Second Quantization: "Theoretical Minimum" (for fermions!)

Consider the many-fermion state

$$|n_{\alpha_1} n_{\alpha_2} \cdots n_{\alpha_j} \cdots\rangle , \qquad (1)$$

where n_{α_i} = number of fermions in the single-fermion state $|\alpha_i\rangle$. By the Pauli principle, $n_{\alpha_i} = 0$ or 1. α_i is a symbolic label for all the quantum numbers that must be specified in order to uniquely specify a single-fermion state. Two (common!) examples:

(I) Spin-polarized electrons (where all electrons have the same spin, and hence there is no need to specify the spin for an individual single-electron state): $\alpha_i \equiv \vec{p}_i = \hbar\vec{k}_i = \{\hbar = 1\} = \vec{k}_i$.

(II) electrons with spin $s_i = +1/2$ or $-1/2$:
$\alpha_i \equiv (\vec{k}_i, s_i)$

The wave function $u_{\alpha_i}(\vec{r})$ corresponding to $|\alpha_i\rangle$ is obtained by taking the inner product $\langle \vec{r} | \alpha_i \rangle$, i.e.

$$u_{\alpha_i}(\vec{r}) = \langle \vec{r} | \alpha_i \rangle \qquad (2)$$

Important case (plane waves):

$$\frac{1}{\sqrt{V}} e^{i\vec{k}_i \cdot \vec{r}} = \langle \vec{r} | \vec{k}_i \rangle \qquad (3)$$

We shall sometimes use the notation $\phi_{\alpha_i}(\vec{r})$ for a wave function. The "standard" quantum mechanics notation for a wave function, $\psi_{\alpha_i}(\vec{r})$ will be avoided, however, since $\psi_{\alpha_i}(\vec{r})$ is conventionally used to denote a so called "field operator" in second quantization.

Importantly, the state in (1) is constructed (from single-fermion states) in such a way that the corresponding many-fermion wavefunction is antisymmetric (as it must be, since we are dealing with fermions!). I showed an example in class when only two single-fermion states $|\alpha_1\rangle$ and $|\alpha_2\rangle$ are occupied.

Next, introduce two kind of operators, c_{α_i} and $c^+_{\alpha_i}$, $i = 1, 2, \ldots$. c_{α_i} is called "annihilation operator". Acting on the state in (1), it removes the particle in the single-fermion state $|\alpha_i\rangle$ if there is a fermion in that state. Otherwise, if there is no fermion in $|\alpha_i\rangle$, the action of c_{α_i} gives zero. In formulas:

$$c_{\alpha_i} | n_{\alpha_1} n_{\alpha_2} \ldots n_{\alpha_i} = 1 \ldots \rangle$$

$$= (-1)^{N_i} | n_{\alpha_1} n_{\alpha_2} \ldots n_{\alpha_i} = 0 \ldots \rangle \qquad (4a)$$

$$c_{\alpha_i} | n_{\alpha_1} n_{\alpha_2} \ldots n_{\alpha_i} = 0 \ldots \rangle = 0 \qquad (4b)$$

where the prefactor $(-1)^{N_i}$, with $N_i = \sum_{j=1}^{i-1} n_{\alpha_j}$, comes from the way the annihilation operator is constructed, to make sure that the new state (with one particle less) also gives rise to an antisymmetric wave function. Turning to the operator $c^+_{\alpha_i}$, we call it a "creation operator" since when acting with it on the state in (1), it adds a fermion to the single-fermion state $|\alpha_i\rangle$ if that state is empty, else it gives zero. In formulas:

$$c^+_{\alpha_i} | n_{\alpha_1} n_{\alpha_2} \dots n_{\alpha_i} = 0 \dots \rangle$$

$$= (-1)^{N_i} | n_{\alpha_1} n_{\alpha_2} \dots n_{\alpha_i} = 1 \dots \rangle \qquad (5a)$$

$$c^+_{\alpha_i} | n_{\alpha_1} n_{\alpha_2} \dots n_{\alpha_i} = 1 \dots \rangle = 0 \qquad (5b)$$

The creation- and annihilation operators satisfy the important anticommutation relations

$$\{ c_{\alpha_i}, c_{\alpha_j} \} = \{ c^+_{\alpha_i}, c^+_{\alpha_j} \} = 0 \qquad (6a)$$

$$\{ c_{\alpha_i}, c^+_{\alpha_j} \} = \delta_{ij} \qquad (6b)$$

These relations tell us that we have to be careful when changing the order of two operators. For example, by (4a), $c_{\alpha_i} c_{\alpha_j} = - c_{\alpha_j} c_{\alpha_i}$.

