B.2. Symmetrized N-Particle Position And Momentum Eigenstates

Consider now the Hamiltonian for N identical particles

$$\hat{H}_N = \sum_{i=1}^{N} h(\hat{\boldsymbol{p}}_i, \hat{r}_i) + \sum_{i<j=1}^{N(N-1)/2} \mathcal{V}(\hat{r}_i, \hat{r}_j) \qquad \hat{r} = (\hat{\boldsymbol{q}}, \hat{s}_z) \tag{B.1}$$

where

$$h(\hat{\boldsymbol{p}}_i, \hat{r}_i) = \frac{\hat{\boldsymbol{p}}_i^2}{2m} + v(\hat{r}_i) \tag{B.1a}$$

is a 1-body Hamiltonian.

Let

$$|\, r \rangle \equiv |\, \boldsymbol{r}, s_z \rangle = |\, \boldsymbol{r} \rangle \otimes |\, s_z \rangle \tag{B.15a}$$

be the simultaneous eigenstate of the position $\hat{\boldsymbol{q}}$ & z-component of spin $\hat{\boldsymbol{s}}_z$ operators, where $\otimes$ is the direct product. Similarly,

$$|\, k \rangle \equiv |\, \boldsymbol{k}, s_z \rangle = |\, \boldsymbol{k} \rangle \otimes |\, s_z \rangle \tag{B.15b}$$

is an eigenstate of the 1-body Hamiltonian with $\boldsymbol{k}$ denoting its complete set of quantum numbers. For example, if $\hat{h}$ is the free particle Hamiltonian, then $\boldsymbol{k}$ is simply the wave vector. If $\hat{h}$ is the Hamiltonian for an electron in an atom, then $\boldsymbol{k} = \{n, l, m\}$.

Since $\{\, |\, r \rangle \}$ is an orthonormal and complete set of states that form a basis for a 1-particle Hilbert space, we can use the set of direct products

$$|\, r_1, r_2, \ldots, r_N \rangle \equiv |\, r_1 \rangle \otimes |\, r_2 \rangle \otimes \ldots \otimes |\, r_N \rangle \tag{B.15}$$

as a basis for a N-particle Hilbert space. Quantities expressed in this basis are called the r-representation. Similarly, for the k-representation, the basis is the set

$$|\, k_1, k_2, \ldots, k_N \rangle \equiv |\, k_1 \rangle \otimes |\, k_2 \rangle \otimes \ldots \otimes |\, k_N \rangle \tag{B.16}$$

It is easily proved that the orthonormality & completeness of the 1-particle basis are directly translated into those for the N-particle basis.

With respect to the basis (B.15), we have

$$\begin{aligned} H(r_1, \ldots, r_N) &\equiv \langle r_1, r_2, \ldots, r_N \,|\, \hat{H}_N \,|\, r_1, r_2, \ldots, r_N \rangle \\ &= \sum_{i=1}^{N} h\left(\frac{\hbar}{i} \nabla_{\boldsymbol{r}_i}, r_i \right) + \sum_{i<j=1}^{N(N-1)/2} \mathcal{V}(r_i, r_j) \end{aligned} \tag{B.17}$$

Reminder: We use ^ to denote an operator on the bras $\langle \ldots |$ & kets $| \ldots \rangle$.
The gradient $\nabla_{\boldsymbol{r}_i}$ is not an operator in this sense.

Let $\hat{P}_{ij}$ be the operator that permute (or exchange) particles i and j. Since the particles are identical, $\hat{H}_N$ must be invariant under $\hat{P}_{ij}$.

$$\hat{P}_{ij}\, \hat{H}_N\, \hat{P}_{ij}^{-1} = \hat{H}_N \quad \rightarrow \quad \hat{P}_{ij}\, \hat{H}_N = \hat{H}_N\, \hat{P}_{ij} \qquad \forall\ i, j = 1, \ldots, N \tag{B.17a}$$

i.e., $\hat{P}_{ij}$ & $\hat{H}_N$ commute.

Let $|\, E \rangle$ be an eigenstate of $\hat{H}_N$ so that

$$\hat{H}_N \,|\, E \rangle = E \,|\, E \rangle \tag{B.17b}$$

Then $\hat{P}_{ij}$ (B.17b) gives

$$\hat{P}_{ij}\hat{H}_N \left| E \right\rangle = E\,\hat{P}_{ij} \left| E \right\rangle$$

$$= \hat{H}_N \hat{P}_{ij} \left| E \right\rangle \qquad \text{[(B.17a) used.]}$$

which means $\hat{P}_{ij} \left| E \right\rangle$ is also an eigenstate of $\hat{H}_N$ with the same eigenvalue E. Similarly, let $| \alpha \rangle$ be an eigenstate of $\hat{P}_{ij}$ so that

$$\hat{P}_{ij} \left| \alpha \right\rangle = \alpha \left| \alpha \right\rangle \qquad \text{(B.17c)}$$

then $\hat{H}_N \left| \alpha \right\rangle$ is also an eigenstate of $\hat{P}_{ij}$ with the same eigenvalue α. Note that α is independent of i & j since the exchange operation should work the same way irregardless of the labelling.

Thus $\hat{P}_{ij}$ & $\hat{H}_N$ share the same eigenstates, which can be designated as $| E, \alpha \rangle$.

