

3. CMS exercise: Calculation of the Resistivity within Linear Response

The aim of this exercise is to compute the resistivity of a material within linear response. For this you will write your own program that evaluates the necessary formulae from the lecture, and apply it to the tight binding model of PbVO₃ that you derived in the second exercise.

After completion, please send your source code and your discussion to jan.tomczak@tuwien.ac.at

Linear Response

In the lecture we derived the Kubo formula for the conductivity of a solid. If we only have one band:

$$\sigma^{\alpha\beta} = \pi^2 \hbar e^2 \int d\omega \left(-\frac{\partial f}{\partial \omega} \right) \frac{1}{VN_{\mathbf{k}}} \sum_{\mathbf{k} \in BZ} A^2(\mathbf{k}, \omega) v^\alpha(\mathbf{k}) v^\beta(\mathbf{k}) \quad (1)$$

where $v^\alpha(\mathbf{k})$ is the Fermi velocity

$$v^\alpha(\mathbf{k}) = \frac{1}{\hbar} \frac{\partial \epsilon_{\mathbf{k}}}{\partial k_\alpha} \quad (2)$$

and

$$f(\omega) = \frac{1}{e^{\beta\omega} + 1} \quad (3)$$

the Fermi-Dirac function at an inverse temperature $\beta = 1/(k_B T)$ ¹, and

$$A(\mathbf{k}, \omega) = -\frac{1}{\pi} \Im G^R(\mathbf{k}, \omega + i0^+) \quad (4)$$

is the spectral function, V is the unit-cell volume and $N_{\mathbf{k}}$ the number of \mathbf{k} -points.² As we have seen in the lecture, for the conductivity to be non-zero, excitations must have a finite lifetime. We therefore supplement the dispersion $\epsilon_{\mathbf{k}}$ with an imaginary part:

$$\epsilon_{\mathbf{k}} \longrightarrow \epsilon_{\mathbf{k}} + i\hbar/\tau \quad (5)$$

where τ constitutes the lifetime of the excitation, that occurs as a damping factor in the Green's function:

$$G(\mathbf{k}, t) = e^{i\epsilon_{\mathbf{k}}t/\hbar} e^{-t/\tau} \quad (6)$$

which corresponds in frequency space to a broadened Lorentzian peak:

$$A(\mathbf{k}, \omega) = -\frac{1}{\pi} \Im G(\mathbf{k}, \omega) = -\frac{1}{\pi} \Im \frac{1}{\omega - \epsilon_{\mathbf{k}} + i\hbar/\tau} = \frac{1}{\pi} \frac{\hbar/\tau}{(\omega - \epsilon_{\mathbf{k}})^2 + (\hbar/\tau)^2} \xrightarrow{\tau \rightarrow \infty} \delta(\omega - \epsilon_{\mathbf{k}}) \quad (7)$$

As discussed in the lecture, in the limit of long lifetimes $\tau \rightarrow \infty$ the conductivity can be simplified to

$$\sigma^{\alpha\beta} = \pi \hbar e^2 (\tau/\hbar) \frac{1}{2VN_{\mathbf{k}}} \sum_{\mathbf{k}} \left(-\frac{\partial f}{\partial \omega} \right)_{\omega=\epsilon_{\mathbf{k}}} v^\alpha(\mathbf{k}) v^\beta(\mathbf{k}) \quad (8)$$

Both equations give σ in units $(\Omega m)^{-1}$ ($\hbar = 6.58212 \cdot 10^{-16}$ eVs, $e = 1.602 \cdot 10^{-19}$ C, $k_B = 8.617 \cdot 10^{-5}$ eV/K, $[\omega] = \text{eV}$, $[A(\mathbf{k}, \omega)] = \text{eV}^{-1}$, $[v(\mathbf{k})] = \text{m/s}$).

¹We measure ω in units of eV!

²compared to the lecture we are using here the convention that A has the unit of an inverse energy. Therefore we have a different power of \hbar as prefactor in Eqs. 1, 8. The unit-cell volume and number of \mathbf{k} -points, previously absorbed in the \sum -symbol, have been put as explicit factors for clarity.

Electronic structure

In the last exercise you obtained that, within DFT, PbVO_3 has a single band near the Fermi level that is well described by the tight-binding relation

$$\epsilon_{\mathbf{k}} = \epsilon_0 + 2t_1 (\cos(k_x a) + \cos(k_y a)) + 4t_2 \cos(k_x a) \cos(k_y a) \quad (9)$$

with the lattice constant $a = 3.8\text{\AA}$, and $\epsilon_0 = 0.03\text{eV}$, $t_1 = -0.154\text{eV}$ and $t_2 = -0.05\text{eV}$. Since the band does not disperse in k_z -direction ($c = 4.67\text{\AA}$), the momentum-sum in the above equations can be restricted to two dimensions (k_x, k_y) with $k_i \in [-\pi/a : \pi/a)$.

Tasks

1. Set up a program (you can choose any available language) that computes the *local* spectral function

$$A^{loc}(\omega) = \frac{1}{N_{\mathbf{k}}} \sum_{\mathbf{k}} A(\mathbf{k}, \omega) \quad (10)$$

using the above electronic structure and assuming a lifetime $\hbar/\tau \sim 0.01$ eV. Given this lifetime, how dense should you at least choose your ω -frequency mesh? Compare the local spectral function to the density of states (DOS) from exercise 2. The comparison can also help to judge how many \mathbf{k} -points are needed to produce a decent spectrum.

2. Given the above dispersion, and the relation Eq. 2 for the Fermi velocities, can you say (without evaluating Eq. 1 on the computer) what is the value of the conductivity σ^{xy} in our case? According to Ohm's law, σ^{xy} is the proportionality between the current measured in x -direction, when applying an external electrical field in y -direction.
3. Now code the Eqs. 1 and 8 and the necessary functions for the Fermi velocities and the derivative of the Fermi function. A few things to consider:
 - Note that $-\partial_{\omega} f(\omega)$ is strongly peaked at low temperatures. The frequency mesh has to be dense enough to resolve features smaller than $\sim k_B T$. You can test the accuracy of your frequency integration by numerically checking that $\int d\omega (-\partial_{\omega} f(\omega)) = 1$.
 - Note that the sum over the *square* of the spectral function will require more \mathbf{k} -points than the spectral function in order to be "smooth".
 - Also note that for constant τ , only the Fermi function is temperature dependent. As a consequence, $\Phi^{\alpha\beta}(\omega) = \sum_{\mathbf{k} \in BZ} A^2(\mathbf{k}, \omega) v^{\alpha}(\mathbf{k}) v^{\beta}(\mathbf{k})$ can be computed once and then used for the frequency integral at various temperatures.

With this in mind

- (a) Compare the conductivities σ of the two equations: plot them as a function of temperature for constant $\hbar/\tau = 0.005, 0.01, 0.05, 0.1$ eV. Identify the regime where there are notable differences in the conductivities.
- (b) Use a temperature dependent $\hbar/\tau = a + bT^2$, with $a = 10^{-3}\text{eV}$ and $b = 10^{-6}\text{eV/K}^2$. What is the resulting temperature dependence of the resistivity $\rho = 1/\sigma$?