B.3.3. Field Operators

There are various formalisms designed to treat the many body problem of identical particles. One approach starts by treating the quantum wave functions of single particles as classical fields. These fields are then "quantized" by treating them as operators obeying the appropriate kind of commutation relations. The ensuing methodology is therefore called quantum field theory. In contrast, the number representation is often called the second quantization method since it deals with the time evolution of a system by tracking the discrete changes of the occupation numbers.

Consider now the 1-particle operator defined by (B.52). Its N-representation is given by (B.53) & (B.72) as

$$\hat{\mathbb{O}}^{(1)} = \sum_{\alpha,\alpha'} \left\langle \alpha \mid \hat{O}^{(1)} \mid \alpha' \right\rangle \hat{a}_\alpha^+ \hat{a}_{\alpha'} \qquad \alpha = (\boldsymbol{k}, \lambda) \tag{B.74a}$$

where λ is the z-component of the spin and [see (B.41b) & (B.61c)]

$$[\, \hat{a}_\alpha , \hat{a}_\beta^+ \,]_\mp = \delta_{\alpha\beta} \qquad [\, a_\alpha^+ , a_\beta^+ \,]_\mp = 0 \qquad [\, \hat{a}_\alpha , \hat{a}_\beta \,]_\mp = 0 \qquad \text{for } \begin{matrix}\text{bosons}\\ \text{fermions}\end{matrix} \tag{B.78}$$

In the r-representation, we set

$$\psi_\alpha(\boldsymbol{r}) = \psi_{\boldsymbol{k}\lambda}(\boldsymbol{r}) = \chi_\lambda \langle \boldsymbol{r} \mid \boldsymbol{k} \rangle = \chi_\lambda\, \phi_{\boldsymbol{k}}(\boldsymbol{r})$$

$$\to \quad \psi_\alpha^+(\boldsymbol{r}) = \psi_{\boldsymbol{k}\lambda}^+(\boldsymbol{r}) = \langle \boldsymbol{k} \mid \boldsymbol{r} \rangle \chi_\lambda^+ = \phi_{\boldsymbol{k}}^*(\boldsymbol{r})\, \chi_\lambda^+ \tag{B.74b}$$

where $\psi_\alpha(\boldsymbol{r})$ & χ_λ are spinors and $\phi_{\boldsymbol{k}}(\boldsymbol{r}) = \langle \boldsymbol{r} \mid \boldsymbol{k} \rangle$. For spin 1/2 fermions,

$$\chi_+ = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad \chi_- = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{B.74c}$$

Note: For a general spinor, the ± components may assume different values.

However, since $\phi_{\boldsymbol{k}}(\boldsymbol{r})$ is a basis state for the spatial parts, it is independent of spin.

Using the completeness of $\{ \mid \boldsymbol{r} \rangle \}$, we have

$$\left\langle \alpha \mid \hat{O}^{(1)} \mid \alpha' \right\rangle = \int d^3 r \int d^3 r' \,\langle \alpha \mid \boldsymbol{r} \rangle \left\langle \boldsymbol{r} \mid \hat{O}^{(1)} \mid \boldsymbol{r}' \right\rangle \langle \boldsymbol{r}' \mid \alpha' \rangle$$

Since $\hat{O}^{(1)}$ operates only on one particle, it must take the form

$$\left\langle \boldsymbol{r} \mid \hat{O}^{(1)} \mid \boldsymbol{r}' \right\rangle = \delta(\boldsymbol{r} - \boldsymbol{r}')\, O^{(1)}(\hat{\boldsymbol{p}}, \boldsymbol{r}, \hat{\boldsymbol{\sigma}}) \tag{B.74d}$$

where $\hat{\boldsymbol{p}} = \frac{\hbar}{i} \nabla_{\boldsymbol{r}}$ and $\hat{\boldsymbol{\sigma}}$ is the spin operator. Hence,

$$\begin{aligned}
\left\langle \alpha \mid \hat{O}^{(1)} \mid \alpha' \right\rangle &= \int d^3 r\, \psi_\alpha^+(\boldsymbol{r})\, O^{(1)}\!\left(\frac{\hbar}{i}\nabla_{\boldsymbol{r}}, \boldsymbol{r}, \hat{\boldsymbol{\sigma}} \right) \psi_{\alpha'}(\boldsymbol{r}) \\
&= \int d^3 r\, \phi_{\boldsymbol{k}}^*(\boldsymbol{r})\, \chi_\lambda^+\, O^{(1)}\!\left(\frac{\hbar}{i}\nabla_{\boldsymbol{r}}, \boldsymbol{r}, \hat{\boldsymbol{\sigma}} \right) \chi_{\lambda'}\, \phi_{\boldsymbol{k}'}(\boldsymbol{r}) \\
&= \int d^3 r\, \phi_{\boldsymbol{k}}^*(\boldsymbol{r})\, O_{\lambda\lambda'}^{(1)}\!\left(\frac{\hbar}{i}\nabla_{\boldsymbol{r}}, \boldsymbol{r}, \hat{\boldsymbol{\sigma}} \right) \phi_{\boldsymbol{k}'}(\boldsymbol{r})
\end{aligned} \tag{B.74e}$$

where

$$O_{\lambda\lambda'}^{(1)}\!\left(\frac{\hbar}{i}\nabla_{\boldsymbol{r}}, \boldsymbol{r}, \hat{\boldsymbol{\sigma}} \right) = \chi_\lambda^+\, O^{(1)}\!\left(\frac{\hbar}{i}\nabla_{\boldsymbol{r}}, \boldsymbol{r}, \hat{\boldsymbol{\sigma}} \right) \chi_{\lambda'} \tag{B.74f}$$

