Transport in the case of anisotropic parabolic band

Wenhao

September 9, 2021

1 Multiband anisotropic transport coefficient

Here, we follow the W. E. Bies et. al.'s derivation of the thermoelectric properties in an anisotropic semiconductor. *PRB, 65, 085208.*

The result of the semiclassical transport theory in the Boltzmann equation in the relaxation-time approximation gives

$$\sigma_{ij} = e^2 \int d\varepsilon \left(-\frac{\partial f_0}{\partial \varepsilon}\right) \Sigma_{ij}(\varepsilon) \tag{1}$$

$$T(\sigma \cdot S)_{ij} = e \int d\varepsilon \left(-\frac{\partial f_0}{\partial \varepsilon}\right) \Sigma_{ij}(\varepsilon)(\varepsilon - \mu) \tag{2}$$

and the transport distribution tensor Σ is given by:

$$\Sigma_{ij}(\varepsilon) = \int \frac{2d^3k}{(2\pi)^3} v_i(k) \sum_l \tau_{jl}(k) v_l(k) \delta[\varepsilon - \varepsilon(k)] \tag{3}$$

where ε is the energy of the electronic states, μ is the chemical potential, $v(k)$ is the electronic velocity and $\tau_{ij}(k) = \tau(\varepsilon)U_{ij}$ is the relaxation time which is explicitly an anisotropic tensor. Instead of considering N degenerate parabolic valleys as in the derivation of Bies. we consider N parabolic valleys with different energy ε_n and effective mass tensor M_{ij} with the electronic dispersion relationship and electronic group velocity is given by:

$$\varepsilon^{(n)}(k) = \varepsilon_n + \frac{\hbar^2}{2} \sum_{ij} (k_i - k_i^{(n)}) M_{ij}^{(n)-1} (k_j - k_j^{(n)}) \tag{4}$$

$$v_i^{(n)}(k) = \hbar \sum_j M_{ij}^{(n)-1} (k_j - k_j^{(n)}) \tag{5}$$

where ε_n is the energy at the bottom of the parabolic valley and k_α^0 with $\alpha = i, j, k$ is the position of the band maximum. Putting the expression of the electronic velocity into the expression for Σ and summing over all N transport valleys, we obtain:

$$\Sigma_{ij}(\varepsilon) = \sum_{n=1}^{N} \tau(\varepsilon) \int \frac{2d^3k}{(2\pi)^3} \hbar^2 \sum_{i',j',l} M_{ii'}^{(n)-1} k_{i'} U_{jj'}^{(n)} M_{j'l}^{(n)-1} k_l \delta[\varepsilon - \varepsilon(k + k^{(n)})] \tag{6}$$

$$= \sum_{n=1}^{N} \frac{2^{3/2} \tau(\varepsilon - \varepsilon_n)(\varepsilon - \varepsilon_n)^{3/2}}{3\pi^2\hbar^3} \sum_l \sqrt{\det \mathbf{M}^{(n)}} U_{jl}^{(n)} M_{li}^{(n)-1} \theta(\varepsilon - \varepsilon_n) \tag{7}$$

which correspond to Eq.(29) with a change of variable from $\varepsilon \to (\varepsilon - \varepsilon_n)$ for different parabolic valleys and A step θ function is included for each band.

Following the notation of the paper, we further write:

$$\Sigma_{ij}(\varepsilon) = \sum_{n=1}^{N} \mathcal{T}^{(n)}(\varepsilon) A_{ij}^{(n)} \tag{8}$$

with a dimensionaless matrix $\mathbf{A}$:

$$\mathbf{A}^{(n)} = \left(m_0^{-1/2}\sqrt{\det \mathbf{M}^{(n)}}\right)\left(\mathbf{U}^{(n)}\mathbf{M}^{(n)-1}\right)^T \tag{9}$$

$$\mathcal{T}^{(n)}(\varepsilon) = \frac{2^{3/2}m_0^{1/2}}{3\pi^2\hbar^3}\tau(\varepsilon-\varepsilon_n)(\varepsilon-\varepsilon_n)^{3/2}\theta(\varepsilon-\varepsilon_n) \tag{10}$$

In the simplest case, we consider $\mathcal{T} = \mathcal{I}$, a 3×3 identity matrix correspond to isotropic scattering and $\mathbf{M}$ diagonal. Then $\mathbf{A}$ is also diagonal and $A_i = A_{ii}$ will simply be:

$$A_i^{(n)} = \left(m_0^{-1/2}\sqrt{M_1M_2M_3}\right)/M_i \tag{11}$$

for $i = 1,2,3$, three eigen direction. We note that $\mathbf{A}$ encode all information about the anisotropy of the electronic bands.

We write the conductivity tensor as:

$$\sigma = e^2\int d\varepsilon\left(-\frac{\partial f_0}{\partial\varepsilon}\right)\mathbf{\Sigma}(\varepsilon) \tag{12}$$

$$= e^2\sum_{n=1}^{N}\int d\varepsilon\left(-\frac{\partial f_0}{\partial\varepsilon}\right)\mathcal{T}^{(n)}(\varepsilon)\mathbf{A}^{(n)} \tag{13}$$

$$= \sum_{n=1}^{N}\sigma_0^{(n)}\mathbf{A}^{(n)} \tag{14}$$

The Seebeck tensor is related to σ by:

$$(\sigma\cdot\mathbf{S}) = (e/T)\sum_{n=1}^{N}\int d\varepsilon\left(-\frac{\partial f_0}{\partial\varepsilon}\right)(\varepsilon-\mu)\mathcal{T}^{(n)}(\varepsilon)\mathbf{A}^{(n)} \tag{15}$$

$$= \sum_{n=1}^{N}\sigma_0^{(n)}S_0^{(n)}\mathbf{A}^{(n)} \tag{16}$$

This two equations follow Eq.(34) and Eq.(35) in the paper but now with different bands have different value of $\mathcal{T}^{(n)}(\varepsilon)$.

In the case when $\mathbf{A}$ is diagonal, we obtain the Seebeck coefficient:

$$S_i = \frac{\sum_{n=1}^{N}\sigma_0^{(n)}S_0^{(n)}A_i^{(n)}}{\sum_{n=1}^{N}\sigma_0^{(n)}A_i^{(n)}} \tag{17}$$

2 Application to $CrSi_2$