Second-quantization Hamiltonian

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

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

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 $H_0 = \frac{p^2}{2m} + V_{ext}$ with a external potential V_{ext}, and V_{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 $\mathbf{r}$, j with $\mathbf{r}'$, k with $\mathbf{r}''$ and l with $\mathbf{r}'''$, and we transform the sums into integrals. In this way, the hamiltonian reads

$$H = \iint d\mathbf{r} d\mathbf{r}'\, \hat{a}_\mathbf{r}^\dagger \langle \mathbf{r}|H_0|\mathbf{r}'\rangle \hat{a}_{\mathbf{r}'} + \frac{1}{2}\iiiint d^3r\, d^3r'\, d^3r''\, d^3r'''\, \hat{a}_\mathbf{r}^\dagger \hat{a}_{\mathbf{r}'}^\dagger \langle \mathbf{r}\mathbf{r}'|V_{int}|\mathbf{r}''\mathbf{r}'''\rangle \hat{a}_{\mathbf{r}''} \hat{a}_{\mathbf{r}'''}. \tag{2}$$

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

$$\langle \mathbf{r}|H_0|\mathbf{r}'\rangle = H_0(\mathbf{r})\delta(\mathbf{r}-\mathbf{r}') \tag{3a}$$

$$\langle \mathbf{r}\mathbf{r}'|V_{int}|\mathbf{r}''\mathbf{r}'''\rangle = V_{int}(\mathbf{r},\mathbf{r}')\delta(\mathbf{r}-\mathbf{r}'')\delta(\mathbf{r}'-\mathbf{r}'''). \tag{3b}$$

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

$$H = \int d^3r\, \hat{\Psi}^\dagger(\mathbf{r}) \left[-\frac{\hbar^2}{2M}\nabla^2 + V_{ext}(\mathbf{r})\right] \hat{\Psi}(\mathbf{r}) + \frac{1}{2}\iint d^3r\, d^3r'\, \hat{\Psi}^\dagger(\mathbf{r})\hat{\Psi}^\dagger(\mathbf{r}')V_{int}(\mathbf{r},\mathbf{r}')\hat{\Psi}(\mathbf{r})\hat{\Psi}(\mathbf{r}'). \tag{4}$$

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

$$\hat{\Psi}(\mathbf{r}) \equiv \langle \mathbf{r}|\hat{a}\rangle = \sum_l \langle \mathbf{r}|l\rangle\langle l|\hat{a}\rangle = \sum_l \psi_l(\mathbf{r})\hat{a}_l. \tag{5}$$

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

$$V_{int}(\mathbf{r},\mathbf{r}') = g\,\delta(\mathbf{r}-\mathbf{r}'). \tag{6}$$

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

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

References

[1] Bruus, "Many-body theory in condensed matter physics"

[2] Fetter, "Quantum theory of many-particle systems"