(B.74a) thus becomes

$$\hat{\mathbb{O}}^{(1)} = \sum_{\alpha,\alpha'} \int d^3 r\;\; \psi_\alpha^*(\boldsymbol{r})\, O^{(1)}\!\left(\frac{\hbar}{i}\nabla_{\boldsymbol{r}}, \boldsymbol{r}, \hat{\boldsymbol{\sigma}} \right) \psi_{\alpha'}(\boldsymbol{r})\;\; \hat{a}_\alpha^+ \hat{a}_{\alpha'}$$

$$= \sum_{\lambda,\lambda'} \int d^3 r\ \hat{\psi}^+_\lambda(\boldsymbol{r})\, O^{(1)}\left(\frac{\hbar}{i} \nabla_{\boldsymbol{r}} , \boldsymbol{r}, \hat{\boldsymbol{\sigma}} \right) \hat{\psi}_{\lambda'}(\boldsymbol{r}) \tag{B.74g}$$

$$= \sum_{\lambda,\lambda'} \int d^3 r\ \hat{\phi}^+_\lambda(\boldsymbol{r})\, \chi^+_\lambda\, O^{(1)}\left(\frac{\hbar}{i} \nabla_{\boldsymbol{r}} , \boldsymbol{r}, \hat{\boldsymbol{\sigma}} \right) \chi_{\lambda'}\, \hat{\phi}_{\lambda'}(\boldsymbol{r})$$

$$= \sum_{\lambda,\lambda'} \int d^3 r\ \hat{\phi}^+_\lambda(\boldsymbol{r})\, O^{(1)}_{\lambda\lambda'}\left(\frac{\hbar}{i} \nabla_{\boldsymbol{r}} , \boldsymbol{r}, \hat{\boldsymbol{\sigma}} \right) \hat{\phi}_{\lambda'}(\boldsymbol{r}) \tag{B.74}$$

where

$$\hat{\psi}_\lambda (\boldsymbol{r}) = \sum_{\boldsymbol{k}} \psi_{\boldsymbol{k}\lambda}(\boldsymbol{r})\, \hat{a}_{\boldsymbol{k}\lambda} = \chi_\lambda \sum_{\boldsymbol{k}} \phi_{\boldsymbol{k}}(\boldsymbol{r})\, \hat{a}_{\boldsymbol{k}\lambda} = \chi_\lambda\, \hat{\phi}_\lambda(\boldsymbol{r}) \qquad \hat{\phi}_\lambda(\boldsymbol{r}) = \sum_{\boldsymbol{k}} \phi_{\boldsymbol{k}}(\boldsymbol{r})\, \hat{a}_{\boldsymbol{k}\lambda} \tag{B.75}$$

$$\to \quad \hat{\psi}^+_\lambda (\boldsymbol{r}) = \sum_{\boldsymbol{k}} \hat{a}^+_{\boldsymbol{k}\lambda}\, \psi^+_{\boldsymbol{k}\lambda}(\boldsymbol{r}) = \sum_{\boldsymbol{k}} \phi^*_{\boldsymbol{k}}(\boldsymbol{r})\, \hat{a}^+_{\boldsymbol{k}\lambda}\, \chi^+_\lambda = \hat{\phi}^+_\lambda(\boldsymbol{r})\, \chi^+_\lambda \qquad \hat{\phi}^+_\lambda(\boldsymbol{r}) = \sum_{\boldsymbol{k}} \phi^*_{\boldsymbol{k}}(\boldsymbol{r})\, \hat{a}^+_{\boldsymbol{k}\lambda} \tag{B.76}$$

