

Consider a set of electrons in a system with volume  $\Omega$  with periodic boundary conditions. To describe such a system, we usually use the second quantization formalism. Therefore, it is necessary to determine the expressions of the different observables in this formalism.

Let's consider the Hilbert space for an electron  $\mathcal{H}^{(1)}$ . A general basis of this space is given by  $|\psi_1\rangle, |\psi_2\rangle, \dots$ . Let  $\hat{O}^{(1)}$  act on  $\mathcal{H}^{(1)}$ , then one can define the operator acting on the  $N$  electron Hilbert space ( $\mathcal{H}^{(N)} = \otimes^N \mathcal{H}^{(1)}$ ) as

$$\hat{O} = \sum_j \hat{O}^{(1)}(j) = (\hat{O}^{(1)} \otimes \mathbf{I} \otimes \dots \otimes \mathbf{I}) + (\mathbf{I} \otimes \hat{O}^{(1)} \otimes \dots \otimes \mathbf{I}) + \dots + (\mathbf{I} \otimes \mathbf{I} \otimes \dots \otimes \hat{O}^{(1)}) \quad (1)$$

where  $\hat{O}^{(1)}(j)$  acts on the  $j$ th particle and leaves the rest intact. In second quantization form  $\hat{O}$  acting on the Fock space reads as

$$\hat{O} = \sum_{\alpha, \beta} \langle \psi_\alpha | \hat{O}^{(1)} | \psi_\beta \rangle c_\alpha^\dagger c_\beta \quad (2)$$

with  $c_\alpha^\dagger$  and  $c_\alpha$  the creation and annihilation operators of an electron in the state  $|\psi_\alpha\rangle$ . Similarly, consider a two-particle operator denoted as  $F^{(2)}$  acting on  $\mathcal{H}^{(2)} = \mathcal{H}^{(1)} \otimes \mathcal{H}^{(1)}$ . Then one can define an operator  $\hat{F}$  acting on the  $N$ -particle Hilbert space  $\mathcal{H}^{(N)}$ :

$$\hat{F} = \frac{1}{2} \sum_{i \neq j} \hat{F}^{(2)}(i, j) \quad (3)$$

where  $F^{(2)}$  acts on the  $i$ th and  $j$ th particle and leaves the rest intact. Then  $\hat{F}$  in second quantization form acting on the full Fock space reads as

$$\hat{F} = \frac{1}{2} \sum_{\alpha, \beta, \gamma, \delta} \left( \hat{f}^{(2)} \right)_{\delta\gamma}^{\alpha\beta} c_\alpha^\dagger c_\beta^\dagger c_\gamma c_\delta, \quad (4)$$

where

$$\begin{aligned} \left( \hat{f}^{(2)} \right)_{\delta\gamma}^{\alpha\beta} &= \langle \psi_\alpha \otimes \psi_\beta | \hat{F}^{(2)} | \psi_\delta \otimes \psi_\gamma \rangle \\ &= \int \int dx_1 dx_2 \psi_\alpha^*(x_1) \psi_\beta^*(x_2) \hat{F}^{(2)}(x_1, x_2) \psi_\delta(x_1) \psi_\gamma(x_2). \end{aligned} \quad (5)$$

In the following exercises we get acquainted with these second quantized forms through various examples.

A special choice of basis over  $\mathcal{H}^{(1)}$  are the plane waves  $\{|\varphi_{\mathbf{k}, \sigma}\rangle\}$ . The wave functions read as

$$\langle \mathbf{r}, \sigma' | \varphi_{\mathbf{k}, \sigma} \rangle = \varphi_{\mathbf{k}, \sigma}(\mathbf{r}, \sigma') = \frac{1}{\sqrt{\Omega}} e^{i\mathbf{k} \cdot \mathbf{r}} \eta_\sigma(\sigma')$$

with  $\eta_\sigma(\sigma') = \langle \sigma' | \sigma \rangle = \delta_{\sigma', \sigma}$  the wave function of the spin as defined in the lecture ( $\sigma = \pm 1/2$ ). Then the second quantized form of  $\hat{O}$  acting on the Fock space reads as

$$\hat{O} = \sum_{\mathbf{k}_1, \mathbf{k}_2} \sum_{\sigma_1, \sigma_2} \langle \varphi_{\mathbf{k}_1, \sigma_1} | \hat{O} | \varphi_{\mathbf{k}_2, \sigma_2} \rangle c_{\mathbf{k}_1, \sigma_1}^\dagger c_{\mathbf{k}_2, \sigma_2} \quad (6)$$

with  $c_{\mathbf{k},\sigma}^\dagger$  and  $c_{\mathbf{k},\sigma}$  the creation and annihilation operators of an electron in the state  $|\varphi_{\mathbf{k},\sigma}\rangle$ . Electrons being fermions, these operators must satisfy fermionic anticommutation relations

$$\begin{aligned} \{c_{\mathbf{k},\sigma}, c_{\mathbf{k}',\sigma'}^\dagger\} &= \delta_{\mathbf{k},\mathbf{k}'} \delta_{\sigma,\sigma'} \\ \{c_{\mathbf{k},\sigma}, c_{\mathbf{k}',\sigma'}\} &= \{c_{\mathbf{k},\sigma}^\dagger, c_{\mathbf{k}',\sigma'}^\dagger\} = 0 \end{aligned} \quad (7)$$

**(A.)** The goal of this exercise is to write the Hamiltonian of an interacting electron system in second quantization language. The Hamiltonian in coordinate representation reads as

$$H = H_{\text{kin}} + H_{\text{ext}} + H_{\text{int}} = \sum_i -\frac{\Delta_i}{2m} + \sum_i U(\mathbf{r}_i) + \frac{1}{2} \sum_{i \neq j} V(\mathbf{r}_i, \mathbf{r}_j) \quad (8)$$

where  $\Delta_i$  stands for the laplacian in the  $i$ th coordinate,  $U(\mathbf{r})$  is an external potential, and  $V(\mathbf{r}_i, \mathbf{r}_j) = V(\mathbf{r}_i - \mathbf{r}_j) = \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|}$  is the Coulomb interaction between electrons.

1. Using Eq. (??), write down the second quantized form of  $H_{\text{kin}}$ , calculate the expectation value explicitly.
2. Find the second quantized form of  $H_{\text{ext}}$ . Simplify the final expression using the Fourier transform  $U(\mathbf{q}) = \frac{1}{\Omega} \int d\mathbf{r} U(\mathbf{r}) e^{-i\mathbf{q}\mathbf{r}}$ .
3. Write down how Eq. (??) looks like in the  $\{|\varphi_{\mathbf{k},\sigma}\rangle\}$  basis. Use this to obtain the second quantized form of  $H_{\text{int}}$ . Explicitly calculate the matrix element using  $\int d\mathbf{r} e^{i\mathbf{q}\mathbf{r}} \frac{1}{|\mathbf{r}|} = \frac{4\pi}{|\mathbf{q}|^2}$  (bonus if you remember how this was obtained). What do you observe about the wave vectors of the creation and annihilation operators? Can you explain why that is?

**(B.)** Let  $\hat{S}_1$  be the spin-1/2 operator acting on  $\mathcal{H}^{(1)}$

$$\begin{cases} \hat{S}_1^x |\varphi_{\mathbf{k},\sigma}\rangle = \frac{1}{2} |\varphi_{\mathbf{k},-\sigma}\rangle \\ \hat{S}_1^y |\varphi_{\mathbf{k},\sigma}\rangle = i\sigma |\varphi_{\mathbf{k},-\sigma}\rangle \\ \hat{S}_1^z |\varphi_{\mathbf{k},\sigma}\rangle = \sigma |\varphi_{\mathbf{k},\sigma}\rangle \end{cases}$$

Show that the total spin operator  $\hat{S}$  acting on the Fock space is given by

$$\begin{aligned} \hat{S}^x &= \frac{1}{2} \sum_{\mathbf{k}} \left( c_{\mathbf{k},\uparrow}^\dagger c_{\mathbf{k},\downarrow} + c_{\mathbf{k},\downarrow}^\dagger c_{\mathbf{k},\uparrow} \right) \\ \hat{S}^y &= \frac{i}{2} \sum_{\mathbf{k}} \left( c_{\mathbf{k},\downarrow}^\dagger c_{\mathbf{k},\uparrow} - c_{\mathbf{k},\uparrow}^\dagger c_{\mathbf{k},\downarrow} \right) \\ \hat{S}^z &= \frac{1}{2} \sum_{\mathbf{k}} \left( c_{\mathbf{k},\uparrow}^\dagger c_{\mathbf{k},\uparrow} - c_{\mathbf{k},\downarrow}^\dagger c_{\mathbf{k},\downarrow} \right) \end{aligned}$$

**(C.)** The particle density operator at the point  $\mathbf{r}$  (denoted  $\hat{n}_1(\mathbf{r})$ ) acting on  $\mathcal{H}^{(1)}$  is given by

$$\hat{n}_1(\mathbf{r}) = |\mathbf{r}\rangle \langle \mathbf{r}|$$

with

$$|\mathbf{r}\rangle \langle \mathbf{r}| \equiv \sum_{\sigma} |\mathbf{r}, \sigma\rangle \langle \mathbf{r}, \sigma|$$

