Lesson 9 - Second Quantization of Matter
Unit 9.3 Hamiltonian in second quantization with interaction

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Structure of Matter - MSc in Physics

First vs second quantization (I)

In first quantization, the non-relativistic quantum Hamiltonian of N interacting identical particles in the external potential $U(\mathbf{r})$ is given by

$$\hat{H}^{(N)} = \sum_{i=1}^{N} \left[-\frac{\hbar^2}{2m} \nabla_i^2 + U(\mathbf{r}_i) \right] + \frac{1}{2} \sum_{\substack{i,j=1 \\ i \neq j}}^{N} V(\mathbf{r}_i - \mathbf{r}_j) = \sum_{i=1}^{N} \hat{h}_i + \frac{1}{2} \sum_{\substack{i,j=1 \\ i \neq j}}^{N} V_{ij} \ , \tag{1}$$

where $V(\mathbf{r} - \mathbf{r}')$ is the inter-particle potential.
In second quantization, the quantum field operator can be written as

$$\hat{\psi}(\mathbf{r}) = \sum_{\alpha} \hat{c}_{\alpha} \ \phi_{\alpha}(\mathbf{r}) \tag{2}$$

where the $\phi_{\alpha}(\mathbf{r}) = \langle \mathbf{r} | \alpha \rangle$ are the eigenfunctions of $\hat{h}$ such that $\hat{h}|\alpha\rangle = \epsilon_{\alpha}|\alpha\rangle$, and $\hat{c}_{\alpha}$ and $\hat{c}_{\alpha}^{+}$ are the annihilation and creation operators of the single-particle state $|\alpha\rangle$.

First vs second quantization (II)

We now introduce the quantum many-body Hamiltonian

$$\hat{H} = \sum_{\alpha} \epsilon_{\alpha} \; \hat{c}_{\alpha}^{+} \hat{c}_{\alpha} + \sum_{\alpha\beta\gamma\delta} V_{\alpha\beta\gamma\delta} \; \hat{c}_{\alpha}^{+} \hat{c}_{\beta}^{+} \hat{c}_{\delta} \hat{c}_{\gamma} \; , \qquad (3)$$

where

$$V_{\alpha\beta\delta\gamma} = \int d^3\mathbf{r} \; d^3\mathbf{r}' \; \phi_{\alpha}^{*}(\mathbf{r}) \; \phi_{\beta}^{*}(\mathbf{r}') \; V(\mathbf{r}-\mathbf{r}') \; \phi_{\delta}(\mathbf{r}') \; \phi_{\gamma}(\mathbf{r}) \; . \qquad (4)$$

This Hamiltonian can be also written as

$$\begin{aligned} \hat{H} \;\; &= \;\; \int d^3\mathbf{r} \; \hat{\psi}^{+}(\mathbf{r}) \left[-\frac{\hbar^2}{2m} \nabla^2 + U(\mathbf{r}) \right] \hat{\psi}(\mathbf{r}) \\ &+ \;\; \frac{1}{2} \int d^3\mathbf{r} \; d^3\mathbf{r}' \; \hat{\psi}^{+}(\mathbf{r}) \; \hat{\psi}^{+}(\mathbf{r}') \; V(\mathbf{r}-\mathbf{r}') \; \hat{\psi}(\mathbf{r}') \; \hat{\psi}(\mathbf{r}) \; . \qquad (5) \end{aligned}$$

First vs second quantization (III)

The meaningful connection between the second-quantization Hamiltonian $\hat{H}$ and the first-quantization Hamiltonian $\hat{H}^{(N)}$, which is given by the formula

$$\hat{H}|\mathbf{r}_1\mathbf{r}_2...\mathbf{r}_N\rangle = \hat{H}^{(N)}|\mathbf{r}_1\mathbf{r}_2...\mathbf{r}_N\rangle \ . \tag{6}$$

