5.9: Appendix I- Second Quantization

Basis States and Creation/Annihilation Operators

Second quantization is a convenient scheme to label basis states of a many particle quantum system. We are ultimately interested in solutions of the many-body Schrödinger equation,

$$\hat{H}\Psi(\mathbf{x}_1,\ldots,\mathbf{x}_N) = E\,\Psi(\mathbf{x}_1,\ldots,\mathbf{x}_N) \tag{5.9.1}$$

where the Hamiltonian is

$$\hat{H} = -\frac{\hbar^2}{2m}\sum_{i=1}^{N}\boldsymbol{\nabla}_i^2 + \sum_{j<k}^{N} V(\mathbf{x}_j - \mathbf{x}_k) \quad . \tag{5.9.2}$$

To the coordinate labels $\{\mathbf{x}_1,\ldots\mathbf{x}_N\}$ we may also append labels for internal degrees of freedom, such as spin polarization, denoted $\{\zeta_1,\ldots,\zeta_N\}$. Since $\big[\hat{H},\sigma\big]=0$ for all permutations $\sigma\in S_N$, the many-body wavefunctions may be chosen to transform according to irreducible representations of the symmetric group S_N. Thus, for any $\sigma\in S_N$,

$$\Psi\big(\mathbf{x}_{\sigma(1)},\ldots,\mathbf{x}_{\sigma(N)}\big) = \begin{Bmatrix} 1 \\ \mathsf{sgn}(\sigma)\end{Bmatrix}\Psi(\mathbf{x}_1,\ldots,\mathbf{x}_N) \quad , \tag{5.9.3}$$

where the upper choice is for Bose-Einstein statistics and the lower sign for Fermi-Dirac statistics. Here $\mathbf{x}_j$ may include not only the spatial coordinates of particle j, but its internal quantum number(s) as well, such as ζ_j.

A convenient basis for the many body states is obtained from the single-particle eigenstates $\big\{|\alpha\rangle\big\}$ of some single-particle Hamiltonian $\hat{H}_0$, with $\langle\,\mathbf{x}\,|\,\alpha\,\rangle = \varphi_\alpha(\mathbf{x})$ and $\hat{H}_0\,|\alpha\rangle = \varepsilon_\alpha\,|\alpha\rangle$. The basis may be taken as orthonormal, $\big\langle\,\alpha\,\big|\,\alpha'\,\big\rangle = \delta_{\alpha\alpha'}$. Now define

$$\Psi_{\alpha_1,\ldots,\alpha_N}(\mathbf{x}_1,\ldots,\mathbf{x}_N) = \frac{1}{\sqrt{N!\prod_\alpha n_\alpha!}}\sum_{\sigma\in S_N}\begin{Bmatrix} 1 \\ \mathsf{sgn}(\sigma)\end{Bmatrix}\varphi_{\alpha_{\sigma(1)}}(\mathbf{x}_1)\cdots\varphi_{\alpha_{\sigma(N)}}(\mathbf{x}_N) \quad . \tag{5.9.4}$$

Here n_α is the number of times the index α appears among the set $\{\alpha_1,\ldots,\alpha_N\}$. For BE statistics, $n_\alpha\in\{0,1,2,\ldots\}$, whereas for FD statistics, $n_\alpha\in\{0,1\}$. Note that the above states are normalized[22]:

$$\begin{aligned}\int\! d^dx_1\cdots\!\int\! d^dx_N\,\big|\Psi_{\alpha_1\cdots\alpha_N}(\mathbf{x}_1,\ldots,\mathbf{x}_N)\big|^2 &= \frac{1}{N!\prod_\alpha n_\alpha!}\sum_{\sigma,\mu\in S_N}\begin{Bmatrix} 1 \\ \mathsf{sgn}(\sigma\mu)\end{Bmatrix}\prod_{j=1}^{N}\int\! d^dx_j\,\varphi^*_{\alpha_{\sigma(j)}}(\mathbf{x}_j)\,\varphi_{\alpha_{\mu(j)}}(\mathbf{x}_j) \\ &= \frac{1}{\prod_\alpha n_\alpha!}\sum_{\sigma\in S_N}\prod_{j=1}^{N}\delta_{\alpha_j,\alpha_{\sigma(j)}} = 1 \quad .\end{aligned}$$

