Second-quantization Hamiltonian

David Chen

January 10, 2014

The second quantization is a powerful tool for studying many-body systems. The Hamiltonian in the second-quantization form is

\[ H = \sum_{i,j} \hat{a}_i^\dagger \langle i | H_0 | j \rangle \hat{a}_j + \frac{1}{2} \sum_{i,j,k,l} \hat{a}_i^\dagger \hat{a}_j^\dagger \langle ij | V_{\text{int}} | kl \rangle \hat{a}_k \hat{a}_l. \]  

(1)

where the indices \( i, j, k, l \) represent a state of the system (position, momentum, lattice site, etc). \( \hat{a}_i^\dagger, \hat{a}_i \) are the creation and annihilation operator of a particle in the state \( i \), \( H_0 \) is the single-particle Hamiltonian \( H_0 = \frac{\hbar^2}{2m} + V_{\text{ext}} \) with an external potential \( V_{\text{ext}} \), and \( V_{\text{int}} \) is a two-body interaction potential. The derivation of eq. (1) is in [1,2].

As a particular case, let us consider eq. (1) in the position space. We identify \( i \) with \( r \), \( j \) with \( r' \), \( k \) with \( r'' \), and \( l \) with \( r''' \), and we transform the sums into integrals. In this way, the Hamiltonian reads

\[ H = \int \int d^3r d^3r' \hat{a}_r^\dagger \langle r | H_0 | r' \rangle \hat{a}_{r'} + \frac{1}{2} \int \int \int d^3r d^3r' d^3r'' d^3r''' \hat{a}_r^\dagger \hat{a}_{r'}^\dagger \langle rr' | V_{\text{int}} | r'' r''' \rangle \hat{a}_{r''} \hat{a}_{r'''} \]  

(2)

The one-particle operator \( H_0 \) and the two-particle potential \( U \) satisfy

\[ \langle r | H_0 | r' \rangle = H_0(r) \delta(r - r') \]  

(3a)

\[ \langle rr' | V_{\text{int}} | r'' r''' \rangle = V_{\text{int}}(r, r') \delta(r - r') \delta(r' - r''). \]  

(3b)

Plugging eqs. (3a) and (3b) into (2), and denoting the field operator \( \hat{a}_r \) as \( \hat{\Psi}(r) \), the Hamiltonian becomes

\[ H = \int d^3r \hat{\Psi}^\dagger(r) \left[ -\frac{\hbar^2}{2M} \nabla^2 + V_{\text{ext}}(r) \right] \hat{\Psi}(r) + \frac{1}{2} \int \int d^3r d^3r' \hat{\Psi}^\dagger(r) \hat{\Psi}^\dagger(r') V_{\text{int}}(r, r') \hat{\Psi}(r) \hat{\Psi}(r'). \]  

(4)
The field operator $\hat{\Psi}(\mathbf{r})$ can be expressed in terms of another basis set $\{|l\rangle\}$

$$\hat{\Psi}(\mathbf{r}) \equiv \langle \mathbf{r}|\hat{a} \rangle = \sum_{l} \langle \mathbf{r}|l\rangle \langle l|\hat{a} \rangle = \sum_{l} \psi_{l}(\mathbf{r}) \hat{a}_{l}.$$  \hspace{1cm} (5)

In the particular case of a dilute gas, the effective two-body potential is

$$V_{\text{int}}(\mathbf{r}, \mathbf{r}') = g \delta(\mathbf{r} - \mathbf{r}).$$  \hspace{1cm} (6)

where $g \equiv 4\pi\hbar^2 a_s / M$. This result arises from scattering calculations.

$$H = \int d^3r \hat{\Psi}^\dagger(\mathbf{r}) \left[ -\frac{\hbar^2}{2M} \nabla^2 + V_{\text{ext}}(\mathbf{r}) \right] \hat{\Psi}(\mathbf{r}) + \frac{g}{2} \int d^3r \hat{\Psi}^\dagger(\mathbf{r}) \hat{\Psi}^\dagger(\mathbf{r}) \hat{\Psi}(\mathbf{r}) \hat{\Psi}(\mathbf{r}).$$  \hspace{1cm} (7)

References