Now, exchanging the same pair of particles twice simply restores the original particle assignments, i.e.,

$$\hat{P}_{ij}\hat{P}_{ij} = \hat{I} \qquad \text{(B.17d)}$$

Therefore, (B.17c) gives

$$\hat{P}_{ij}\hat{P}_{ij} \left| \alpha \right\rangle = \alpha^2 \left| \alpha \right\rangle = | \alpha \rangle \qquad \text{[(B.17d) used.]}$$

$$\rightarrow \quad \alpha = \pm 1 \qquad \text{(B.17e)}$$

Hence, the eigenstates of $\hat{H}_N$ must be either symmetric ($\alpha = 1$) or anti-symmetric ($\alpha = -1$) under $\hat{P}_{ij}\ \forall\ i, j$. Identical particles whose eigenstates are symmetric (anti-symmetric) under particle exchanges are called bosons (fermions).

B.2.1. Symmetrized Momentum Eigenstates for Bose-Einstein Particles

The particle exchange $i \leftrightarrow j$ results in an exchange of the corresponding occupied states

$$\hat{P}_{ij} \left| \;\ldots, k_i,\ \ldots, k_j,\ \ldots \right\rangle = \left| \;\ldots, k_j,\ \ldots, k_i,\ \ldots \right\rangle \qquad \text{(B.18)}$$

By definition, a state ψ_N for N bosons must satisfy

$$\hat{P}_{ij} \left| \psi_N \right\rangle = \left| \psi_N \right\rangle \qquad \forall\ i, j \qquad \text{(B.18a)}$$

Now, an arbitrary sequence of pair-wise exchanges among N-particles can be represented concisely by a single permutation $\hat{\mathcal{P}}$. Furthermore, while the number of possible sequences of pair-wise exchanges is infinite, the number of distinct permutations is finite. Therefore, the following discussions will be in terms of permutations. (B.18a) is therefore re-phrased as

$$\hat{\mathcal{P}} \left| \psi_N \right\rangle = \left| \psi_N \right\rangle \qquad \forall\ \mathcal{P} \qquad \text{(B.18b)}$$

Since we can always expand $\left| \psi_N \right\rangle$ as a linear combination of the basis $| k_1, \ldots, k_N \rangle$, it suffices to consider only the latter.

While the number of distinct permutations of the particle labels is always $N!$, that of the resultant states depends on the number n_j of k's that have the same value k_j. In general, the number of distinct permutations of $| k_1, \ldots, k_N \rangle$ is $\dfrac{N!}{\prod_j n_j!}$, where j runs over the distinct k values present.

For example, $\{n_1, n_2, n_3\} = \{1,1,1\}$ gives $\frac{N!}{\prod_j n_j!} = \frac{3!}{1!\cdot 1!\cdot 1!} = 6$ distinct terms so that

$$\sum_{\mathcal{P}} \hat{\mathcal{P}} \left| k_1 k_2 k_3 \right\rangle = \left| k_1 k_2 k_3 \right\rangle + \left| k_1 k_3 k_2 \right\rangle + \left| k_3 k_2 k_1 \right\rangle + \left| k_2 k_1 k_3 \right\rangle + \left| k_2 k_3 k_1 \right\rangle + \left| k_3 k_1 k_2 \right\rangle \tag{B.20}$$

and $\{n_1, n_2\} = \{2,1\}$ gives $\frac{N!}{\prod_j n_j!} = \frac{3!}{2!\cdot 1!} = 3$ distinct terms so that

$$\sum_{\mathcal{P}} \hat{\mathcal{P}} \left| k_1 k_1 k_2 \right\rangle = \left| k_1 k_1 k_2 \right\rangle + \left| k_1 k_2 k_1 \right\rangle + \left| k_2 k_1 k_1 \right\rangle \tag{B.20a}$$

Note that the subscript j in k_j merely denotes different values of k, and the n_j's in the formula $\frac{N!}{\prod_j n_j!}$ counts only those k_j's listed in $| k_1, \ldots, k_N \rangle$.

Orthonormality of the 1-particle states leads to that of the direct product states of (B.15):

$$\left\langle k_1, \ldots, k_N \,\middle|\, k_1', \ldots, k_N' \right\rangle = \langle k_1 | k_1' \rangle \ldots \langle k_N | k_N' \rangle = \delta_{k_1 k_1'} \ldots \delta_{k_N k_N'} \tag{B.21}$$

The condition (B.18b) can be satisfied if we expand $| \psi_N \rangle$ in terms of the symmetrized basis

$$\left| k_1, \ldots, k_N \right\rangle^{(S)} \equiv \sqrt{\frac{\prod_j n_j!}{N!}} \sum_{\mathcal{P}} \hat{\mathcal{P}} \left| k_1, \ldots, k_N \right\rangle \tag{B.22}$$

The orthonormality & completeness of this basis follows from those of the 1-particle states:

$$^{(S)}\left\langle k_1, \ldots, k_N \,\middle|\, k_1', \ldots, k_N' \right\rangle^{(S)} = \delta_{k_1 k_1'} \ldots \delta_{k_N k_N'} \tag{B.23}$$

$$\sum_{k_1, \ldots, k_N} \frac{\prod_j n_j!}{N!} \left| k_1, \ldots, k_N \right\rangle^{(S)} {}^{(S)}\left\langle k_1, \ldots, k_N \right| = \hat{1} \tag{B.24}$$

where the factor $\frac{\prod_j n_j!}{N!}$ is inserted to counteract the over-counting in the summations. This is necessary because any permutation among the indices in the summations will lead to the same symmetrized state.