Thus,

$$\left[\hat{\psi}_\lambda (\boldsymbol{r}), \hat{\psi}^+_{\lambda'} (\boldsymbol{r}') \right]_\mp = \sum_{\boldsymbol{k},\boldsymbol{k}'} \psi_{\boldsymbol{k}\lambda}(\boldsymbol{r}) \left[\hat{a}_{\boldsymbol{k}\lambda}, \hat{a}^+_{\boldsymbol{k}'\lambda'} \right]_\mp \psi^+_{\boldsymbol{k}'\lambda'}(\boldsymbol{r}')$$

$$= \sum_{\boldsymbol{k},\boldsymbol{k}'} \phi_{\boldsymbol{k}\lambda}(\boldsymbol{r})\, \chi_\lambda \left[\hat{a}_{\boldsymbol{k}\lambda}, \hat{a}^+_{\boldsymbol{k}'\lambda'} \right]_\mp \chi^+_{\lambda'}\, \phi^*_{\boldsymbol{k}'\lambda}(\boldsymbol{r}')$$

$$= \delta_{\lambda\lambda'}\, \mathbb{I} \sum_{\boldsymbol{k},\boldsymbol{k}'} \phi_{\boldsymbol{k}}(\boldsymbol{r})\, \phi^*_{\boldsymbol{k}'}(\boldsymbol{r}') \left[\hat{a}_{\boldsymbol{k}\lambda}, \hat{a}^+_{\boldsymbol{k}'\lambda} \right]_\mp \qquad [\ \mathbb{I} = \text{identity in spin space.}\ ]$$

$$= \delta_{\lambda\lambda'} \sum_{\boldsymbol{k},\boldsymbol{k}'} \phi_{\boldsymbol{k}}(\boldsymbol{r})\, \phi^*_{\boldsymbol{k}'}(\boldsymbol{r}')\, \delta_{\boldsymbol{k}\boldsymbol{k}'} \qquad [\ \text{(B.78) used. } \mathbb{I} \text{ omitted.}\ ]$$

$$= \delta_{\lambda\lambda'} \sum_{\boldsymbol{k}} \phi_{\boldsymbol{k}}(\boldsymbol{r})\, \phi^*_{\boldsymbol{k}'}(\boldsymbol{r}')$$

$$= \delta_{\lambda\lambda'}\ \delta(\boldsymbol{r} - \boldsymbol{r}') \qquad [\ \{\phi_{\boldsymbol{k}}(\boldsymbol{r})\} \text{ is complete.}\ ] \tag{B.79}$$

$$\left[\hat{\phi}_\lambda (\boldsymbol{r}), \hat{\phi}^+_{\lambda'} (\boldsymbol{r}') \right]_\mp = \delta_{\lambda\lambda'}\ \delta(\boldsymbol{r} - \boldsymbol{r}') \tag{B.79a}$$

Similarly,

$$\left[\hat{\psi}^+_\lambda(\boldsymbol{r}), \hat{\psi}^+_{\lambda'} (\boldsymbol{r}') \right]_\mp = \left[\hat{\psi}_\lambda (\boldsymbol{r}), \hat{\psi}_{\lambda'} (\boldsymbol{r}') \right]_\mp = 0 \tag{B.79b}$$

$$\left[\hat{\phi}^+_\lambda(\boldsymbol{r}), \hat{\phi}^+_{\lambda'} (\boldsymbol{r}') \right]_\mp = \left[\hat{\phi}_\lambda (\boldsymbol{r}), \hat{\phi}_{\lambda'} (\boldsymbol{r}') \right]_\mp = 0 \tag{B.79c}$$

Consider next the 2-body operator (B.58) or (B.73),

$$\hat{\mathbb{O}}^{(2)} = \frac{1}{2} \sum_{\alpha,\alpha',\beta,\beta'} \left\langle \alpha\beta \mid \hat{O}^{(2)} \mid \alpha'\beta' \right\rangle \hat{a}^+_\alpha\, \hat{a}^+_\beta\, \hat{a}_{\beta'}\, \hat{a}_{\alpha'} \tag{B.77a}$$

where

$$\left\langle \alpha\beta \mid \hat{O}^{(2)} \mid \alpha'\beta' \right\rangle = \int d^3 r_1 \int d^3 r_2 \int d^3 r_1' \int d^3 r_2' \langle \alpha\beta \mid \boldsymbol{r}_1 \boldsymbol{r}_2 \rangle \left\langle \boldsymbol{r}_1 \boldsymbol{r}_2 \mid \hat{O}^{(2)} \mid \boldsymbol{r}_1' \boldsymbol{r}_2' \right\rangle \langle \boldsymbol{r}_1' \boldsymbol{r}_2' \mid \alpha'\beta' \rangle$$

Since $\hat{O}^{(2)}$ operates only on two particles, it must take the form

$$\left\langle \boldsymbol{r}_1 \boldsymbol{r}_2 \mid \hat{O}^{(2)} \mid \boldsymbol{r}_1' \boldsymbol{r}_2' \right\rangle = \delta(\boldsymbol{r}_1 - \boldsymbol{r}_1')\, \delta(\boldsymbol{r}_2 - \boldsymbol{r}_2')\, O^{(2)}(\hat{\boldsymbol{p}}_1, \boldsymbol{r}_1, \hat{\boldsymbol{\sigma}}_1;\ \hat{\boldsymbol{p}}_2, \boldsymbol{r}_2, \hat{\boldsymbol{\sigma}}_2) \tag{B.77b}$$