The second-quantized formalism becomes really powerful when using it to express a many-fermion Hamiltonian. The case that we shall mostly study in the first part of the course is that of spin-polarized electrons (where we can forget about spin!). Long and cumbersome algebra (not part of the course) yields the result that the many-electron Hamiltonian

$$H = H_{\text{kinetic}} + H_{\substack{e\text{-}e \\ \text{interaction}}} \qquad (7)$$

takes the form where

$$H_{\text{kinetic}} = \sum_{\vec{k}} \varepsilon_{\vec{k}} c^{+}_{\vec{k}} c_{\vec{k}} \qquad (8)$$

$$\varepsilon_{\vec{k}} = \frac{\hbar^2 k^2}{2m}$$

and

$$H_{\substack{e\text{-}e \\ \text{interaction}}} = \frac{1}{2} \sum_{\vec{k},\vec{k}',\vec{q}} V_{\vec{q}} \, c^{+}_{\vec{k}-\vec{q}} \, c^{+}_{\vec{k}'+\vec{q}} \, c_{\vec{k}'} \, c_{\vec{k}} \qquad (9)$$

$$V_{\vec{q}} = \frac{1}{V} \int_{\text{volume}} e^{i\vec{q}\cdot\vec{r}} V(\vec{r}) \, d\vec{r}$$

$$= \left\{ V(\vec{r}) = \frac{e^2}{|\vec{r}|}, \text{ Coulomb} \right\}$$

$$= \frac{4\pi e^2}{V q^2} . \qquad (10)$$

To get rid of the nasty $q = 0$ component in (10), we embedd the electrons in a uniform positively charged background (JELLIUM MODEL ! THE WORLD'S SIMPLEST CONDENSED MATTER SYSTEM !). This background "stands in" for the positively charged ions in a crystal. As I mentioned in class, by having charge neutrality (electrons + background), the $q = 0$ component in (10) gets cancelled.

To make the formula in (9) look less cluttered, the index "i" labelling the different possible momenta has been removed. If you wish, you can put it back : $\vec{k} \to \vec{k}_i$, $\vec{k}' = \vec{k}_j$, $\vec{q} = \vec{q}_\ell$, $\Sigma_{\vec{k}} \to \Sigma_i$, $\Sigma_{\vec{k}'} \to \Sigma_j$, $\Sigma_{\vec{q}} \to \Sigma_\ell$.

The formula for the Hamiltonian in (7) - (9) is quite intuitive and easy to understand. No need (in this course !) to go through all the gory details in the derivation.

First, look at the kinetic part, H_{kinetic} in (8). Pull out one term from the sum, $\varepsilon_{\vec{k}_i} c^+_{\vec{k}_i} c_{\vec{k}_i}$ (having reinserted the index "i" for convenience). Let it act on the state $|n_{\vec{k}_1} n_{\vec{k}_2} \dots n_{\vec{k}_i} \dots\rangle$. $c^+_{\vec{k}_i} c_{\vec{k}_i} = \hat{n}_{\vec{k}_i}$ is a "number operator" with $n_{\vec{k}_i}$ as eigenvalue. Thus, if there is a fermion in $|\vec{k}_i\rangle$, it will contribute a kinetic energy ε_{k_i}. If not, no contribution. Quite simple and transparent!

Next, look at the interaction term $H_{e\text{-}e\ \text{interaction}}$ in (9)! Pull out one term from the sum:

$$V_{\vec{q}}\, c^{\dagger}_{\vec{k}-\vec{q}}\, c^{\dagger}_{\vec{k}'+\vec{q}}\, c_{\vec{k}'}\, c_{\vec{k}} \qquad (10)$$

Here $\vec{q}$, $\vec{k}$, and $\vec{k}'$ are fixed momenta, in contrast to how they appear in the sum in (9), where they are summed over. If you find this confusing, insert indices i, j, and l, and proceed!

Now let the operator in (10) act on the state

$$|\ldots\ n_{\vec{k}}\ \ldots\ n_{\vec{k}'}\ \ldots\rangle \qquad (11)$$

(where, as above, ... denote occupation numbers for all the other single-fermion momentum states).