For example,

$$\begin{aligned}
\sum_{k_1=1}^{3} \sum_{k_2=1}^{3} \sum_{k_2=1}^{3} \left| k_1 k_2 k_3 \right\rangle &= \sum_{k_1=1}^{3} \sum_{k_2=1}^{3} \left(\left| k_1 k_2 1 \right\rangle + \left| k_1 k_2 2 \right\rangle + \left| k_1 k_2 3 \right\rangle \right) \\
&= \sum_{k_1=1}^{3} \left(\left| k_1 11 \right\rangle + \left| k_1 21 \right\rangle + \left| k_1 31 \right\rangle + \left| k_1 12 \right\rangle + \left| k_1 22 \right\rangle + \left| k_1 32 \right\rangle + \left| k_1 13 \right\rangle + \left| k_1 23 \right\rangle + \left| k_1 33 \right\rangle \right) \\
&= \left| 111 \right\rangle + \left| 211 \right\rangle + \left| 311 \right\rangle + \left| 121 \right\rangle + \left| 221 \right\rangle + \left| 321 \right\rangle \\
&\quad + \left| 131 \right\rangle + \left| 231 \right\rangle + \left| 331 \right\rangle + \left| 112 \right\rangle + \left| 212 \right\rangle + \left| 312 \right\rangle \\
&\quad + \left| 122 \right\rangle + \left| 222 \right\rangle + \left| 322 \right\rangle + \left| 132 \right\rangle + \left| 232 \right\rangle + \left| 332 \right\rangle \\
&\quad + \left| 113 \right\rangle + \left| 213 \right\rangle + \left| 313 \right\rangle + \left| 123 \right\rangle + \left| 223 \right\rangle + \left| 323 \right\rangle
\end{aligned}$$

$$+\left|133\right\rangle+\left|233\right\rangle+\left|333\right\rangle$$

Grouping states that lead to the same symmetrized state together, we have

$$\sum_{k_1=1}^{3}\sum_{k_2=1}^{3}\sum_{k_2=1}^{3}\left|k_1\,k_2\,k_3\right\rangle=\left|111\right\rangle+\left|222\right\rangle+\left|333\right\rangle$$
$$+\left(\left|211\right\rangle+\left|121\right\rangle+\left|112\right\rangle\right)+\left(\left|311\right\rangle+\left|131\right\rangle+\left|113\right\rangle\right)$$
$$+\left(\left|221\right\rangle+\left|212\right\rangle+\left|122\right\rangle\right)+\left(\left|322\right\rangle+\left|232\right\rangle+\left|223\right\rangle\right)$$
$$+\left(\left|331\right\rangle+\left|313\right\rangle+\left|133\right\rangle\right)+\left(\left|332\right\rangle+\left|233\right\rangle+\left|323\right\rangle\right)$$
$$+\left(\left|321\right\rangle+\left|231\right\rangle+\left|312\right\rangle+\left|132\right\rangle+\left|213\right\rangle+\left|123\right\rangle\right)$$

Hence, for all three k's the same, there are 3 groups, each consisting of $\frac{N!}{\prod_j n_j!}=\frac{3!}{3!}=1$ state. For two k's the same, there are 6 groups, each consisting of $\frac{N!}{\prod_j n_j!}=\frac{3!}{2!\cdot 1!}=3$ states. Finally, for all three k's different, there is only 1 group of $\frac{N!}{\prod_j n_j!}=\frac{3!}{1!\cdot 1!\cdot 1!}=6$ states. In total, there are

$$3\times 1+6\times 3+1\times 6=27 \text{ states}$$
$$=3\times 3\times 3 = \text{Numbers of terms in } \sum_{k_1=1}^{3}\sum_{k_2=1}^{3}\sum_{k_2=1}^{3}$$

However, there are only

$$3+6+1=10 \text{ independent symmetrized states}$$

which can be taken as

$$\left|111\right\rangle^{(S)},\ \left|222\right\rangle^{(S)},\ \left|333\right\rangle^{(S)}$$
$$\left|112\right\rangle^{(S)},\ \left|113\right\rangle^{(S)},\ \left|122\right\rangle^{(S)},\ \left|223\right\rangle^{(S)},\ \left|133\right\rangle^{(S)},\ \left|233\right\rangle^{(S)} \qquad \text{(B.24a)}$$
$$\left|123\right\rangle^{(S)}$$

B.2.2. Antisymmetrized Momentum Eigenstates for Fermi-Dirac Particles

A state ϕ_N for N fermions must satisfy [c.f.(B.18b)]

$$\hat{\mathcal{P}}\left|\phi_N\right\rangle=(-)^{\mathcal{P}}\left|\phi_N\right\rangle \qquad \forall\ \mathcal{P} \qquad \text{(B.25a)}$$

where $(-)^{\mathcal{P}}$ equals to $+1$ (-1) if $\mathcal{P}$ is a product of an even (odd) number of 2-particle exchanges.

The condition (B.25a) can be satisfied if we expand $|\ \phi_N\ \rangle$ in terms of the antisymmetrized basis

$$\left|k_1,\ \ldots,\ k_N\right\rangle^{(A)}\equiv\frac{1}{\sqrt{N!}}\sum_{\mathcal{P}}(-)^{\mathcal{P}}\,\hat{\mathcal{P}}\left|k_1,\ldots,k_N\right\rangle \qquad \text{(B.25)}$$

The orthonormality & completeness of this basis follows from those of the 1-particle states:

$${}^{(A)}\!\left\langle k_1,\ \ldots,\ k_N\,\middle|\,k_1',\ \ldots,\ k_N'\right\rangle^{(A)}=\delta_{k_1 k_1'}\ldots\delta_{k_N k_N'} \qquad \text{(B.27)}$$

$$\sum_{k_1,\ldots,k_N}\frac{1}{N!}\left|k_1,\ \ldots,\ k_N\right\rangle^{(A)}\ {}^{(A)}\!\left\langle k_1,\ \ldots,\ k_N\right|=\hat{1} \qquad \text{(B.28)}$$

where the factor $\frac{1}{N!}$ is inserted to counteract the over-counting in the summations.