so that

$$\left\langle \alpha\beta \mid \hat{O}^{(2)} \mid \alpha'\beta' \right\rangle = \int d^3 r_1 \int d^3 r_2\ \psi^+_\alpha(\boldsymbol{r}_1)\, \psi^+_\beta(\boldsymbol{r}_2)\, O^{(2)}(\hat{\boldsymbol{p}}_1, \boldsymbol{r}_1, \hat{\boldsymbol{\sigma}}_1;\ \hat{\boldsymbol{p}}_2, \boldsymbol{r}_2, \hat{\boldsymbol{\sigma}}_2)\, \psi_{\alpha'}(\boldsymbol{r}_1)\, \psi_{\beta'}(\boldsymbol{r}_2)$$

$$= \int d^3 r_1 \int d^3 r_2\ \phi^*_\alpha(\boldsymbol{r}_1)\, \phi^*_\beta(\boldsymbol{r}_2)\, O^{(2)}_{\lambda_1\lambda_2,\lambda_1'\lambda_2'}\, \phi_{\alpha'}(\boldsymbol{r}_1)\, \phi_{\beta'}(\boldsymbol{r}_2)$$

where

$$O^{(2)}_{\lambda_1\lambda_2,\lambda_1'\lambda_2'} = \chi^+_{\lambda_1}\, \chi^+_{\lambda_2}\, O^{(2)}(\hat{\boldsymbol{p}}_1, \boldsymbol{r}_1, \hat{\boldsymbol{\sigma}}_1;\ \hat{\boldsymbol{p}}_2, \boldsymbol{r}_2, \hat{\boldsymbol{\sigma}}_2)\, \chi_{\lambda_1'}\, \chi_{\lambda_2'} \tag{B.77c}$$

Setting

$$\alpha = (\boldsymbol{k}_1, \lambda_1) \qquad \beta = (\boldsymbol{k}_2, \lambda_2) \qquad \alpha' = (\boldsymbol{k}_1', \lambda_1') \qquad \beta' = (\boldsymbol{k}_2', \lambda_2')$$

we have

$$\hat{\mathbb{O}}^{(2)} = \frac{1}{2} \sum_{\alpha,\alpha',\beta,\beta'} \int d^3 r_1 \int d^3 r_2 \; \psi_\alpha^+(\boldsymbol{r}_1)\, \psi_\beta^+(\boldsymbol{r}_2)\; O^{(2)}\; \psi_{\alpha'}(\boldsymbol{r}_1)\, \psi_{\beta'}(\boldsymbol{r}_2)\;\; \hat{a}_\alpha^+\, \hat{a}_\beta^+\, \hat{a}_{\beta'}\, \hat{a}_{\alpha'}$$

$$= \frac{1}{2} \sum_{\lambda_1 \lambda_2 \lambda_1' \lambda_2'} \int d^3 r_1 \int d^3 r_2 \; \hat{\psi}_{\lambda_1}^+(\boldsymbol{r}_1)\, \hat{\psi}_{\lambda_2}^+(\boldsymbol{r}_2)\; O^{(2)}\; \hat{\psi}_{\lambda_2'}(\boldsymbol{r}_2)\, \hat{\psi}_{\lambda_1'}(\boldsymbol{r}_1) \qquad \text{(B.77)}$$

$$= \frac{1}{2} \sum_{\substack{\boldsymbol{k}_1 \boldsymbol{k}_2 \boldsymbol{k}_1' \boldsymbol{k}_2' \\ \lambda_1 \lambda_2 \lambda_1' \lambda_2'}} \int d^3 r_1 \int d^3 r_2 \; \phi_{\boldsymbol{k}_1 \lambda_1}^*(\boldsymbol{r}_1)\, \phi_{\boldsymbol{k}_2 \lambda_2}^*(\boldsymbol{r}_2)\, O^{(2)}_{\lambda_1 \lambda_2,\, \lambda_1' \lambda_2'}\, \phi_{\boldsymbol{k}_1' \lambda_1'}(\boldsymbol{r}_1)\, \phi_{\boldsymbol{k}_2' \lambda_2'}(\boldsymbol{r}_2)\, \hat{a}_{\boldsymbol{k}_1 \lambda_1}^+\;\, \hat{a}_{\boldsymbol{k}_2 \lambda_2}^+\;\, \hat{a}_{\boldsymbol{k}_2' \lambda_2'}\, \hat{a}_{\boldsymbol{k}_1' \lambda_1'}$$

$$= \frac{1}{2} \sum_{\lambda_1 \lambda_2 \lambda_1' \lambda_2'} \int d^3 r_1 \int d^3 r_2 \; \hat{\phi}_{\lambda_1}^+(\boldsymbol{r}_1)\, \hat{\phi}_{\lambda_2}^+(\boldsymbol{r}_2)\; O^{(2)}_{\lambda_1 \lambda_2\,,\, \lambda_1' \lambda_2'}\; \hat{\phi}_{\lambda_2'}(\boldsymbol{r}_2)\, \hat{\phi}_{\lambda_1'}(\boldsymbol{r}_1) \qquad \text{(B.77e)}$$

The number density operator at position $\boldsymbol{r}$ in an N-particle system is defined (in the r-representation) as

$$\hat{\rho}_N(\boldsymbol{r}) = \sum_{i=1}^{N} \delta(\boldsymbol{r} - \hat{\boldsymbol{q}}_i) = \sum_{i=1}^{N} \delta(\boldsymbol{r} - \boldsymbol{r}_i) \qquad [\; \hat{O}_N^{(1)} \to \hat{\rho}_N(\boldsymbol{r}) \;] \qquad \text{(B.81a)}$$

where $\boldsymbol{r}_i$ is the position of particle i. This corresponds to a number operator

$$\hat{N}_N = \int d^3 r\, \hat{\rho}_N(\boldsymbol{r}) \qquad [\; \hat{O}_N^{(1)} \to \hat{N}_N \;]$$

$$= \sum_{i=1}^{N} \int d^3 r\, \delta(\boldsymbol{r} - \boldsymbol{r}_i) \qquad [\text{ (B.81a) used. }]$$

$$= \sum_{i=1}^{N} 1 = N \qquad \text{(B.80a)}$$

Hence,

$$\langle \boldsymbol{k}\, \lambda \mid \hat{\rho}_i \mid \boldsymbol{k}'\, \lambda' \rangle = \int d^3 r\, \phi_{\boldsymbol{k}}^*(\boldsymbol{r})\, \chi_\lambda^+ \chi_{\lambda'}\, \delta(\boldsymbol{r} - \boldsymbol{r}_i)\, \phi_{\boldsymbol{k}'}(\boldsymbol{r}) \qquad [\; \hat{O}_i = \hat{\rho}_i \;]$$

$$= \delta_{\lambda \lambda'}\;\; \phi_{\boldsymbol{k}}^*(\boldsymbol{r}_i)\;\, \phi_{\boldsymbol{k}'}(\boldsymbol{r}_i)$$

$$\langle \boldsymbol{k}\, \lambda \mid \hat{\rho} \mid \boldsymbol{k}'\, \lambda' \rangle = \delta_{\lambda \lambda'}\;\; \phi_{\boldsymbol{k}}^*(\boldsymbol{r})\;\, \phi_{\boldsymbol{k}'}(\boldsymbol{r}) \qquad [\; \hat{O}^{(1)} = \hat{\rho} \;] \qquad \text{(B.81b)}$$

Using $\hat{\mathbb{n}}(\boldsymbol{r})$ to denote the N-representation of $\hat{\rho}_N(\boldsymbol{r})$, we have [see (B.53) or (B.72)]

$$\hat{\mathbb{n}}(\boldsymbol{r}) = \sum_{\boldsymbol{k}, \lambda, \boldsymbol{k}', \lambda'} \langle \boldsymbol{k}\, \lambda \mid \hat{\rho} \mid \boldsymbol{k}'\, \lambda' \rangle\, \hat{a}_{\boldsymbol{k},\lambda}^+\, \hat{a}_{\boldsymbol{k}',\lambda'}$$

$$= \sum_{\boldsymbol{k}, \lambda, \boldsymbol{k}', \lambda'} \delta_{\lambda \lambda'}\;\; \phi_{\boldsymbol{k}}^*(\boldsymbol{r})\;\, \phi_{\boldsymbol{k}'}(\boldsymbol{r})\, \hat{a}_{\boldsymbol{k},\lambda}^+\, \hat{a}_{\boldsymbol{k}',\lambda'}$$

$$= \sum_{\boldsymbol{k}, \lambda, \boldsymbol{k}'} \phi_{\boldsymbol{k}}^*(\boldsymbol{r})\;\, \phi_{\boldsymbol{k}'}(\boldsymbol{r})\, \hat{a}_{\boldsymbol{k},\lambda}^+\, \hat{a}_{\boldsymbol{k}',\lambda} \qquad \text{(B.81c)}$$

$$= \sum_{\lambda} \hat{\phi}_\lambda^+(\boldsymbol{r})\, \hat{\phi}_\lambda(\boldsymbol{r}) \qquad [\text{ (B.75-6) used. }] \qquad \text{(B.81d)}$$

If the system is confined in a box of volume V, then

$$\phi_{\boldsymbol{k}}(\boldsymbol{r}) = \frac{1}{\sqrt{V}}\, e^{i\, \boldsymbol{k} \cdot \boldsymbol{r}} \qquad \phi_{\boldsymbol{k}}^*(\boldsymbol{r}) = \frac{1}{\sqrt{V}}\, e^{-i\, \boldsymbol{k} \cdot \boldsymbol{r}}$$

and (B.81c) becomes

$$\hat{n}(\boldsymbol{r}) = \frac{1}{V}\sum_{\boldsymbol{k},\boldsymbol{k}',\lambda} e^{i(\boldsymbol{k}'-\boldsymbol{k})\cdot\boldsymbol{r}}\,\hat{a}^{+}_{\boldsymbol{k},\lambda}\,\hat{a}_{\boldsymbol{k}',\lambda} \tag{B.81}$$

$$= \sum_{\lambda}\int \frac{d^3 k}{(2\pi)^3}\, e^{i(\boldsymbol{k}'-\boldsymbol{k})\cdot\boldsymbol{r}}\,\hat{a}^{+}_{\boldsymbol{k},\lambda}\,\hat{a}_{\boldsymbol{k}',\lambda} \qquad [\text{ For } V \to \infty.\ ]$$

