vec{x}-\vec{y})\, \psi_j^{*}(\vec{y})\, \psi_i(\vec{y})$$

The two-body interaction can be represented graphically by the Feynman diagram: