1 Review of second quantization for electrons

a. Field operators

Consider a system of electrons, or more generally of identical fermions having spin $\frac{1}{2}$. By definition, the creation operator $\hat{c}^\dagger_{k\sigma}$ creates (and the annihilation operator $\hat{c}_{k\sigma}$ annihilates) a particle of momentum $\hbar k$ and spin σ ($\uparrow$ or $\downarrow$). If $|0\rangle$ is the vacuum state,

$$\hat{c}^\dagger_{k\sigma}|0\rangle = |k\sigma\rangle \qquad \text{with } |k\sigma\rangle = |k\rangle|\sigma\rangle \tag{1}$$

The field operators $\hat{\psi}_\sigma(r)$ and $\hat{\psi}^\dagger_\sigma(r)$ are defined as

$$\hat{\psi}_\sigma(r) = \sum_k \langle r|k\rangle\, \hat{c}_{k\sigma} = \frac{1}{\sqrt{V}}\sum_k e^{ik\cdot r}\hat{c}_{k\sigma} \tag{2}$$

$$\hat{\psi}^\dagger_\sigma(r) = \sum_k \langle k|r\rangle\, \hat{c}^\dagger_{k\sigma} = \frac{1}{\sqrt{V}}\sum_k e^{-ik\cdot r}\hat{c}^\dagger_{k\sigma} \tag{3}$$

We have used normalization in a finite box of volume V. From (1) and (3), it follows that $\hat{\psi}^\dagger_\sigma(r)$ creates a particle of spin σ at point r, or $\hat{\psi}^\dagger_\sigma(r)|0\rangle = |r\sigma\rangle$.

The anticommutation relations

$$\hat{c}_{k\sigma}\hat{c}_{k'\sigma'} + \hat{c}_{k'\sigma'}\hat{c}_{k\sigma} = 0 \qquad\qquad \hat{c}^\dagger_{k\sigma}\hat{c}^\dagger_{k'\sigma'} + \hat{c}^\dagger_{k'\sigma'}\hat{c}^\dagger_{k\sigma} = 0 \tag{4}$$

$$\hat{c}_{k\sigma}\hat{c}^\dagger_{k'\sigma'} + \hat{c}^\dagger_{k'\sigma'}\hat{c}_{k\sigma} = \delta_{kk'}\delta_{\sigma\sigma'} \tag{5}$$

imply, in particular, that $\left(\hat{c}^\dagger_{k\sigma}\right)^2 = 0$ and $(\hat{c}_{k\sigma})^2 = 0$, meaning that it is impossible to have two particles, or two holes, with the same spin and momentum. Thus the exclusion principle is built into the relations (4).

From eqs. (2)-(5) it follows that

$$\hat{\psi}_\sigma(r)\hat{\psi}_{\sigma'}(r') + \hat{\psi}_{\sigma'}(r')\hat{\psi}_\sigma(r) = 0 \qquad \hat{\psi}^\dagger_\sigma(r)\hat{\psi}^\dagger_{\sigma'}(r') + \hat{\psi}^\dagger_{\sigma'}(r')\hat{\psi}^\dagger_\sigma(r) = 0 \tag{6}$$

$$\hat{\psi}_\sigma(r)\hat{\psi}^\dagger_{\sigma'}(r') + \hat{\psi}^\dagger_{\sigma'}(r')\hat{\psi}_\sigma(r) = \delta(r - r')\delta_{\sigma\sigma'} \tag{7}$$

b. Density and density fluctuation operators

All operators of interest can be expressed in terms of $\hat{\psi}_\sigma(r)$ and $\hat{\psi}^\dagger_\sigma(r)$, or equivalently in terms of $\hat{c}_{k\sigma}$ and $\hat{c}^\dagger_{k\sigma}$. When an operator is expressed in terms of the field operators, it is said to be in second-quantized form. There is a general prescription for doing so, but often one can guess what the second-quantized form of a familiar operator should be, and then confirm the guess by checking that it gives all the correct matrix elements for a complete set of states. It is instructive to work out explicitly some of the cases of interest to us. For instance, we reasonably guess that the second-quantized form of the number density operator will be

$$\hat\rho(\mathbf{r}) = \sum_{\sigma} \hat\psi^{\dagger}_{\sigma}(\mathbf{r})\hat\psi_{\sigma}(\mathbf{r}) = \frac{1}{V}\sum_{\mathbf{k}_1\mathbf{k}_2\sigma} e^{i(\mathbf{k}_2-\mathbf{k}_1)\cdot\mathbf{r}}\, \hat c^{\dagger}_{\mathbf{k}_1\sigma}\, \hat c_{\mathbf{k}_2\sigma} \tag{8}$$

To confirm our guess, we compare $\hat\rho(\mathbf{r})$ with the usual number density operator for an N-particle system:

$$\rho(\hat{\mathbf{r}}_1;\ldots;\hat{\mathbf{r}}_N;\mathbf{r}) = \sum_{\alpha=1}^{N} \delta(\mathbf{r}-\hat{\mathbf{r}}_\alpha) = \sum_{\alpha=1}^{N}\sum_{\mathbf{k}} \frac{1}{V} e^{i\mathbf{k}\cdot(\mathbf{r}-\hat{\mathbf{r}}_\alpha)} \tag{9}$$

where $\hat{\mathbf{r}}_\alpha$ is the position operator for the α-th particle. We show below that, for a system containing N particles, $\hat\rho(\mathbf{r})$ is equivalent to $\rho(\hat{\mathbf{r}}_1;\ldots;\hat{\mathbf{r}}_N;\mathbf{r})$.

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Proof of the equivalence between (6) and (7) -

Instead of working with $\hat\rho(\mathbf{r})$, we introduce its Fourier transform, the density fluctuation operator

$$\hat\rho_{\mathbf{q}} = \int d^3r\, e^{-i\mathbf{q}\cdot\mathbf{r}}\, \hat\rho(\mathbf{r}) = \sum_{\mathbf{k}\sigma} \hat c^{\dagger}_{\mathbf{k}-\mathbf{q}\sigma}\, \hat c_{\mathbf{k}\sigma} \tag{10}$$

which will be useful later. Analogously, we define

$$\rho_{\mathbf{q}}(\hat{\mathbf{r}}_1;\ldots;\hat{\mathbf{r}}_N) = \int d^3r\, e^{-i\mathbf{q}\cdot\mathbf{r}}\, \rho(\hat{\mathbf{r}}_1;\ldots;\hat{\mathbf{r}}_N;\mathbf{r}) = \sum_{\alpha=1}^{N} e^{-i\mathbf{q}\cdot\hat{\mathbf{r}}_\alpha} \tag{11}$$

The effect of $\hat\rho_{\mathbf{q}}$ on a state describing N free particles is to produce the sum of all possible states in which the momentum of one of the particles has been decreased by $\hbar\mathbf{q}$. Clearly the operator (11) has precisely the same effect. But any state can be written as a linear combination of free-particle states. Therefore, for N particles, the two operators are equivalent. Since the second-quantized form (10) is valid for all N, it encompasses all the operators (11) (each of which is restricted to a specific N).

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We will in the following use an equal sign to denote this type of equivalence between an operator and its second-quantized form. However, as we see from the above example, the second-quantized form of an operator applies to systems with any number of particles. Often it is convenient to consider a variable number of particles: for instance, it is advantageous to do statistical physics in the grand canonical ensemble. In these cases the second-quantized formalism is the natural one.

The operator that gives the total number of particles is

$$\hat N = \int d^3r\, \hat\rho(\mathbf{r}) = \sum_{\mathbf{k}\sigma} \hat c^{\dagger}_{\mathbf{k}\sigma}\, \hat c_{\mathbf{k}\sigma} \tag{12}$$

Note that $\hat{N}$ is the same as $\hat{\rho}_q$ for $q = 0$ and that, more generally, $\hat{\rho}_q$ is dimensionless, while $\hat{\rho}(\mathbf{r})$ has dimensions of inverse volume.

c. External potential energy and kinetic energy operators

In an external potential $U(\mathbf{r})$, the potential energy is

$$\hat{U} = \int d^3r\, U(\mathbf{r})\,\hat{\rho}(\mathbf{r}) = \frac{1}{V}\sum_{\mathbf{k}} U(\mathbf{k})\,\hat{\rho}_{-\mathbf{k}} \tag{13}$$

with

$$U(\mathbf{k}) = \int d^3r\, U(\mathbf{r})\, e^{-i\mathbf{k}\cdot\mathbf{r}} \tag{14}$$

The kinetic energy can obviously be written

$$\hat{K} = \sum_{\mathbf{k}\sigma} \frac{\hbar^2 k^2}{2m}\,\hat{c}^\dagger_{\mathbf{k}\sigma}\,\hat{c}_{\mathbf{k}\sigma} \tag{15}$$

Using the inverse of eq. (2),

$$\hat{c}_{\mathbf{k}\sigma} = \frac{1}{\sqrt{V}}\int d^3r\,\hat{\psi}_\sigma(\mathbf{r})\,e^{-i\mathbf{k}\cdot\mathbf{r}} \tag{16}$$

we also have

$$\hat{K} = -\frac{\hbar^2}{2m}\int d^3r \sum_\sigma \hat{\psi}^\dagger_\sigma(\mathbf{r})\nabla^2\hat{\psi}_\sigma(\mathbf{r}) = \frac{\hbar^2}{2m}\int d^3r \sum_\sigma \nabla\hat{\psi}^\dagger_\sigma(\mathbf{r})\cdot\nabla\hat{\psi}_\sigma(\mathbf{r}) \tag{17}$$

d. Interaction potential energy operator

We start from

$$\hat{V} = \frac{1}{2}\sum_{\alpha\neq\beta} V(\hat{\mathbf{r}}_\alpha;\hat{\mathbf{r}}_\beta) = \frac{1}{2}\left[\sum_{\alpha\beta} V(\hat{\mathbf{r}}_\alpha;\hat{\mathbf{r}}_\beta) - \sum_\alpha V(\hat{\mathbf{r}}_\alpha;\hat{\mathbf{r}}_\alpha)\right] =$$

$$\frac{1}{2}\left[\int d^3r\,d^3r' \sum_\alpha \delta(\mathbf{r}-\hat{\mathbf{r}}_\alpha)\sum_\beta \delta(\mathbf{r}'-\hat{\mathbf{r}}_\beta)V(\mathbf{r};\mathbf{r}') - \int d^3r \sum_\alpha \delta(\mathbf{r}-\hat{\mathbf{r}}_\alpha)V(\mathbf{r};\mathbf{r})\right] =$$

$$\frac{1}{2}\left\{\int d^3r\,d^3r'\,\hat{\rho}(\mathbf{r})\hat{\rho}(\mathbf{r}')V(\mathbf{r};\mathbf{r}') - \int d^3r\,\hat{\rho}(\mathbf{r})V(\mathbf{r};\mathbf{r})\right\} =$$

$$\frac{1}{2}\left[\int d^3r\,d^3r' \sum_{\sigma\sigma'} \hat{\psi}^\dagger_\sigma(\mathbf{r})\hat{\psi}_\sigma(\mathbf{r})\hat{\psi}^\dagger_{\sigma'}(\mathbf{r}')\hat{\psi}_{\sigma'}(\mathbf{r}')V(\mathbf{r};\mathbf{r}') - \int d^3r \sum_\sigma \hat{\psi}^\dagger_\sigma(\mathbf{r})\hat{\psi}_\sigma(\mathbf{r})V(\mathbf{r};\mathbf{r})\right] \tag{18}$$

Using the last of the anticommutation relations (??) we find

$$\hat{V} = -\frac{1}{2}\int d^3r\, d^3r' \sum_{\sigma\sigma'} \hat{\psi}^\dagger_\sigma(r)\hat{\psi}^\dagger_{\sigma'}(r')\hat{\psi}_\sigma(r)\hat{\psi}_{\sigma'}(r')V(r;r') \tag{19}$$

and finally, using again anticommutation,

$$\hat{V} = \frac{1}{2}\int d^3r\, d^3r' \sum_{\sigma\sigma'} \hat{\psi}^\dagger_\sigma(r)\hat{\psi}^\dagger_{\sigma'}(r')\hat{\psi}_{\sigma'}(r')\hat{\psi}_\sigma(r)V(r;r') \tag{20}$$

To express $\hat{V}$ in terms of $\hat{c}$ and $\hat{c}^\dagger$ operators insert

$$\tilde{\psi}^\dagger_\sigma(r) = \frac{1}{V}\sum_p e^{-ip\cdot r}\hat{c}^\dagger_{p\sigma} \qquad \tilde{\psi}^\dagger_{\sigma'}(r') = \frac{1}{V}\sum_{p'} e^{-ip'\cdot r'}\hat{c}^\dagger_{p'\sigma'}$$

$$\hat{\psi}_\sigma(r) = \frac{1}{V}\sum_k e^{ik\cdot r}\hat{c}_{k\sigma} \qquad \hat{\psi}_{\sigma'}(r') = \frac{1}{V}\sum_{k'} e^{ik'\cdot r'}\hat{c}_{k'\sigma'}$$