In the r-representation, (B.25) becomes

$$\begin{aligned}\phi_N(\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_N) &= \left\langle \boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_N \,\middle|\, k_1, \ldots, k_N \right\rangle^{(A)} \\ &= \frac{1}{\sqrt{N!}} \sum_{\mathcal{P}} (-)^{\mathcal{P}} \left\langle \boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_N \,\middle|\, \hat{\mathcal{P}} \,\middle|\, k_1, \ldots, k_N \right\rangle \\ &= \frac{1}{\sqrt{N!}} \det \begin{vmatrix} \langle \boldsymbol{r}_1 | k_1 \rangle & \langle \boldsymbol{r}_1 | k_2 \rangle & \cdots & \langle \boldsymbol{r}_1 | k_N \rangle \\ \langle \boldsymbol{r}_2 | k_1 \rangle & \langle \boldsymbol{r}_2 | k_2 \rangle & \cdots & \langle \boldsymbol{r}_2 | k_N \rangle \\ \vdots & \vdots & \ddots & \vdots \\ \langle \boldsymbol{r}_N | k_1 \rangle & \langle \boldsymbol{r}_N | k_2 \rangle & \cdots & \langle \boldsymbol{r}_N | k_N \rangle \end{vmatrix} \qquad \text{(B.29)} \\ &= \frac{1}{\sqrt{N!}} \det \begin{vmatrix} \phi_{k_1}(\boldsymbol{r}_1) & \phi_{k_2}(\boldsymbol{r}_1) & \cdots & \phi_{k_N}(\boldsymbol{r}_1) \\ \phi_{k_1}(\boldsymbol{r}_2) & \phi_{k_2}(\boldsymbol{r}_2) & \cdots & \phi_{k_N}(\boldsymbol{r}_2) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_{k_1}(\boldsymbol{r}_N) & \phi_{k_2}(\boldsymbol{r}_N) & \cdots & \phi_{k_N}(\boldsymbol{r}_N) \end{vmatrix}\end{aligned}$$

where

$$\phi_{k_i}(\boldsymbol{r}_j) = \phi_{\boldsymbol{k}_i, s_i}(\boldsymbol{r}_j)$$

The determinant in (B.29) is known as a Slater determinant.

B.2.3. Partition Functions & Expectation Values

With respect to the basis (B.22), the partition function for an N boson system is

$$Z_N = \operatorname{Tr} e^{-\beta \hat{H}_N} = \sum_{k_1, \ldots, k_N} \frac{\prod_j n_j!}{N!} \, {}^{(S)}\!\left\langle k_1, \ldots, k_N \,\middle|\, e^{-\beta \hat{H}_N} \,\middle|\, k_1, \ldots, k_N \right\rangle^{(S)} \qquad \text{(B.30a)}$$

where the factor $\frac{\prod_j n_j!}{N!}$ serves the same purpose as that in (B.24).

Since $\hat{H}_N$ is invariant under $\hat{\mathcal{P}}$,

$$\begin{aligned}\left\langle k_1, \ldots, k_N \,\middle|\, e^{-\beta \hat{H}_N} \,\middle|\, k_1, \ldots, k_N \right\rangle^{(S)} &= \left\langle k_1, \ldots, k_N \,\middle|\, \hat{\mathcal{P}} e^{-\beta \hat{H}_N} \hat{\mathcal{P}}^{-1} \,\middle|\, k_1, \ldots, k_N \right\rangle^{(S)} \\ &= \left\langle k_1, \ldots, k_N \,\middle|\, \hat{\mathcal{P}} e^{-\beta \hat{H}_N} \,\middle|\, k_1, \ldots, k_N \right\rangle^{(S)} \qquad \text{(B.30b)}\end{aligned}$$

because $\left| k_1, \ldots, k_N \right\rangle^{(S)}$ is invariant under $\hat{\mathcal{P}}^{-1}$. Since $\hat{\mathcal{P}}$ must be Hermitian, each term, $\left\langle k_1, \ldots, k_N \right| \hat{\mathcal{P}}$, in ${}^{(S)}\!\left\langle k_1, \ldots, k_N \right|$ gives the same contribution to (B.30a).

Putting (B.22) into (B.30a) gives

$$\begin{aligned}Z_N &= \sum_{k_1, \ldots, k_N} \frac{\prod_j n_j!}{N!} \sqrt{\frac{\prod_j n_j!}{N!}} \sum_{\mathcal{P}} \left\langle k_1, \ldots, k_N \,\middle|\, \hat{\mathcal{P}} e^{-\beta \hat{H}_N} \,\middle|\, k_1, \ldots, k_N \right\rangle^{(S)} \\ &= \sum_{k_1, \ldots, k_N} \frac{\prod_j n_j!}{N!} \sqrt{\frac{\prod_j n_j!}{N!}} \frac{N!}{\prod_j n_j!} \left\langle k_1, \ldots, k_N \,\middle|\, e^{-\beta \hat{H}_N} \,\middle|\, k_1, \ldots, k_N \right\rangle^{(S)} \qquad \text{[(B.30b) used.]} \\ &= \sum_{k_1, \ldots, k_N} \sqrt{\frac{\prod_j n_j!}{N!}} \left\langle k_1, \ldots, k_N \,\middle|\, e^{-\beta \hat{H}_N} \,\middle|\, k_1, \ldots, k_N \right\rangle^{(S)} \qquad \text{(B.30c)}\end{aligned}$$

