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Tutorial VI
Second quantization

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I. Equation of motion of an operator in the Heisenberg representation.

Consider the Hamiltonian of a boson field (representing photons or phonons)

$$\hat{H} = \sum_k \hbar\omega_k c_k^\dagger c_k$$

Write and solve the equations of motion for the creation and annihilation operators in the Heisenberg representation. For a boson field, we recall the commutation relationships : $[c_k, c_{k'}^\dagger = \delta_{k,k'}$, $[c_k, c_{k'}] = [c_k^\dagger, c_{k'}^\dagger] = 0$.

In Heisenberg representation, we can define the evolution operator,

$$U(0,t) = \exp\left(\frac{i}{\hbar}\hat{H}t\right)$$

which is **not the same** as the interaction picture,

$$H = H_0 + H_1 \longrightarrow H_0 = \exp\left(\frac{i}{\hbar}\hat{H}_0 t\right)$$

The Heisenberg representation can be written from the Schrödinger one using,

$$\hat{Q}_H(t) = \hat{U}^\dagger(t)\hat{Q}_S\hat{U}(t)$$

Thus,

$$c_{k,H}(t) = \hat{U}^\dagger c_k \hat{U} = \exp\left(\frac{i}{\hbar}\hat{H}t\right) c_k \exp\left(-\frac{i}{\hbar}\hat{H}t\right)$$

And so,

$$i\hbar\frac{\partial}{\partial t}c_{k,H}(t) = \left[c_{k,H}(t), \hat{H}\right]$$

and thus,

$$i\hbar\frac{\partial}{\partial t}c_{k,H}(t) = \exp\left(\frac{i}{\hbar}\hat{H}t\right)[C_k, \hat{H}]\exp\left(-\frac{i}{\hbar}\hat{H}t\right)$$

Thus, we just need to calculate the commutator,

$$\begin{aligned}
[c_k, \hat{H}] &= \sum_{k'} \hbar\omega_{k'}[c_{k'}, c_k^\dagger c_k] \\
&= \sum_{k'} \hbar\omega_{k'}\left[[c_{k'}, c_k^\dagger]c_k + c_k^\dagger[c_{k'}, c_k]\right] \\
&= \hbar\omega_k c_k
\end{aligned}$$

And so,

$$i\hbar\frac{\partial}{\partial t}c_{k,H}(t) = \exp\left(\frac{i}{\hbar}\hat{H}t\right)\hbar\omega_k c_k \exp\left(-\frac{i}{\hbar}\hat{H}t\right) = \omega_k c_{k,H}(t)$$

leading to,

$$c_{k,H}(t) = c_{k,H}(t=0)\exp(-i\omega_k t) = c_k e^{-i\omega_k t}$$

and similarly,

$$c^{\dagger}_{k,H}(t) = c^{\dagger}_k \exp(i\omega_k t)$$

For the field operators,

$$\hat{\psi}(\vec{r}) = \sum_k \psi_k(r) c_k$$

$$\frac{\partial\hat{\psi}}{\partial t}(\vec{r},t) = \sum_k \psi_k(\vec{r})\frac{\partial c_k}{\partial t} = i\sum_k \psi_k(\vec{r})\omega_k c_k$$

For one particle Hamiltonian,

$$H_{1p} = \frac{p^2}{2m} + V(\vec{r})$$

And thus,

$$-\frac{\hbar^2}{2m}\Delta + V(\vec{r})$$

leading to,

$$i\hbar\frac{\partial\hat{\psi}}{\partial t} = \left[-\frac{\hbar^2}{2m}\Delta + V(\vec{r})\right]\hat{\psi}$$

which is formally identical to a Schrödinger equation except that $\hat{\psi}$ is the field operator.

II. Fermionic Hamiltonian in second quantization.

Consider the Hamiltonian of an N-fermion system

$$H = \sum_{j=1}^{N} T(x_j) + \frac{1}{2}\sum_{j\neq l}^{N} U(x_j, x_l),$$

given by the sum of one-particle operators T (kinetic energy, impurity potential, etc) and two-particle operators U (particle interactions). The Hamiltonian operator in second quantization is given by

$$\hat{H} = \sum_{k,k'} c_k^\dagger \langle k| T |k'\rangle c_{k'} + \frac{1}{2} \sum_{kk',ll'} c_k^\dagger c_{k'}^\dagger \langle kk'| U |ll'\rangle c_{l'} c_l$$

The creation and annihilation operators for fermions follow the anticommutation relationships : $\{c_k, c_{k'}^\dagger\} = \delta_{k,k'}$, $\{c_k, c_{k'}\} = \{c_k^\dagger, c_{k'}^\dagger\} = 0$. The field operators are given by linear combinations of the annihilation and creation operators (in a complete basis) with the wave-functions as coefficients :

$$\hat{\psi}(x) = \sum_k \psi_k(x) c_k, \qquad \hat{\psi}^\dagger(x) = \sum_k \psi_k^*(x) c_k^\dagger$$

1. Give the anticommutation relations of the field operators $\{\hat{\psi}(x), \hat{\psi}^\dagger(x')\}$, $\{\hat{\psi}(x), \hat{\psi}(x')\}$ and $\{\hat{\psi}^\dagger(x), \hat{\psi}^\dagger(x')\}$.

$$\begin{aligned}
\{\hat{\psi}(x), \hat{\psi}^\dagger(x')\} &= \sum_{kk'} \psi_k(x) c_k \psi_{k'}^*(x') c_{k'}^\dagger + \sum_{kk'} \psi_k^\dagger(x') c_k^\dagger \psi_{k'}(x) c_{k'} \\
&= \sum_{kk'} \psi_k(x) \psi_{k'}^*(x') \{c_k, c_{k'}^*\} \\
&= \sum_k psi_k(x) \psi_k^*(x') \\
&= \delta(x - x')
\end{aligned}$$

which is analogous to what we know from ladder operators. The other relations are trivial to derive from the anticommutation relation.