Suppose now that $V(r;r')$ depends only on $r - r'$. Put

$$r = R + \frac{1}{2}s \qquad r' = R - \frac{1}{2}s \tag{21}$$

$$\text{or} \qquad R = \frac{1}{2}(r + r') \qquad s = r - r'$$

We can check that $d^3r\,d^3r' = d^3R\,d^3s$. The integral over R gives

$$\int d^3R\, e^{i(k+k'-p-p')\cdot R} = V\delta_{k+k'-p-p'}$$

This means that, if we put $p = k + q$, the sum over p' reduces to the term $p' = k' - q$. We obtain then

$$\hat{V} = \frac{1}{2V}\sum_{kk'q}\sum_{\sigma\sigma'} \hat{c}^\dagger_{k+q\sigma}\hat{c}^\dagger_{k'-q\sigma'}\hat{c}_{k'\sigma'}\hat{c}_{k\sigma}; \tag{22}$$

where

$$V(q) = \int d^3s\, e^{-iq\cdot s}V(s):$$

e. Equations of motion

The evolution of any operator $\hat{O}$ is of course given by the Heisenberg equation

$$i\hbar\partial\hat{O}/\partial t = \hat{O}\hat{H} - \hat{H}\hat{O}$$

If the Hamiltonian $\hat{H}$ is of the general form (from Eqs. (13), (17), and (18)

$$\hat{H} = (\hbar^2/2m)\sum_\sigma \int d^3r\, \nabla\hat{\psi}^\dagger_\sigma(r)\cdot\nabla\hat{\psi}_\sigma(r) +$$
$$\frac{1}{2}\sum_{\sigma\sigma'}\int d^3r\, d^3r'\,\hat{\psi}^\dagger_\sigma(r)\hat{\psi}^\dagger_{\sigma'}(r')V(r;r')\hat{\psi}_{\sigma'}(r')\hat{\psi}_\sigma(r)$$
$$+\sum_\sigma\int d^3r\,\hat{\psi}^\dagger_\sigma(r)U(r)\hat{\psi}_\sigma(r) \qquad (23)$$

where $V(r;r')$ is the interparticle potential and $U(r)$ is the external potential, the Heisenberg equation for $\hat{\psi}_\sigma(r)$ takes the form

$$i\hbar\partial\hat{\psi}_\sigma(r;t)/\partial t = -(\hbar^2/2m)\nabla^2\hat{\psi}_\sigma(r;t) + \int d^3r'\hat{\rho}(r';t)V(r;r')\hat{\psi}_\sigma(r;t) + U(r)\hat{\psi}_\sigma(r;t)$$

Amazingly, this looks just like the one-particle Schrödinger equation, although $\hat{\psi}_\sigma(r;t)$ is a field operator, not a wave function, and the effective potential $\int d^3r'\hat{\rho}(r')V(r;r')$ depends non-linearly on $\hat{\psi}_\sigma(r)$.

f. The particle current and the continuity equation

Using eq. (25) and its Hermitian conjugate equation for $\hat{\psi}^\dagger_\sigma(r;t)$, we obtain, as in elementary quantum mechanics:

$$i\hbar\partial\hat{\rho}/\partial t = -(\hbar^2/2m)\sum_\sigma [\nabla^2\hat{\psi}^\dagger_\sigma]\hat{\psi}_\sigma - \hat{\psi}^\dagger_\sigma[\nabla^2\hat{\psi}_\sigma]$$
$$= -(\hbar^2/2m)\sum_\sigma \nabla\cdot\left([\nabla\hat{\psi}^\dagger_\sigma]\hat{\psi}_\sigma - \hat{\psi}^\dagger_\sigma[\nabla\hat{\psi}_\sigma]\right)$$

If we define the current density operator as

$$\hat{\jmath}(r;t) = (i\hbar/2m)\sum_\sigma\left([\nabla\hat{\psi}^\dagger_\sigma(r;t)]\hat{\psi}_\sigma(r;t) - \hat{\psi}^\dagger_\sigma(r;t)[\nabla\hat{\psi}_\sigma(r;t)]\right)$$

we obtain

$$\partial\hat{\rho}/\partial t + \nabla\cdot\hat{\jmath} = 0. \qquad (24)$$

Since $\rho(r;t) = \langle\hat{\rho}(r;t)\rangle$ and $J(r;t) = \left\langle\hat{\jmath}(r;t)\right\rangle$, where the expectation value is taken over any initial state or ensemble of states, we have established the continuity equation $\partial\rho/\partial t + \nabla\cdot J = 0$ under the most general conditions.

The current density fluctuation operator, analogously to eq. (9), is

$$\hat{\jmath}_q = \int d^3r\, e^{-iq\cdot r}\hat{\jmath}(r) = \sum_{k\sigma}(\hbar/m)(k + q/2)\hat{c}^\dagger_{k\sigma}\hat{c}_{k+q\sigma}$$

In particular, for $q = 0$; we have the total current

$$\hat{J}_0 = \int d^3r\, \hat{J}(r) = \sum_{k\sigma} (\hbar k/m)\hat{c}^\dagger_{k\sigma}\hat{c}_{k+q\sigma}$$

Reference: G. Mahan, Many-particle Physics, Section 1.2.