Quantum theory of condensed matter II

Mesoscopic physics (Quantum transport)

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Tue	8:00 - 10:00	9.2.01
Fri	12:00 - 14:00	9.2.01
Tue	10:00 - 12:00	5.0.21

Sheet 6

1. Operators in second quantization

The general expression of a one particle operator in second quantization reads:

$$\hat{O} = \sum_{\mu\nu} \hat{d}^\dagger_\mu \langle \mu|\hat{o}|\nu\rangle \hat{d}_\nu$$

where $\{|\mu\rangle\}$ is a complete basis for the single particle Hilbert space and $\hat{o}$ is the single particle operator. The first quantization expression of the density and current density operators (including the paramagnetic and diamagnetic components for the current) read:

$$\hat{\rho}(\mathbf{r}) = \sum_i \delta(\mathbf{r} - \hat{\mathbf{r}}_i),$$

$$\hat{\mathbf{J}}_P(\mathbf{r}) = \frac{1}{2m} \sum_i \left[\hat{\mathbf{p}}_i \delta(\mathbf{r} - \hat{\mathbf{r}}_i) + \delta(\mathbf{r} - \hat{\mathbf{r}}_i)\hat{\mathbf{p}}_i\right],$$

$$\hat{\mathbf{J}}_D(\mathbf{r}) = -\frac{1}{m}\mathbf{A}(\mathbf{r}) \sum_\sigma \delta(\mathbf{r} - \hat{\mathbf{r}}_i).$$

1. Starting from the first quantization operators given above, derive the following second quantization expressions of the density and current density operators in position representation:

$$\hat{\rho}(\mathbf{r}) = \sum_\sigma \hat{\psi}^\dagger_\sigma(\mathbf{r})\hat{\psi}_\sigma(\mathbf{r}),$$

$$\hat{\mathbf{J}}_P(\mathbf{r}) = \sum_\sigma -i\frac{\hbar}{2m}\left[\hat{\psi}^\dagger_\sigma(\mathbf{r})\nabla\hat{\psi}_\sigma(\mathbf{r}) - (\nabla\hat{\psi}^\dagger_\sigma(\mathbf{r}))\hat{\psi}(\mathbf{r})\right],$$

$$\hat{\mathbf{J}}_D(\mathbf{r}) = -\frac{1}{m}\mathbf{A}(\mathbf{r}) \sum_\sigma \hat{\psi}^\dagger_\sigma(\mathbf{r})\hat{\psi}_\sigma(\mathbf{r}).$$

   Hint: Remember that the position and momentum operators read, in position representation,

$$\langle \mathbf{x}|\hat{\mathbf{r}}|\mathbf{x}'\rangle := \delta(\mathbf{x} - \mathbf{x}'), \qquad \langle \mathbf{x}|\hat{\mathbf{p}}|\mathbf{x}'\rangle := -i\hbar\delta(\mathbf{x} - \mathbf{x}')\nabla_{\mathbf{x}}.$$

   (2 Points)

2. Which is the expression of the density and current density operators in the momentum representation?
   (2 Points)

Bitte wenden

2. Pure vs. mixed states

Consider the two orbital interacting model for a molecule described by the following Hamiltonian:

$$H = \varepsilon \hat{N} + J \hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_2 \tag{1}$$

where $\hat{N} = \hat{N}_1 + \hat{N}_2$ with $\hat{N}_i = \sum_\tau \hat{c}^\dagger_{i\tau} \hat{c}_{i\tau}$ counts the number of electrons in the system and $\hat{c}_{i\tau}$ destroys an electron of spin τ and orbital i. Moreover $\hat{S}_{i,\alpha}$ is the component $\alpha = x, y, z$ of the spin vector operator associated to the orbital i and reads:

$$\hat{S}_{i,\alpha} = \frac{\hbar}{2} \sum_{\tau\tau'} \hat{c}^\dagger_{i\tau} \sigma^\alpha_{\tau\tau'} \hat{c}_{i\tau'}$$

where $\{\sigma^\alpha\}$ are the 2x2 Pauli matrices.

1. Consider the set of operators $\mathcal{S} = \{\hat{N}_1, \hat{N}_2, \hat{S}^2, \hat{S}_z\}$, where $\hat{S}^2 = (\hat{\mathbf{S}}_1 + \hat{\mathbf{S}}_2) \cdot (\hat{\mathbf{S}}_1 + \hat{\mathbf{S}}_2)$ and, correspondingly $\hat{S}_z = \hat{S}_{1,z} + \hat{S}_{2,z}$ is the z component of the total spin operator. Prove that $\mathcal{S}$ is a complete set of operators for the entire Fock space of the system.

2. Prove that the measurement of $\langle \hat{N}_1 \rangle = 2$ and $\langle \hat{N}_2 \rangle = 0$ gives full knowledge over the state of the molecule.

3. How many paramenters (*i.e.* observables) are needed, in general, to fully characterize the quantum state of the molecule? How does this number change if we measure $\langle \hat{N}_1 \rangle = \langle \hat{N}_2 \rangle = 1$? Why? What about the case in which the previous result in the measurement of the particle numbers is obtained *without* any dispersion?

Frohes Schaffen!