Setting

$$\left| k_1, \ldots, k_N \right\rangle^{(+)} \equiv \sum_{\mathcal{P}} \hat{\mathcal{P}} \left| k_1, \ldots, k_N \right\rangle \tag{B.31}$$

$$= \sqrt{\frac{N!}{\prod_j n_j!}} \left| k_1, \ldots, k_N \right\rangle^{(S)}$$

(B.30c) becomes, for N bosons,

$$Z_N = \sum_{k_1, \ldots, k_N} \frac{\prod_j n_j!}{N!} \left\langle k_1, \ldots, k_N \right| e^{-\beta \hat{H}_N} \left| k_1, \ldots, k_N \right\rangle^{(+)} \tag{B.30}$$

Note that the factor $\frac{\prod_j n_j!}{N!}$ is the same as that in (B.30a), and serves the same purpose.

The partition function for an N fermion system is

$$Z_N = \mathrm{Tr}\, e^{-\beta \hat{H}_N} = \frac{1}{N!} \sum_{k_1, \ldots, k_N} {}^{(A)}\!\left\langle k_1, \ldots, k_N \right| e^{-\beta \hat{H}_N} \left| k_1, \ldots, k_N \right\rangle^{(A)} \tag{B.32a}$$

where the factor $\frac{1}{N!}$ serves the same purpose as that in (B.28).

Since $\mathcal{P}$ & $\mathcal{P}^{-1}$ are decomposed into the same number of 2-particle exchanges, $(-)^{\mathcal{P}} = (-)^{\mathcal{P}^{-1}}$. This in turn implies

$$\hat{\mathcal{P}}^{-1} \left| k_1, \ldots, k_N \right\rangle^{(A)} = (-)^{\mathcal{P}} \left| k_1, \ldots, k_N \right\rangle^{(A)} \qquad \forall\, \mathcal{P} \tag{B.32b}$$

Therefore, the fermion version of (B.30b) is

$$\left\langle k_1, \ldots, k_N \right| e^{-\beta \hat{H}_N} \left| k_1, \ldots, k_N \right\rangle^{(A)} = \left\langle k_1, \ldots, k_N \right| \hat{\mathcal{P}} e^{-\beta \hat{H}_N} \hat{\mathcal{P}}^{-1} \left| k_1, \ldots, k_N \right\rangle^{(A)}$$

$$= (-)^{\mathcal{P}} \left\langle k_1, \ldots, k_N \right| \hat{\mathcal{P}} e^{-\beta \hat{H}_N} \left| k_1, \ldots, k_N \right\rangle^{(A)} \tag{B.32c}$$

Thus, each term, $(-)^{\mathcal{P}} \left\langle k_1, \ldots, k_N \right| \hat{\mathcal{P}}$, in ${}^{(A)}\!\left\langle k_1, \ldots, k_N \right|$ gives the same contribution to (B.32a).

Putting (B.25) into (B.32a) gives

$$Z_N = \sum_{k_1, \ldots, k_N} \frac{1}{N!} \frac{1}{\sqrt{N!}} \sum_{\mathcal{P}} (-)^{\mathcal{P}} \left\langle k_1, \ldots, k_N \right| \hat{\mathcal{P}} e^{-\beta \hat{H}_N} \left| k_1, \ldots, k_N \right\rangle^{(A)}$$

$$= \sum_{k_1, \ldots, k_N} \frac{1}{\sqrt{N!}} \left\langle k_1, \ldots, k_N \right| e^{-\beta \hat{H}_N} \left| k_1, \ldots, k_N \right\rangle^{(A)} \qquad \text{[(B.32c) use.d]}$$

$$= \sum_{k_1, \ldots, k_N} \frac{1}{N!} \left\langle k_1, \ldots, k_N \right| e^{-\beta \hat{H}_N} \left| k_1, \ldots, k_N \right\rangle^{(-)} \tag{B.32}$$

where

$$\left| k_1, \ldots, k_N \right\rangle^{(-)} \equiv \sum_{\mathcal{P}} (-)^{\mathcal{P}} \hat{\mathcal{P}} \left| k_1, \ldots, k_N \right\rangle \tag{B.33}$$

$$= \sqrt{N!} \left| k_1, \ldots, k_N \right\rangle^{(A)}$$

To check the correctness of (B.30), consider the case of two particles & two 1-particle states. (B.30a) & (B.30) become

$$Z_2 = \sum_{k_1=a}^{b} \sum_{k_2=a}^{b} \frac{\prod_j n_j!}{N!} \; {}^{(S)}\Big\langle k_1, k_2 \;\Big|\; e^{-\beta \hat{H}_2} \;\Big|\; k_1, k_2 \Big\rangle^{(S)} \qquad \text{(a)}$$

$$= \sum_{k_1=a}^{b} \sum_{k_2=a}^{b} \frac{\prod_j n_j!}{N!} \; \Big\langle k_1, k_2 \;\Big|\; e^{-\beta \hat{H}_2} \;\Big|\; k_1, k_2 \Big\rangle^{(+)} \qquad \text{(b)}$$