The N-representation of (B.80a) thus becomes

$$\hat{N} = \int d^3 r\, \hat{n}(\boldsymbol{r})$$

$$= \frac{1}{V}\sum_{\boldsymbol{k},\boldsymbol{k}',\lambda}\int d^3 r\, e^{i(\boldsymbol{k}'-\boldsymbol{k})\cdot\boldsymbol{r}}\,\hat{a}^{+}_{\boldsymbol{k},\lambda}\,\hat{a}_{\boldsymbol{k}',\lambda}$$

$$= \frac{(2\pi)^3}{V}\sum_{\boldsymbol{k},\boldsymbol{k}',\lambda}\delta_{\boldsymbol{k}\boldsymbol{k}'}\,\hat{a}^{+}_{\boldsymbol{k},\lambda}\,\hat{a}_{\boldsymbol{k}',\lambda}$$

$$= \frac{(2\pi)^3}{V}\sum_{\boldsymbol{k},\lambda}\hat{a}^{+}_{\boldsymbol{k},\lambda}\,\hat{a}_{\boldsymbol{k},\lambda} \tag{B.80}$$

$$= \sum_{\lambda}\int d^3 k\,\hat{a}^{+}_{\boldsymbol{k},\lambda}\,\hat{a}_{\boldsymbol{k},\lambda} \qquad [\text{ For } V \to \infty.\ ]$$

Similarly, the spin density operator at position $\boldsymbol{r}$ in an N-particle system is defined (in the r-representation) as

$$\hat{\boldsymbol{S}}_N(\boldsymbol{r}) = \sum_{i=1}^{N}\hat{\boldsymbol{\sigma}}_i\,\delta(\boldsymbol{r}-\hat{\boldsymbol{q}}_i) = \sum_{i=1}^{N}\hat{\boldsymbol{\sigma}}_i\,\delta(\boldsymbol{r}-\boldsymbol{r}_i) \qquad [\ \hat{O}^{(1)}_N \to \hat{\boldsymbol{S}}_N(\boldsymbol{r})\ ] \tag{B.82a}$$

where, for spin 1/2 fermions, $\hat{\boldsymbol{\sigma}} = (\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z)$ are the Pauli matrices.

Hence,

$$\langle \boldsymbol{k}\lambda \mid \hat{\boldsymbol{S}}_i \mid \boldsymbol{k}'\lambda' \rangle = \int d^3 r\,\phi^{*}_{\boldsymbol{k}}(\boldsymbol{r})\,\chi^{+}_{\lambda}\,\hat{\boldsymbol{\sigma}}_i\,\chi_{\lambda'}\,\delta(\boldsymbol{r}-\boldsymbol{r}_i)\,\phi_{\boldsymbol{k}'}(\boldsymbol{r}) \qquad [\ \hat{O}_i = \hat{\boldsymbol{S}}_i\ ]$$

$$= \chi^{+}_{\lambda}\,\hat{\boldsymbol{\sigma}}_i\,\chi_{\lambda'}\ \ \phi^{*}_{\boldsymbol{k}}(\boldsymbol{r}_i)\ \phi_{\boldsymbol{k}'}(\boldsymbol{r}_i)$$

$$\langle \boldsymbol{k}\lambda \mid \hat{\boldsymbol{S}} \mid \boldsymbol{k}'\lambda' \rangle = \chi^{+}_{\lambda}\,\hat{\boldsymbol{\sigma}}\,\chi_{\lambda'}\ \ \phi^{*}_{\boldsymbol{k}}(\boldsymbol{r})\ \phi_{\boldsymbol{k}'}(\boldsymbol{r}) \qquad [\ \hat{O}^{(1)} = \hat{\boldsymbol{S}}\ ] \tag{B.82b}$$

$$\to\quad \hat{\mathbb{S}}(\boldsymbol{r}) = \sum_{\boldsymbol{k},\lambda,\boldsymbol{k}',\lambda'}\langle \boldsymbol{k}\lambda \mid \hat{\boldsymbol{S}} \mid \boldsymbol{k}'\lambda' \rangle\,\hat{a}^{+}_{\boldsymbol{k},\lambda}\,\hat{a}_{\boldsymbol{k}',\lambda'}$$