In fact, after some calculations one finds that

$$\hat{\psi}^{+}(\mathbf{r})\,\hat{h}(\mathbf{r})\,\hat{\psi}(\mathbf{r})\,|\mathbf{r}_1\mathbf{r}_2...\mathbf{r}_N\rangle = \sum_{i=1}^{N} \hat{h}(\mathbf{r}_i)\delta(\mathbf{r}-\mathbf{r}_i)\,|\mathbf{r}_1\mathbf{r}_2...\mathbf{r}_N\rangle \tag{7}$$

and also

$$\begin{aligned} & \hat{\psi}^{+}(\mathbf{r})\,\hat{\psi}^{+}(\mathbf{r}')\,V(\mathbf{r},\mathbf{r}')\,\hat{\psi}(\mathbf{r}')\,\hat{\psi}(\mathbf{r})\,|\mathbf{r}_1\mathbf{r}_2...\mathbf{r}_N\rangle \\ = & \sum_{\substack{i,j=1 \\ i\neq j}}^{N} V(\mathbf{r}_i,\mathbf{r}_i)\delta(\mathbf{r}-\mathbf{r}_i)\,\delta(\mathbf{r}'-\mathbf{r}_j)\,|\mathbf{r}_1\mathbf{r}_2...\mathbf{r}_N\rangle \ . \end{aligned} \tag{8}$$

From these two expressions Eq. (6) follows immediately, after space integration.

Coherent states for bosons (I)

The classical analog of the bosonic quantum field operator

$$\hat{\psi}(\mathbf{r}) = \sum_j \phi_j(\mathbf{r})\ \hat{c}_j \tag{9}$$

is the complex classical field

$$\psi(\mathbf{r}) = \sum_j \phi_\alpha(\mathbf{r})\ c_j \tag{10}$$

such that

$$\hat{\psi}(\mathbf{r})|\psi\rangle = \psi(\mathbf{r})|\psi\rangle\ , \tag{11}$$

where

$$|\psi\rangle = \prod_j |c_j\rangle \tag{12}$$

is the bosonic coherent state of the system, $|c_j\rangle$ is the coherent state of the bosonic operator $\hat{c}_j$, and c_j is its complex eigenvalue, namely

$$\hat{c}_j|c_j\rangle = c_j|c_j\rangle\ . \tag{13}$$

Coherent states for fermions (I)

Similarly, one can introduce the pseudo-classical Grassmann analog of the fermionic field operator by using fermionic coherent states. Thus, the classical analog of the fermionic quantum field operator

$$\hat{\psi}(\mathbf{r}) = \sum_j \phi_j(\mathbf{r}) \ \hat{c}_j \tag{14}$$

is the Grassmann classical field

$$\psi(\mathbf{r}) = \sum_j \phi_\alpha(\mathbf{r}) \ c_j \tag{15}$$

such that

$$\hat{\psi}(\mathbf{r})|\psi\rangle = \psi(\mathbf{r})|\psi\rangle \ , \tag{16}$$

where

$$|\psi\rangle = \prod_j |c_j\rangle \tag{17}$$

is the fermionic coherent state of the system, $|c_j\rangle$ is the coherent state of the fermionic operator $\hat{c}_j$, and c_j is its Grassmann eigenvalue, namely

$$\hat{c}_j|c_j\rangle = c_j|c_j\rangle \ . \tag{18}$$

Coherent states for fermions (II)

In the case of fermions, it is immedate to verify that, for mathematical consistency, this eigenvalue c_j must satisfy the following relationships

$$c_j \bar{c}_j + \bar{c}_j c_j = 1 \; , \qquad c_j^2 = \bar{c}_j^2 = 0 \; , \tag{19}$$

where $\bar{c}_j$ is such that

$$\langle c | \hat{c}_j^+ = \bar{c}_j \langle c | \; . \tag{20}$$

Obviously c_j and $\bar{c}_j$ are not complex numbers. They are instead Grassmann numbers, namely elements of the Grassmann linear algebra $\{1, c_j, \bar{c}_j, \bar{c}_j c_j\}$ characterized by the independent basis elements 1, c_j, $\bar{c}_j$, with 1 the identity (neutral) element.

The most general function on this Grassmann algebra is given by

$$f(\bar{c}, c) = f_{11} + f_{12}\; c + f_{21}\; \bar{c} + f_{22}\; \bar{c} c \; , \tag{21}$$

where f_{11}, f_{12}, f_{21}, f_{22} are complex numbers. In fact, the function $f(\bar{c}, c)$ does not have higher powers of c, $\bar{c}$ and $\bar{c}c$ because they are identically zero.