where, with self-explaining notations,

$$\hat{H}_2 = \hat{h}(1) + \hat{h}(2) + \hat{\mathcal{V}}(1,2)$$

Using (a) and $\mid a\,b \rangle^{(S)} = \mid b\,a \rangle^{(S)}$, we have

$$Z_2 = {}^{(S)}\Big\langle a\,a \;\Big|\; e^{-\beta \hat{H}_2} \;\Big|\; a\,a \Big\rangle^{(S)} + {}^{(S)}\Big\langle a\,b \;\Big|\; e^{-\beta \hat{H}_2} \;\Big|\; a\,b \Big\rangle^{(S)} + {}^{(S)}\Big\langle b\,b \;\Big|\; e^{-\beta \hat{H}_2} \;\Big|\; b\,b \Big\rangle^{(S)}$$

$$= \Big\langle a\,a \;\Big|\; e^{-\beta \hat{H}_2} \;\Big|\; a\,a \Big\rangle + \frac{1}{2}\Big(\Big\langle a\,b \;\Big| + \Big\langle b\,a \;\Big| \Big) e^{-\beta \hat{H}_2} \Big(\;\Big|\; a\,b \Big\rangle + \Big|\; b\,a \Big\rangle \Big) \qquad \text{(c)}$$

$$+ \Big\langle b\,b \;\Big|\; e^{-\beta \hat{H}_2} \;\Big|\; b\,b \Big\rangle$$

Using (b), we have

$$Z_2 = \Big\langle a\,a \;\Big|\; e^{-\beta \hat{H}_2} \;\Big|\; a\,a \Big\rangle^{(+)} + \frac{1}{2}\Big\langle a\,b \;\Big|\; e^{-\beta \hat{H}_2} \;\Big|\; a\,b \Big\rangle^{(+)} + \frac{1}{2}\Big\langle b\,a \;\Big|\; e^{-\beta \hat{H}_2} \;\Big|\; b\,a \Big\rangle^{(+)}$$

$$+ \Big\langle b\,b \;\Big|\; e^{-\beta \hat{H}_2} \;\Big|\; b\,b \Big\rangle^{(+)}$$

$$= \Big\langle a\,a \;\Big|\; e^{-\beta \hat{H}_2} \;\Big|\; a\,a \Big\rangle + \frac{1}{2}\Big\langle a\,b \;\Big|\; e^{-\beta \hat{H}_2} \Big(\;\Big|\; a\,b \Big\rangle + \Big|\; b\,a \Big\rangle \Big) \qquad \text{(d)}$$

$$+ \frac{1}{2}\Big\langle b\,a \;\Big|\; e^{-\beta \hat{H}_2} \Big(\;\Big|\; b\,a \Big\rangle + \Big|\; a\,b \Big\rangle \Big) + \Big\langle b\,b \;\Big|\; e^{-\beta \hat{H}_2} \;\Big|\; b\,b \Big\rangle$$

which is the same as (c). (B.30) is correct at least for $N = 2$.

For fermions, $\mid a\,a \rangle$ & $\mid b\,b \rangle$ do not contribute. The fermion version of (c) is therefore

$$Z_2 = {}^{(A)}\Big\langle a\,b \;\Big|\; e^{-\beta \hat{H}_2} \;\Big|\; a\,b \Big\rangle^{(A)}$$

$$= \frac{1}{2}\Big(\Big\langle a\,b \;\Big| - \Big\langle b\,a \;\Big| \Big) e^{-\beta \hat{H}_2} \Big(\;\Big|\; a\,b \Big\rangle - \Big|\; b\,a \Big\rangle \Big) \qquad \text{(e)}$$

while that of (d) is

$$Z_2 = \frac{1}{2}\Big\langle a\,b \;\Big|\; e^{-\beta \hat{H}_2} \;\Big|\; a\,b \Big\rangle^{(-)} + \frac{1}{2}\Big\langle b\,a \;\Big|\; e^{-\beta \hat{H}_2} \;\Big|\; b\,a \Big\rangle^{(-)}$$

$$= \frac{1}{2}\Big\langle a\,b \;\Big|\; e^{-\beta \hat{H}_2} \Big(\;\Big|\; a\,b \Big\rangle - \Big|\; b\,a \Big\rangle \Big) + \frac{1}{2}\Big\langle b\,a \;\Big|\; e^{-\beta \hat{H}_2} \Big(\;\Big|\; b\,a \Big\rangle - \Big|\; a\,b \Big\rangle \Big)$$

which is the same as (e). (B.32) is correct at least for $N = 2$.

Consider now a 1-body operator in an N-particle system.

$$\hat{O}_N^{(1)} = \sum_{i=1}^{N} \hat{O}_i \qquad\qquad \hat{O}_i = O\Big(\hat{\boldsymbol{p}}_i\,,\; \hat{r}_i\Big) \qquad \text{(B.34)}$$

Its expectation value is given by its ensemble average as

$$\Big\langle O^{(1)} \Big\rangle = \mathrm{Tr}\Big(\hat{O}_N^{(1)}\, \hat{\rho}_N \Big) \qquad\qquad \Big[\; \hat{\rho}_N = \frac{1}{Z_N} e^{-\beta \hat{H}_N} \;\Big]$$

$$= \sum_{k_1, \ldots, k_N} \frac{\prod_j n_j!}{N!} \; {}^{(S)}\Big\langle k_1, \;\ldots, k_N \;\Big|\; \hat{O}_N^{(1)}\, \hat{\rho}_N \;\Big|\; k_1, \;\ldots, k_N \Big\rangle^{(S)} \qquad [\text{ c.f. (B.30a). }]$$

$$= \sum_{k_1,\ldots,k_N} \frac{\prod_j n_j!}{N!} \sum_{k_1',\ldots,k_N'} \frac{\prod_{j'} n_{j'}!}{N!} {}^{(S)}\Big\langle k_1, \ldots, k_N \Big| \hat{O}_N^{(1)} \Big| k_1', \ldots, k_N' \Big\rangle^{(S)}$$