Note that

$$\begin{aligned}\sum_{\sigma\in S_N}\varphi_{\alpha_{\sigma(1)}}(\mathbf{x}_1)\cdots\varphi_{\alpha_{\sigma(N)}}(\mathbf{x}_N) &\equiv \mathsf{per}\big\{\varphi_{\alpha_i}(\mathbf{x}_j)\big\} \\ \sum_{\sigma\in S_N}\mathsf{sgn}(\sigma)\,\varphi_{\alpha_{\sigma(1)}}(\mathbf{x}_1)\cdots\varphi_{\alpha_{\sigma(N)}}(\mathbf{x}_N) &\equiv \mathsf{det}\big\{\varphi_{\alpha_i}(\mathbf{x}_j)\big\} \quad ,\end{aligned}$$

which stand for *permanent* and *determinant*, respectively. We may now write

$$\Psi_{\alpha_1\cdots\,\alpha_N}(\mathbf{x}_1,\ldots,\mathbf{x}_N) = \big\langle\,\mathbf{x}_1,\cdots,\mathbf{x}_N\,\big|\,\alpha_1\cdots\alpha_N\,\big\rangle \quad , \tag{5.9.5}$$

where

$$\big|\,\alpha_1\cdots\,\alpha_N\,\big\rangle = \frac{1}{\sqrt{N!\prod_\alpha n_\alpha!}}\sum_{\sigma\in S_N}\begin{Bmatrix} 1 \\ \mathsf{sgn}(\sigma)\end{Bmatrix}\big|\,\alpha_{\sigma(1)}\big\rangle\otimes\big|\,\alpha_{\sigma(2)}\big\rangle\otimes\cdots\otimes\big|\,\alpha_{\sigma(N)}\big\rangle \quad . \tag{5.9.6}$$

Note that $\big|\,\alpha_{\sigma(1)}\cdots\alpha_{\sigma(N)}\,\big\rangle = (\pm 1)^\sigma\,\big|\,\alpha_1\cdots\alpha_N\,\big\rangle$, where by $(\pm1)^\sigma$ we mean 1 in the case of BE statistics and $sgn\,(\sigma)$ in the case of FD statistics.

We may express $|\,\alpha_1 \cdots \alpha_N\,\rangle$ as a product of creation operators acting on a vacuum $|\,0\,\rangle$ in *Fock space*. For bosons,

$$|\,\alpha_1 \cdots \alpha_N\,\rangle = \prod_\alpha \frac{(b^\dagger_\alpha)^{n_\alpha}}{\sqrt{n_\alpha!}}\,|\,0\,\rangle \equiv |\,\{n_\alpha\}\,\rangle \quad , \tag{5.9.7}$$

with

$$\big[b_\alpha\,,\,b_\beta\big] = 0 \qquad , \qquad \big[b^\dagger_\alpha\,,\,b^\dagger_\beta\big] = 0 \qquad , \qquad \big[b_\alpha\,,\,b^\dagger_\beta\big] = \delta_{\alpha\beta} \quad , \tag{5.9.8}$$

where $[\,\bullet\,,\bullet\,]$ is the commutator. For fermions,

$$|\,\alpha_1 \cdots \alpha_N\,\rangle = c^\dagger_{\alpha_1} c^\dagger_{\alpha_2} \cdots c^\dagger_{\alpha_N}\,|\,0\,\rangle \equiv |\,\{n_\alpha\}\,\rangle \quad , \tag{5.9.9}$$

with

$$\big\{c_\alpha\,,\,c_\beta\big\} = 0 \qquad , \qquad \big\{c^\dagger_\alpha\,,\,c^\dagger_\beta\big\} = 0 \qquad , \qquad \big\{c_\alpha\,,\,c^\dagger_\beta\big\} = \delta_{\alpha\beta} \quad , \tag{5.9.10}$$

where $\{\bullet\,,\bullet\}$ is the anticommutator.