$$= \sum_{\boldsymbol{k},\lambda,\boldsymbol{k}',\lambda'}\chi^{+}_{\lambda}\,\hat{\boldsymbol{\sigma}}\,\chi_{\lambda'}\ \ \phi^{*}_{\boldsymbol{k}}(\boldsymbol{r})\ \phi_{\boldsymbol{k}'}(\boldsymbol{r})\,\hat{a}^{+}_{\boldsymbol{k},\lambda}\,\hat{a}_{\boldsymbol{k}',\lambda'} \tag{B.82c}$$

$$= \sum_{\lambda,\lambda'}\chi^{+}_{\lambda}\,\hat{\boldsymbol{\sigma}}\,\chi_{\lambda'}\ \ \hat{\phi}^{+}_{\boldsymbol{\lambda}}(\boldsymbol{r})\ \hat{\phi}_{\boldsymbol{\lambda}'}(\boldsymbol{r}) \qquad [\ (\text{B.75-6}) \text{ used.}\ ] \tag{B.82d}$$

$$= \frac{1}{V}\sum_{\boldsymbol{k},\lambda,\boldsymbol{k}',\lambda'}\chi^{+}_{\lambda}\,\hat{\boldsymbol{\sigma}}\,\chi_{\lambda'}\ \ e^{i(\boldsymbol{k}'-\boldsymbol{k})\cdot\boldsymbol{r}}\,\hat{a}^{+}_{\boldsymbol{k},\lambda}\,\hat{a}_{\boldsymbol{k}',\lambda'}$$

For the kinetic energy,

$$\hat{T}_N = \sum_{i=1}^{N}\frac{\hat{\boldsymbol{p}}_i^2}{2m} \qquad [\ \hat{O}^{(1)}_N \to \hat{T}_N\ ] \tag{B.83a}$$

Hence,

$$\langle \boldsymbol{k}\lambda \mid \hat{T} \mid \boldsymbol{k}'\lambda' \rangle = \int d^3 r\,\phi^{*}_{\boldsymbol{k}}(\boldsymbol{r})\,\chi^{+}_{\lambda}\,\chi_{\lambda'}\left(-\frac{\hbar^2}{2m}\nabla^2_{\boldsymbol{r}}\right)\phi_{\boldsymbol{k}'}(\boldsymbol{r}) \qquad [\ \hat{O}_i = \hat{T}\ ] \tag{B.83b}$$

$$= \delta_{\lambda\lambda'}\ \ \delta_{\boldsymbol{k}\boldsymbol{k}'}\ \frac{\hbar^2\,\boldsymbol{k}^2}{2m} \tag{B.83c}$$

$$\rightarrow \quad \hat{\mathbb{T}} = \sum_{\boldsymbol{k},\lambda,\boldsymbol{k}',\lambda'} \left\langle \boldsymbol{k}\,\lambda \mid \hat{T} \mid \boldsymbol{k}'\,\lambda' \right\rangle \hat{a}^{+}_{\boldsymbol{k},\lambda}\,\hat{a}_{\boldsymbol{k}',\lambda'}$$

$$= \sum_{\boldsymbol{k},\lambda,\boldsymbol{k}',\lambda'} \delta_{\lambda\lambda'}\;\delta_{\boldsymbol{k}\boldsymbol{k}'}\;\frac{\hbar^2\boldsymbol{k}^2}{2\,m}\,\hat{a}^{+}_{\boldsymbol{k},\lambda}\,\hat{a}_{\boldsymbol{k}',\lambda'} \qquad \text{[(B.83c) used.]}$$

$$= \sum_{\boldsymbol{k},\lambda} \frac{\hbar^2\boldsymbol{k}^2}{2\,m}\,\hat{a}^{+}_{\boldsymbol{k},\lambda}\,\hat{a}_{\boldsymbol{k},\lambda} \qquad \text{(B.83d)}$$

$$= \sum_{\boldsymbol{k},\lambda,\boldsymbol{k}',\lambda'} \int d^3 r\,\phi^{*}_{\boldsymbol{k}}(\boldsymbol{r})\,\chi^{+}_{\lambda}\,\chi_{\lambda'}\left(-\frac{\hbar^2}{2\,m}\,\nabla^2_{\boldsymbol{r}}\right)\phi_{\boldsymbol{k}'}(\boldsymbol{r})\;\hat{a}^{+}_{\boldsymbol{k},\lambda}\,\hat{a}_{\boldsymbol{k}',\lambda'} \qquad \text{[(B.83b) used.]}$$

$$= \sum_{\boldsymbol{k},\lambda,\boldsymbol{k}',\lambda'} \int d^3 r\,\phi^{*}_{\boldsymbol{k}}(\boldsymbol{r})\,\delta_{\lambda\lambda'}\left(-\frac{\hbar^2}{2\,m}\,\nabla^2_{\boldsymbol{r}}\right)\phi_{\boldsymbol{k}'}(\boldsymbol{r})\;\hat{a}^{+}_{\boldsymbol{k},\lambda}\,\hat{a}_{\boldsymbol{k}',\lambda'}$$