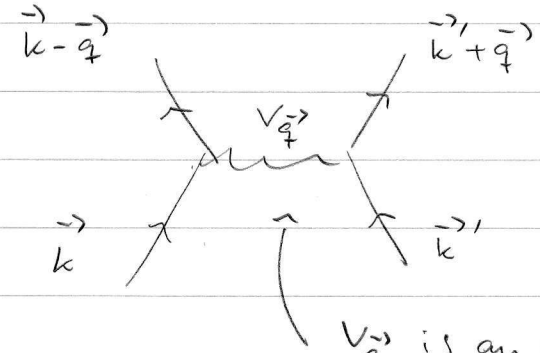
Clearly, only if $n_{\vec{k}} = n_{\vec{k}'} = 1$ and $n_{\vec{k}-\vec{q}} = n_{\vec{k}'+\vec{q}} = 0$ will the result be nonzero. Explicitly,

$$V_{\vec{q}}\, c^{\dagger}_{\vec{k}-\vec{q}}\, c^{\dagger}_{\vec{k}'+\vec{q}}\, c_{\vec{k}'}\, c_{\vec{k}}\ \Big|\ldots n_{\vec{k}-\vec{q}}=0 \ldots n_{\vec{k}}=1 \ldots n_{\vec{k}'}=1 \ldots n_{\vec{k}'+\vec{q}}=0\ldots\Big\rangle$$

$$= V_{\vec{q}}\ \Big|\ldots n_{\vec{k}-\vec{q}}=1 \ldots n_{\vec{k}}=0 \ldots n_{\vec{k}'}=0 \ldots n_{\vec{k}'+\vec{q}}=1 \ldots\Big\rangle \qquad (12)$$

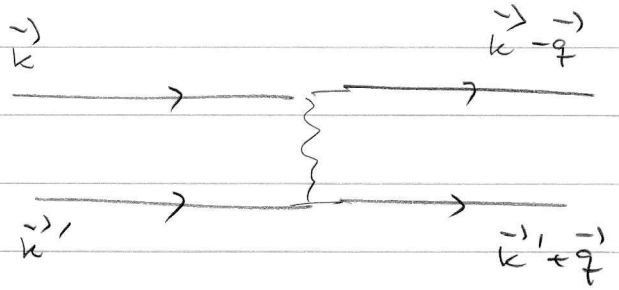
All other occupation numbers (denoted by ...) are untouched by the action of $V_{\vec{q}}\, c^{\dagger}_{\vec{k}-\vec{q}}\, c^{\dagger}_{\vec{k}'+\vec{q}}\, c_{\vec{k}'}\, c_{\vec{k}}$.

The important thing to realize is that the physical process encoded by (12) is that of scattering between two particles with momentum transfer $\vec{q}$.
It is instructive to illustrate it in a picture, a "Feynman diagram":



$V_{\vec{q}}$ is an amplitude which measures how likely a scattering event with momentum $\vec{q}$ is.

Nota Bene! How you draw the Feynman diagram is up to you. It's only a symbolic illustration!
Another way to draw

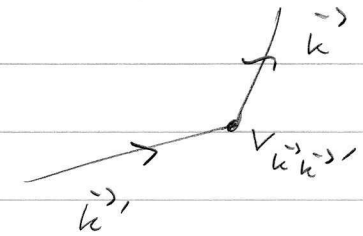


One final thing: I also discussed "single-fermion operators" in my lecture:

$$\sum_{\vec{k},\vec{k}'} V_{\vec{k}\vec{k}'} \, c^{+}_{\vec{k}} c_{\vec{k}'} \qquad (13)$$

$$V_{\vec{k}\vec{k}'} = \frac{1}{V} \int_{\text{volume}} e^{i(\vec{k}'-\vec{k})\cdot\vec{r}} V(\vec{r}) \, d\vec{r}$$

The action of a single term in (13) can also be illustrated diagrammatically:



Here a single fermion with momentum $\vec{k}'$ is scattered into a new state $\vec{k}$ by the potential. The amplitude for this process is $V_{\vec{k}\vec{k}'}$. Obviously, this is the only contribution: If $n_{\vec{k}}' = 0$ and/or $n_{\vec{k}} = 1$ the result of acting with the single term $V_{\vec{k}\vec{k}'} c^{+}_{\vec{k}} c_{\vec{k}'}$ on $|\ldots n_{\vec{k}}, \ldots n_{\vec{k}'} \ldots\rangle$ will give zero.

This is all you need to know about second quantization in this course!