Second Quantized Operators

Now consider the action of permutation-symmetric first quantized operators such as $\hat T = -\frac{\hbar^2}{2m}\sum_{i=1}^N \boldsymbol{\nabla}^2_i$ and $\hat V = \sum_{i<j}^N \hat v(\mathbf{x}_i - \mathbf{x}_j)$. For a one-body operator such as $\hat T$, we have

$$\begin{aligned}\langle\,\alpha_1 \cdots \alpha_N\,|\,\hat T\,|\,\alpha'_1 \cdots \alpha'_N\,\rangle &= \int\! d^dx_1 \cdots \!\int\! d^dx_N \,\Big(\prod_\alpha n_\alpha!\Big)^{-1/2}\Big(\prod_\alpha n'_\alpha!\Big)^{-1/2}\times \\ &\qquad \sum_{\sigma\in S_N} (\pm 1)^\sigma \varphi^*_{\alpha_{\sigma(1)}}(\mathbf{x}_1)\cdots\varphi^*_{\alpha_{\sigma(N)}}(\mathbf{x}_N)\,\sum_{k=1}^N \hat T_i\,\varphi_{\alpha'_{\sigma(1)}}(\mathbf{x}_1)\cdots\varphi_{\alpha'_{\sigma(N)}} \\ &= \sum_{\sigma\in S_N}(\pm 1)^\sigma\,\Big(\prod_\alpha n_\alpha!\,n'_\alpha!\Big)^{-1/2}\sum_{i=1}^N \prod_{\substack{j\\(j\neq i)}} \delta_{\alpha_j,\alpha'_{\sigma(j)}}\int\! d^dx_1\,\varphi^*_{\alpha_i}(\mathbf{x}_1)\,\hat T_1\,\varphi_{\alpha'_{\sigma(i)}}(\mathbf{x}_1) \quad .\end{aligned}$$

One may verify that any permutation-symmetric one-body operator such as $\hat T$ is faithfully represented by the second quantized expression,

$$\hat T = \sum_{\alpha,\beta} \langle\,\alpha\,|\,\hat T\,|\,\beta\,\rangle\,\psi^\dagger_\alpha\,\psi_\beta \quad , \tag{5.9.11}$$

where $\psi^\dagger_\alpha$ is $b^\dagger_\alpha$ or $c^\dagger_\alpha$ as the application determines, and

$$\langle\,\alpha\,|\,\hat T\,|\,\beta\,\rangle = \int\! d^dx_1\,\varphi^*_\alpha(\mathbf{x}_1)\,\hat T_1\,\varphi_\beta(\mathbf{x}_1) \quad . \tag{5.9.12}$$

Similarly, two-body operators such as $\hat V$ are represented as

$$\hat V = \frac{1}{2}\sum_{\alpha,\beta,\gamma,\delta} \langle\,\alpha\beta\,|\,\hat V\,|\,\gamma\delta\,\rangle\,\psi^\dagger_\alpha\,\psi^\dagger_\beta\,\psi_\delta\,\psi_\gamma \quad , \tag{5.9.13}$$

where

$$\langle\,\alpha\beta\,|\,\hat V\,|\,\gamma\delta\,\rangle = \int\! d^dx_1\!\int\! d^dx_2\,\varphi^*_\alpha(\mathbf{x}_1)\,\varphi^*_\beta(\mathbf{x}_2)\,v(\mathbf{x}_1-\mathbf{x}_2)\,\varphi_\delta(\mathbf{x}_2)\,\varphi_\gamma(\mathbf{x}_1) \quad . \tag{5.9.14}$$

The general form for an n-body operator is then

$$\hat R = \frac{1}{n!}\sum_{\substack{\alpha_1\cdots\,\alpha_n\\ \beta_1\cdots\,\beta_n}} \langle\,\alpha_1\cdots\alpha_n\,|\,\hat R\,|\,\beta_1\cdots\beta_n\,\rangle\,\psi^\dagger_{\alpha_n}\cdots\psi^\dagger_{\alpha_n}\,\psi_{\beta_n}\cdots\psi_{\beta_1} \quad . \tag{5.9.15}$$

Finally, if the Hamiltonian is noninteracting, consisting solely of one-body operators $\hat H = \sum_{i=1}^N \hat h_i$, then

$$\hat{H} = \sum_{\alpha} \varepsilon_{\alpha} \, \psi^{\dagger}_{\alpha} \, \psi_{\alpha} \quad , \tag{5.9.16}$$

where $\{\varepsilon_{\alpha}\}$ is the spectrum of each single particle Hamiltonian $\hat{h}_i$.