$$\times {}^{(S)}\Big\langle k_1', \ldots, k_N' \Big| \hat{\rho}_N \Big| k_1, \ldots, k_N \Big\rangle^{(S)} \qquad \text{[Completeness used.]}$$

$$= \sum_{k_1,\ldots,k_N} \frac{\prod_j n_j!}{N!} \sum_{k_1',\ldots,k_N'} \frac{\prod_{j'} n_{j'}!}{N!} \Big\langle k_1, \ldots, k_N \Big| \hat{O}_N^{(1)} \Big| k_1', \ldots, k_N' \Big\rangle^{(+)}$$

$$\times \Big\langle k_1', \ldots, k_N' \Big| \hat{\rho}_N \Big| k_1, \ldots, k_N \Big\rangle^{(+)} \qquad \text{[c.f. (B.30).]} \qquad \text{(B.34a)}$$

$$= \sum_{k_1,\ldots,k_N} \frac{\prod_j n_j!}{N!} \sum_{k_1',\ldots,k_N'} \frac{\prod_{j'} n_{j'}!}{N!} \sum_{i=1}^{N} \Big[\Big\langle k_i \Big| \hat{O}_i \Big| k_i' \Big\rangle \prod_{m \neq i} \delta_{k_m k_m'} \Big]$$

$$\times \Big\langle k_1', \ldots, k_N' \Big| \hat{\rho}_N \Big| k_1, \ldots, k_N \Big\rangle^{(+)} \qquad \text{(B.34b)}$$

Since the factor $\frac{\prod_{j'} n_{j'}!}{N!}$ serves to ensure every non-equivalent term in the sums appear only once, we have

$$\Big\langle O^{(1)} \Big\rangle = \sum_{k_1,\ldots,k_N} \frac{\prod_j n_j!}{N!} \sum_{i=1}^{N} \sum_{k_i'} \Big\langle k_i \Big| \hat{O}_i \Big| k_i' \Big\rangle \Big\langle k_1, \ldots, k_i \to k_i', \ldots, k_N \Big| \hat{\rho}_N \Big| k_1, \ldots, k_N \Big\rangle^{(+)}$$

where we have used $k_i \to x$ to denote replacing k at position i with x.

Since

$$\Big\langle k_i \Big| \hat{O}_i \Big| k_i' \Big\rangle = \Big\langle k_i \Big| \hat{O}^{(1)} \Big| k_i' \Big\rangle$$

we have

$$\Big\langle O^{(1)} \Big\rangle = \sum_{k_1,\ldots,k_N} \frac{\prod_j n_j!}{N!} \sum_{i=1}^{N} \sum_{k'} \Big\langle k_i \Big| \hat{O}^{(1)} \Big| k_i' \Big\rangle \Big\langle k_1, \ldots, k_i \to k', \ldots, k_N \Big| \hat{\rho}_N \Big| k_1, \ldots, k_i \ldots, k_N \Big\rangle^{(+)}$$

$$= \sum_{k_1,\ldots,k,\ldots,k_N} \frac{\prod_j n_j!}{N!} \sum_{i=1}^{N} \sum_{k'} \Big\langle k \Big| \hat{O}^{(1)} \Big| k' \Big\rangle \Big\langle k', \overbrace{k_1, \ldots, k_N}^{k_i \text{ term missing}} \Big| \hat{\rho}_N \Big| k, \overbrace{k_1, \ldots, k_N}^{k_i \text{ term missing}} \Big\rangle^{(+)}$$

where we have renamed $k_i \to k$ & $k_i' \to k'$, then taken advantage of the invariance of $\hat{\rho}_N$ & $| \ldots \rangle^{(+)}$ to move both k & k' to the 1st positions.

Renaming

$$\{k_1, \ldots, k_{i-1}\} \to \{k_2, \ldots, k_i\} \qquad \forall\ i \qquad \text{(B.34c)}$$

we have

$$\Big\langle O^{(1)} \Big\rangle = \sum_{i=1}^{N} \sum_{k,k'} \Big\langle k \Big| \hat{O}^{(1)} \Big| k' \Big\rangle \sum_{k_2,\ldots,k_N} \frac{\prod_j n_j!}{N!} \big\langle k', k_2, \ldots, k_N \big| \hat{\rho}_N \big| k, k_2, \ldots, k_N \big\rangle^{(+)}$$

$$= \sum_{k,k'} \Big\langle k \Big| \hat{O}^{(1)} \Big| k' \Big\rangle \sum_{k_2,\ldots,k_N} \frac{\prod_j n_j!}{(N-1)!} \big\langle k', k_2, \ldots, k_N \big| \hat{\rho}_N \big| k, k_2, \ldots, k_N \big\rangle^{(+)}$$

Setting

$$\Big\langle k' \Big| \hat{\rho}^{(1)} \Big| k \Big\rangle = \sum_{k_2,\ldots,k_N} \frac{\prod_j n_j!}{(N-1)!} \big\langle k', k_2, \ldots, k_N \big| \hat{\rho}_N \big| k, k_2, \ldots, k_N \big\rangle^{(+)} \qquad \text{(B.37)}$$

we get

$$\Big\langle O^{(1)} \Big\rangle = \sum_{k} \sum_{k'} \Big\langle k \Big| \hat{O}^{(1)} \Big| k' \Big\rangle \Big\langle k' \Big| \hat{\rho}^{(1)} \Big| k \Big\rangle \qquad \text{(B.36)}$$

Completeness of the 1-particle states allows us to write (B.36) as

$$\left\langle O^{(1)} \right\rangle = \sum_{k_1} \left\langle k_1 \,\middle|\, \hat{O}^{(1)} \hat{\rho}^{(1)} \,\middle|\, k_1 \right\rangle$$
$$= \mathrm{Tr}\left(\hat{O}^{(1)} \hat{\rho}^{(1)} \right) \qquad \text{(B.36c)}$$

so that $\hat{\rho}^{(1)}$ is the probability density operator if the system were a 1-body system. It is therefore simply $\hat{\rho}_N$ averaged over the states of $N-1$ bodies, and hence called the reduced 1-body probability density operator.

