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Solid State Theory I

1. Exercise Sheet

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1 One-particle operators in second quantization

A one-particle operator in a many-body system is an operator that acts on the state of a single particle at a time. It is defined as $\hat{B} = \sum_{i=1}^{N} \hat{B}_i$ where $\hat{B}_i$ is given by

$$\hat{B}_i = \mathbb{1}_1 \otimes \ldots \otimes \mathbb{1}_{i-1} \otimes \sum_{\nu,\mu} \langle\nu|\hat{b}|\mu\rangle |\nu\rangle\langle\mu|_i \otimes \mathbb{1}_{i+1} \otimes \ldots \otimes \mathbb{1}_N, \tag{1.1}$$

where $\langle\nu|\hat{b}|\mu\rangle$ are the matrix elements in one-particle quantum mechanics. In other words, $\hat{B}_i$ acts trivially in all Hilbert spaces, except in that of particle i.

(a) Applying $\hat{B}$ to the state $\big|\alpha_1, \alpha_2, \ldots, \alpha_N\big\}$ introduced above, show that one obtains

$$\hat{B}\big|\alpha_1, \alpha_2, \ldots, \alpha_N\big\} = \frac{1}{\sqrt{N!}} \sum_{\mu,\nu} \langle\nu|\hat{b}|\mu\rangle \times \sum_{i,P} \xi^{\sigma(P)} \delta_{\mu,\alpha_{P(i)}} |\alpha_{P(1)}\rangle_1 \otimes \ldots \otimes |\nu\rangle_i \otimes \ldots \otimes |\alpha_{P(N)}\rangle_N. \tag{1.2}$$

Note that we have explicitly labeled the one-particle states with a subscript to identify the subspace they belong to within the tensor product (**??**), *e.g.* $|\nu\rangle_i$belongs to the subspace of particle i.
(2 points)

(b) Show that one can write the last summation in (1.2) as

$$\sum_{i,P} \xi^{\sigma(P)} \delta_{\mu,\alpha_{P(i)}} |\alpha_{P(1)}\rangle_1 \otimes \ldots \otimes |\nu\rangle_i \otimes \ldots \otimes |\alpha_{P(N)}\rangle_N = \tag{1.3}$$

$$\sum_{j,P} \xi^{\sigma(P)} \delta_{\mu,\alpha_j} |\alpha_{P(1)}\rangle_1 \otimes \ldots \otimes |\nu\rangle_{P^{-1}(j)} \otimes \ldots \otimes |\alpha_{P(N)}\rangle_N. \tag{1.4}$$

(2 points)
Hint: Note that $\sum_j \delta_{j,P(i)} = 1$ for fixed i, as $P(i) = j$ for some $j, \varepsilon\{1, \ldots, N\}$ since any P is a bijective mapping of $\{1, \ldots, N\}$ in itself.

(c) Consider again

$$\big|\alpha_1, \ldots, \alpha_j, \ldots, \alpha_N\big\} = \frac{1}{\sqrt{N!}} \sum_P \xi^{\sigma(P)} |\alpha_{P(1)}\rangle_1 \otimes \ldots \otimes |\nu_{P(j)}\rangle_j \otimes \ldots \otimes |\alpha_{P(N)}\rangle_N. \tag{1.5}$$

In which position in each of these terms is α_j located? Note that I am not asking where $\alpha_{P(j)}$ is located, which is obviously at position j. From this observation and using (1.3), prove the identity

$$\frac{1}{\sqrt{N!}} \sum_{i,P} \xi^{\sigma(P)} \delta_{\mu,\alpha_{P(i)}} |\alpha_{P(1)}\rangle_1 \otimes \ldots \otimes |\nu\rangle_i \otimes \ldots \otimes |\alpha_{P(N)}\rangle_N = \tag{1.6}$$

$$\sum_j \delta_{\mu,\alpha_j} \big|\alpha_1, \ldots, \alpha_{j-1}, \nu, \alpha_{j+1} \ldots, \alpha_N\big\}. \tag{1.7}$$

(2 points)

(d) Show that

$$c_\nu^\dagger c_\mu \big|\alpha_1, \ldots, \alpha_N\big\} = \sum_j \delta_{\mu,\alpha_j} \big|\alpha_1, \ldots, \alpha_{j-1}, \nu, \alpha_{j+1} \ldots, \alpha_N\big\}. \tag{1.8}$$

(2 points)
Hint: Use (**??**) and the symmetry properties of the wave-function under interchange of particles.