$$= \sum_{\boldsymbol{k},\lambda,\boldsymbol{k}'} \int d^3 r\,\phi^{*}_{\boldsymbol{k}}(\boldsymbol{r})\left(-\frac{\hbar^2}{2\,m}\,\nabla^2_{\boldsymbol{r}}\right)\phi_{\boldsymbol{k}'}(\boldsymbol{r})\;\hat{a}^{+}_{\boldsymbol{k},\lambda}\,\hat{a}_{\boldsymbol{k}',\lambda}$$

$$= \sum_{\lambda} \int d^3 r\,\hat{\phi}^{+}_{\lambda}(\boldsymbol{r})\left(-\frac{\hbar^2}{2\,m}\,\nabla^2_{\boldsymbol{r}}\right)\hat{\phi}_{\lambda}(\boldsymbol{r}) \qquad \text{[(B.75-6) used.]} \qquad \text{(B.83)}$$

Finally, for a spin-independent 2-body potential energy operator [see (B.57)]

$$\hat{V}_N = \sum_{i<j}^{N(N-1)/2} \hat{V}_{ij} \qquad [\ \hat{O}^{(2)}_N = \hat{V}_N\ ]$$

(B.77c) simplifies to

$$V_{\lambda_1\lambda_2,\lambda_1'\lambda_2'} = \chi^{+}_{\lambda_1}\,\chi_{\lambda_1'}\,\chi^{+}_{\lambda_2}\,\chi_{\lambda_2'}\,V(\boldsymbol{r}_1-\boldsymbol{r}_2) = \delta_{\lambda_1\lambda_1'}\,\delta_{\lambda_2\lambda_2'}\,V(\boldsymbol{r}_1-\boldsymbol{r}_2) \qquad \text{(B.84a)}$$

so that (B.77a & e) become

$$\hat{\mathbb{V}} = \frac{1}{2}\sum_{\substack{\boldsymbol{k}_1,\lambda_1,\boldsymbol{k}_1',\lambda_1' \\ \boldsymbol{k}_2,\lambda_2,\boldsymbol{k}_2',\lambda_2'}} \delta_{\lambda_1\lambda_1'}\,\delta_{\lambda_2\lambda_2'}\left\langle \boldsymbol{k}_1\,\boldsymbol{k}_2 \mid V \mid \boldsymbol{k}_1'\,\boldsymbol{k}_2' \right\rangle\;\hat{a}^{+}_{\boldsymbol{k}_1,\lambda_1}\;\hat{a}^{+}_{\boldsymbol{k}_2,\lambda_2}\;\hat{a}_{\boldsymbol{k}_2',\lambda_2'}\,\hat{a}_{\boldsymbol{k}_1',\lambda_1'}$$

$$= \frac{1}{2}\sum_{\substack{\boldsymbol{k}_1,\lambda_1,\boldsymbol{k}_1' \\ \boldsymbol{k}_2,\lambda_2,\boldsymbol{k}_2'}} \left\langle \boldsymbol{k}_1\,\boldsymbol{k}_2 \mid V \mid \boldsymbol{k}_1'\,\boldsymbol{k}_2' \right\rangle\;\hat{a}^{+}_{\boldsymbol{k}_1,\lambda_1}\;\hat{a}^{+}_{\boldsymbol{k}_2,\lambda_2}\;\hat{a}_{\boldsymbol{k}_2',\lambda_2}\,\hat{a}_{\boldsymbol{k}_1',\lambda_1}$$

$$= \frac{1}{2}\sum_{\substack{\boldsymbol{k}_1,\lambda_1,\boldsymbol{k}_1' \\ \boldsymbol{k}_2,\lambda_2,\boldsymbol{k}_2'}} \int d^3 r_1 \int d^3 r_2\;\phi^{*}_{\boldsymbol{k}_1}(\boldsymbol{r}_1)\,\phi^{*}_{\boldsymbol{k}_2}(\boldsymbol{r}_2)\;V(\boldsymbol{r}_1-\boldsymbol{r}_2)\;\phi_{\boldsymbol{k}_1'}(\boldsymbol{r}_1)\,\phi_{\boldsymbol{k}_2'}(\boldsymbol{r}_2)\;\hat{a}^{+}_{\boldsymbol{k}_1,\lambda_1}\;\hat{a}^{+}_{\boldsymbol{k}_2,\lambda_2}\;\hat{a}_{\boldsymbol{k}_2',\lambda_2}\,\hat{a}_{\boldsymbol{k}_1',\lambda_1}$$

$$= \frac{1}{2}\sum_{\lambda_1\lambda_2} \int d^3 r_1 \int d^3 r_2\;\hat{\phi}^{+}_{\lambda_1}(\boldsymbol{r}_1)\,\hat{\phi}^{+}_{\lambda_2}(\boldsymbol{r}_2)\;V(\boldsymbol{r}_1-\boldsymbol{r}_2)\,\hat{\phi}_{\lambda_2}(\boldsymbol{r}_2)\,\hat{\phi}_{\lambda_1}(\boldsymbol{r}_1) \qquad \text{(B.84)}$$