University of Regensburg Summer Term 2018

Quantum Theory of Condensed Matter I

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Sheet 7

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1. The Kubo Formula for the Conductivity I .... [8P]

In this exercise, we study the electrical conductivity tensor in more detail which is of great importance in transport theory. The appearing operators are to be considered in the Heisenberg picture.

(a)(2P) Prove the Kubo-identity:

$$\mathrm{i}[A(t),\rho] = \rho \int_0^\beta \mathrm{d}\lambda\, \dot{A}(t-\mathrm{i}\lambda), \tag{1}$$

with $\rho = \exp(-\beta H)/\mathrm{Tr}[\exp(-\beta H)]$ the statistical operator with $\beta \equiv 1/(k_B T)$.

(b)(2P) By means of (a), show that one can rewrite the retarded Green's function as

$$\langle\langle A(t)B(t')\rangle\rangle^{\mathrm{ret}} = -\hbar\theta(t-t') \int_0^\beta \mathrm{d}\lambda\, \langle \dot{B}(t'-\mathrm{i}\hbar\lambda)A(t)\rangle. \tag{2}$$

(c)(2P) Show that in case of a Hamiltonian which does not depend on time explicitly the *correlation function* depends only on the time difference, i.e.,

$$\langle A(t)B(t')\rangle = \langle A(t-t')B(0)\rangle. \tag{3}$$

(d)(2P) Rewrite the conductivity tensor at finite frequencies ω (due to an applied electric field), i.e.,

$$\sigma^{\beta\alpha}(\omega) = -\frac{1}{\hbar}\int_{-\infty}^{\infty} \mathrm{d}t\, \langle\langle j^\beta(0), P^\alpha(-t)\rangle\rangle^{\mathrm{ret}} \exp(\mathrm{i}(\omega + i0^+)t) \tag{4}$$

with the current operator $\mathbf{j} = \dot{\mathbf{P}}/V$, the dipole moment operator $\mathbf{P}$, and the volume of the sample V as

$$\sigma^{\beta\alpha}(\omega) = V\int_0^\beta \mathrm{d}\lambda \int_0^\infty \mathrm{d}t\, \mathrm{Tr}[\rho\, j^\alpha(0) j^\beta(t+\mathrm{i}\hbar\lambda)] \exp(\mathrm{i}(\omega+i0^+)t). \tag{5}$$

2. Conductivity Tensor in the Tight Binding Model .... [8P]

The interacting electron system for which we are going to calculate the conductivity tensor is given by the Hamiltonian

$$H = \sum_{i,j,\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + \sum_{i,j,\sigma,\sigma'} V_{ij\sigma\sigma'} n_{i\sigma} n_{j\sigma'}, \tag{6}$$

with $c^\dagger_{i\sigma}(c_{i\sigma})$ the creation (annihilation) operator of an electron at site i with spin σ. Further, assume that the electrons are tightly bound to the crystal ions, thus

$$\int \mathrm{d}^3 r\, w^*_\sigma(\mathbf{r}-\mathbf{R}_i)\mathbf{r} w_\sigma(\mathbf{r}-\mathbf{R}_j) \simeq \mathbf{R}_i \delta_{ij}, \tag{7}$$

where $w_\sigma(\mathbf{r}-\mathbf{R}_i)$ is a Wannier function which is localized at $\mathbf{R}_i$.

(a)(4P) Write down the dipole moment operator

$$\mathbf{P} = q \sum_i \hat{\mathbf{r}}_i, \quad q\text{: charge at position } \mathbf{r}_i \tag{8}$$

and with this the current density operator $\mathbf{j} = \dot{\mathbf{P}}/V$ in second quantization using Wannier states.

(b)(4P) Using (a), write down the conductivity tensor $\sigma^{\alpha\beta}(E)$, with $\alpha, \beta \in \{x, y, z\}$, in the tight binding approximation and determine the appearing Green's function.