(e) Thus, show that

$$\hat{B}\big|\alpha_1, \ldots, \alpha_N\big\} = \sum_{\mu,\nu} \langle\nu|\hat{b}|\mu\rangle c_\nu^\dagger c_\mu \big|\alpha_1, \ldots, \alpha_N\big\}. \tag{1.9}$$

(1 point)

Since the state $\big|\alpha_1, \ldots, \alpha_N\big\}$ is arbitrary, we conclude that a one-particle operator is given, in second quantisation, by

$$\hat{B} = \sum_{\mu,\nu} \langle\nu|\hat{b}|\mu\rangle c_\nu^\dagger c_\mu. \tag{1.10}$$

2 The density operator in second quantization

For a system of N identical particles (fermions) enclosed in a volume V with periodic boundary conditions, the density operator at position r is defined (in its first quantised form), as

$$\hat{\rho}(\boldsymbol{r}) = \sum_{i=1}^{N} \delta(\boldsymbol{r} - \hat{\boldsymbol{r}}_i), \tag{2.1}$$

where $\hat{\boldsymbol{r}}_i$ is the position operator of particle i. Note that $\boldsymbol{r}$ is not an operator.

(a) Show that the Fourier transform $\hat{\rho}_q = \int_V d^3r e^{-iq\cdot r} \hat{\rho}(\boldsymbol{r})$ is given by

$$\hat{\rho}_q = \sum_{i=1}^{N} e^{-iq\cdot\hat{r}_i}. \tag{2.2}$$

(1 point)

(b) The second quantisation representation of $\hat{\rho}(\boldsymbol{r})$, as follows from (1.10), is given by

$$\hat{\rho}(\boldsymbol{r}) = \sum_{\sigma',\sigma} \int_V d^3x' \int_V d^3x \langle \boldsymbol{x}'\sigma' | \delta(\boldsymbol{r} - \hat{\boldsymbol{r}}) | \boldsymbol{x}\sigma \rangle \hat{\psi}^\dagger_{\sigma'}(\boldsymbol{x}') \hat{\psi}_\sigma(\boldsymbol{x}), \tag{2.3}$$

where $\hat{\psi}_\sigma(\boldsymbol{x})$ and $\hat{\psi}^\dagger_\sigma(\boldsymbol{x})$ are the annihilation and creation operators for a fermion, with spin projection along z equal to σ, at point $\boldsymbol{x}$. Show from (2.3) that $\hat{\rho}(\boldsymbol{r})$ is given by

$$\hat{\rho}(\boldsymbol{r}) = \sum_{\sigma} \hat{\psi}^\dagger_\sigma(\boldsymbol{r}) \hat{\psi}_\sigma(\boldsymbol{r}). \tag{2.4}$$

(2 points)

(c) Show that in second quantization the FT of $\hat{\rho}(\boldsymbol{r})$ is given by

$$\hat{\rho}_q = \sum_{i=1}^{N} \hat{c}^\dagger_{k-q,\sigma} \hat{c}_{k,\sigma}. \tag{2.5}$$

(2 points)
Hint: Substitute the relations $\hat{\psi}_\sigma(\boldsymbol{r}) = \frac{1}{\sqrt{V}} \sum_k e^{ik\cdot r} \hat{c}_{\boldsymbol{k},\sigma}$, $\hat{\psi}^\dagger_\sigma(\boldsymbol{r}) = \frac{1}{\sqrt{V}} \sum_k e^{-ik\cdot r} \hat{c}^\dagger_{\boldsymbol{k},\sigma}$, see (**??**), in the definition of the Fourier transform given above. Note that $\int_V d^3r e^{-i(k-k')\cdot r} = V\delta_{k,k'}$.

(d) Show that $\hat{\rho}^\dagger_q = \hat{\rho}_{-q}$.
(1 point)

(e) Show that $\left[\hat{\rho}_q, \hat{\rho}_{q'}\right] = 0$.
(2 points)
Hint: Use the identities $\left[\hat{A}, \hat{B}, \hat{C}\right]_- = \left[\hat{A}, \hat{B}\right]_{-\xi} \hat{C} + \xi \hat{B} \left[\hat{A}, \hat{C}\right]_{-\xi}$ where $\xi = \pm 1$.

(f) Use the first quantisation representation of $\hat{\rho}_q$, as given in equation (2.2), to show the previous identity.
(2 points)
Hint: What is $\left[\hat{\boldsymbol{r}}_i, \hat{\boldsymbol{r}}_j\right]$ for arbitrary i, j?

(g) What is $\hat{\rho}_{q=0}$?
(1 point)