Show that the particle density operator in the point  $\mathbf{r}$  acting on the Fock space is given by

$$\hat{n}(\mathbf{r}) = \sum_{\sigma} \Psi^{\dagger}(\mathbf{r}, \sigma) \Psi(\mathbf{r}, \sigma)$$

with the  $\Psi^{\dagger}(\mathbf{r}, \sigma)$  and  $\Psi(\mathbf{r}, \sigma)$  field operators defined as

$$\begin{cases} \Psi(\mathbf{r}, \sigma) = \sum_{\mathbf{k}, \sigma'} \varphi_{\mathbf{k}, \sigma'}(\mathbf{r}, \sigma) c_{\mathbf{k}, \sigma'} \\ \Psi^{\dagger}(\mathbf{r}, \sigma) = \sum_{\mathbf{k}, \sigma'} \varphi_{\mathbf{k}, \sigma'}^*(\mathbf{r}, \sigma) c_{\mathbf{k}, \sigma'}^{\dagger} \end{cases}$$

(D.) The particle current operator at the point  $\mathbf{r}$  (denoted  $\hat{\mathbf{J}}_1(\mathbf{r})$ ) acting on  $\mathcal{H}^{(1)}$  is given by

$$\hat{\mathbf{J}}_1(\mathbf{r}) = \frac{1}{2m} \left( |\mathbf{r}\rangle \langle \mathbf{r}| \hat{\mathbf{P}}_1 + \hat{\mathbf{P}}_1 |\mathbf{r}\rangle \langle \mathbf{r}| \right)$$

with  $\hat{\mathbf{P}}_1$  the momentum operator. For a system in presence of a static magnetic field  $\mathbf{B}(\mathbf{r}) = \nabla \times \mathbf{A}(\mathbf{r})$ , we have

$$\langle \mathbf{r}, \sigma | \hat{\mathbf{P}}_1 | \psi \rangle = \left( -i\nabla - \frac{e}{c} \mathbf{A}(\mathbf{r}) \right) \psi(\mathbf{r}, \sigma) \quad \forall \psi$$

Show that the particle current operator at the point  $\mathbf{r}$  acting on the Fock space is given by

$$\hat{\mathbf{J}}(\mathbf{r}) = \hat{\mathbf{J}}_a(\mathbf{r}) + \hat{\mathbf{J}}_b(\mathbf{r})$$

with

$$\hat{\mathbf{J}}_a(\mathbf{r}) = \frac{i}{2m} \sum_{\sigma} \left\{ (\nabla \Psi^{\dagger}(\mathbf{r}, \sigma)) \Psi(\mathbf{r}, \sigma) - \Psi^{\dagger}(\mathbf{r}, \sigma) (\nabla \Psi(\mathbf{r}, \sigma)) \right\}$$

and

$$\hat{\mathbf{J}}_b(\mathbf{r}) = -\frac{e}{mc} \mathbf{A}(\mathbf{r}) \sum_{\sigma} \Psi^{\dagger}(\mathbf{r}, \sigma) \Psi(\mathbf{r}, \sigma) = -\frac{e}{mc} \mathbf{A}(\mathbf{r}) \hat{n}(\mathbf{r})$$

where  $\hat{n}(\mathbf{r})$  is the particle density operator.  $\hat{\mathbf{J}}(\mathbf{r})$  thus can be written in terms of field operators in the form

$$\hat{\mathbf{J}}(\mathbf{r}) = \frac{1}{2m} \sum_{\sigma} \left\{ \left[ \left( i\nabla - \frac{e}{c} \mathbf{A}(\mathbf{r}) \right) \Psi^{\dagger}(\mathbf{r}, \sigma) \right] \Psi(\mathbf{r}, \sigma) + \Psi^{\dagger}(\mathbf{r}, \sigma) \left( -i\nabla - \frac{e}{c} \mathbf{A}(\mathbf{r}) \right) \Psi(\mathbf{r}, \sigma) \right\}$$

Let  $\hat{\mathbf{J}}_a(\mathbf{q})$  be the Fourier transform of  $\hat{\mathbf{J}}_a(\mathbf{r})$

$$\hat{\mathbf{J}}_a(\mathbf{q}) = \int d^3\mathbf{r} e^{-i\mathbf{q}\cdot\mathbf{r}} \hat{\mathbf{J}}_a(\mathbf{r})$$

Show that

$$\hat{\mathbf{J}}_a(\mathbf{q}) = \frac{1}{2m} \sum_{\mathbf{k}, \sigma} (2\mathbf{k} - \mathbf{q}) c_{\mathbf{k}-\mathbf{q}, \sigma}^{\dagger} c_{\mathbf{k}, \sigma}$$

Finally, compute the current expectation values for the following states, and justify physically your results.

1.  $|1\rangle = \prod_{\mathbf{k} \in \text{BZ}} c_{\mathbf{k}}^{\dagger} |0\rangle$ ,
2.  $|2\rangle = \prod_{|\mathbf{k}| < k_F} c_{\mathbf{k}}^{\dagger} |0\rangle$ ,
3.  $|3\rangle = \prod_{|\mathbf{k}| < k_F} c_{\mathbf{k}+\mathbf{q}}^{\dagger} |0\rangle$ .