By now, it should be obvious that the fermion version can be easily obtained from the boson one by setting

$$\prod_j n_j \to 1 \qquad (S) \to (A) \qquad (+) \to (-)$$

while watching out diligently for sign changes due to particle exchanges. By comparing (B.32) with (B30), we can deduce that the fermion version of (B.36a) is simply

$$\left\langle O^{(1)} \right\rangle = \sum_{k_1,\dots,k_N} \frac{1}{N!} \sum_{k_1',\dots,k_N'} \frac{1}{N!} \left\langle k_1, \dots, k_N \,\middle|\, \hat{O}_N^{(1)} \,\middle|\, k_1', \dots, k_N' \right\rangle^{(-)}$$
$$\times \left\langle k_1', \dots, k_N' \,\middle|\, \hat{\rho}_N \,\middle|\, k_1, \dots, k_N \right\rangle^{(-)}$$
$$= \sum_{k_1,\dots,k_N} \frac{1}{N!} \sum_{k_1',\dots,k_N'} \frac{1}{N!} \sum_{i=1}^{N} \left[\left\langle k_i \,\middle|\, \hat{O}_i \,\middle|\, k_i' \right\rangle (-)^{i+1} \prod_{m \neq i} \delta_{k_m k_m'} \right]$$
$$\times \left\langle k_1', \dots, k_N' \,\middle|\, \hat{\rho}_N \,\middle|\, k_1, \dots, k_N \right\rangle^{(-)}$$

where the factor $(-)^{i+1}$ comes from the position of k_i' in $\left| k_1', \dots, k_N' \right\rangle^{(-)}$.

Following the same path used in the boson case, we have

$$\left\langle O^{(1)} \right\rangle = \sum_{k_1,\dots,k_N} \frac{1}{N!} \sum_{i=1}^{N} \sum_{k'} (-)^{i+1} \left\langle k_i \,\middle|\, \hat{O}^{(1)} \,\middle|\, k_i' \right\rangle \left\langle k_1, \dots, k_i \to k', \dots, k_N \,\middle|\, \hat{\rho}_N \,\middle|\, k_1, \dots, k_i \dots, k_N \right\rangle^{(-)}$$
$$= \sum_{k_1,\dots,k,\dots,k_N} \frac{1}{N!} \sum_{i=1}^{N} \sum_{k'} \left\langle k \,\middle|\, \hat{O}^{(1)} \,\middle|\, k' \right\rangle \left\langle k', \overbrace{k_1, \dots, k_N}^{k_i \text{ term missing}} \,\middle|\, \hat{\rho}_N \,\middle|\, k, \overbrace{k_1, \dots, k_N}^{k_i \text{ term missing}} \right\rangle^{(-)}$$

where moving k_i up to the 1st position in $\left| k, \overbrace{k_1, \dots, k_N}^{k_i \text{ term missing}} \right\rangle^{(-)}$ produces another $(-)^{i+1}$ factor that cancels out the existing one.

After applying the relabeling (B.34c), we get

$$\left\langle O^{(1)} \right\rangle = \sum_{i=1}^{N} \sum_{k,k'} \left\langle k \,\middle|\, \hat{O}^{(1)} \,\middle|\, k' \right\rangle \sum_{k_2,\dots,k_N} \frac{1}{N!} \left\langle k', k_2, \dots, k_N \,\middle|\, \hat{\rho}_N \,\middle|\, k, k_2, \dots, k_N \right\rangle^{(-)}$$
$$= \sum_{k,k'} \left\langle k \,\middle|\, \hat{O}^{(1)} \,\middle|\, k' \right\rangle \sum_{k_2,\dots,k_N} \frac{1}{(N-1)!} \left\langle k', k_2, \dots, k_N \,\middle|\, \hat{\rho}_N \,\middle|\, k, k_2, \dots, k_N \right\rangle^{(-)}$$

Hence, (B.36) is also applicable for fermions if we replace (B.37) with

$$\left\langle k' \,\middle|\, \hat{\rho}^{(1)} \,\middle|\, k \right\rangle = \sum_{k_2,\dots,k_N} \frac{1}{(N-1)!} \left\langle k', k_2, \dots, k_N \,\middle|\, \hat{\rho}_N \,\middle|\, k, k_2, \dots, k_N \right\rangle^{(-)} \qquad \text{(B.38)}$$

Note that of the two $(-)^{i+1}$ factors, one comes from the completeness of the anti-symmetrized basis. Thus, if we had used the completeness of the basis $| k_1, \ldots, k_N \rangle$ instead, the results would be erroneous. This is because the basis $| k_1, \ldots, k_N \rangle$, which contains symmetrized components, is over-complete in the anti-symmetrized Hilbert subspace.

Following Reichl's instruction, we leave the derivation for $\langle O^{(2)} \rangle$ as an exercise.