2. Show that $\hat{H}$ can be written as

$$\hat{H} = \int \mathrm{d}^3x \hat{\psi}^\dagger(x) T(x) \hat{\psi}(x) + \frac{1}{2} \iint \mathrm{d}^3x \mathrm{d}^3x' \hat{\psi}^\dagger(x) \hat{\psi}^\dagger(x') U(x,x') \hat{\psi}(x') \hat{\psi}(x)$$

$$\begin{aligned}
\langle k| T |k'\rangle &= \int \mathrm{d}x \int \mathrm{d}x' \langle k|x\rangle \langle x| T |x'\rangle \langle x'|k'\rangle \\
&= \int \mathrm{d}x \psi_k^*(x) T(x) \psi_{k'}(x)
\end{aligned}$$

$$\begin{aligned}
\sum_{kk'} c_k^\dagger \langle k| T |k'\rangle c_k &= \int \mathrm{d}x \sum_{kk'} c_k^\dagger \psi_k^\dagger T(x) c_{k'} \psi_{k'} \\
&= \int \mathrm{d}x \hat{\psi}^\dagger(x) T(x) \hat{\psi}(x) \\
&\equiv T
\end{aligned}$$

$$\langle kk'| U |ll'\rangle = \int \mathrm{d}x \int \mathrm{d}x' \psi_k^*(x)\psi_{k'}(x')U(x,x')\psi_{l'}(x')\psi_l(x)$$
$$= \frac{1}{2}\int \mathrm{d}x\mathrm{d}x' \hat{\psi}^\dagger(x)\hat{\psi}^\dagger(x')U(x,x')\hat{\psi}(x')\hat{\psi}(x)$$
$$= U$$

Thus,

$$\hat{H} = T + U$$

III. Density and number of particle operators.

Consider the operators representing the particle-density $n(x) = \sum_{j=1}^{N} \delta(x - x_j)$ and the number of particles $N = \int \mathrm{d}^3 x n(x)$.

1. Give their expressions in second quantization.

2. Write $n(x)$ and N in terms of the field operators.

$$\hat{n} = \sum_{kk'} c_k^\dagger \langle k| n |k'\rangle c_{k'}$$

$$\langle k| n |k'\rangle = \int \mathrm{d}x' \psi_k^\dagger(x')\delta(x - x')\psi_{k'}(x)$$

and from previous exercise,

$$\langle k| n |k'\rangle = \psi_k^*(x)\psi_{k'}(x)$$

thus,

$$\hat{n} = \hat{\psi}^\dagger\hat{\psi}$$

$$\hat{N} = \int \mathrm{d}x \hat{n}(x) = \int \mathrm{d}x \hat{\psi}^\dagger(x)\hat{\psi}(x) = \sum_k c_k^\dagger c_k$$

3. Show that $\hat{N}$ commutes with the Hamiltonian $\hat{H}$ of the previous exercise.

We want to confirm that the number of particles in conserved, which is equivalent to say that $[\hat{H}, \hat{N}] = 0$,

$$[\hat{H}, \hat{N}] = [\hat{T} + \hat{U}, \hat{N}]$$

$$\begin{aligned}[\hat{T}, \hat{N}] &= \sum kk'lT_{kk'}[c_k^\dagger c_{k'}, c_l^\dagger c_l] \\ &= \sum_{kk'l} T_{kk'}[\delta_{k'l} c_k^\dagger c_l - \delta_{kl} c_l^\dagger c_k] \\ &= \sum_{kl} T_{kl}(c_k^\dagger c_l - c_l^\dagger c_k)\end{aligned}$$

but we can change the index and so $[\hat{T}, \hat{N}] = 0$.

IV. Current operator and the perturbation by an electromagnetic field (optional).

Consider the current density operator for N particles

$$J_N(x,t) = \frac{e}{2m}\sum_{j=1}^{N}[(p_j - eA(x,t))\delta(x - x_j) + \delta(x - x_j)(p_j - eA(x,t))]$$

Where the vector $A(x,t)$ represents the vector-potential of the electromagnetic field. Show that the matrix element of the one-particle operator $J(x,t)$ between two states $|k\rangle$ and $|k'\rangle$ is given by

$$J_{kk'}(x,t) = \langle k| J(x,t) |k'\rangle = \frac{e}{2mi}[\psi_k^*(x)\nabla\psi_{k'}(x) - \psi_{k'}(x)\nabla\psi_k^*(x)] - \frac{e^2}{m}A(x,t)\psi_k^*(x)\psi_{k'}(x)$$

Consider the Hamiltonian of the perturbation

$$H^{\text{ex}} = \frac{e}{2m}(pA + Ap) - \frac{e^2}{2m}A^2$$

Neglecting the term quadratic in A and the last term (diamagnetic) in $J_{kk'}$, show that

$$\langle k| H^{\text{ex}} |k'\rangle = \int \mathrm{d}^3x A(x,t) J_{kk'}(x)$$

Write the operators $\hat{J}$ and $\hat{H}^{\text{ex}}$ in second quantization and show the relationship

$$\hat{H}^{\text{ex}} = -\int \mathrm{d}^3x A(x,t)\hat{J}(x)$$