Boltzmann equation and the like

Jinyuan Wu

January 18, 2023

1 Boltzmann equation for electrons in a crystal

We define

$$\# \text{ of band } n \text{ electrons in } \Delta\Omega, \Delta V = \frac{\Delta V}{V} \sum_{\boldsymbol{k} \in \Delta\Omega} f_n(\boldsymbol{r}, \boldsymbol{k}, t), = \Delta V \int_{\Delta\Omega} \frac{\mathrm{d}^3 \boldsymbol{k}}{(2\pi)^3} f_n(\boldsymbol{r}, \boldsymbol{k}, t),$$

and therefore when the $\boldsymbol{k}$-grid is dense enough, i.e. when $V \to \infty$, we have

$$\# \text{ of band } n \text{ electrons in } \mathrm{d}^3\boldsymbol{r}\, \mathrm{d}^3\boldsymbol{k} = f_n(\boldsymbol{r}, \boldsymbol{k}, t)\, \mathrm{d}^3\boldsymbol{r}\, \frac{\mathrm{d}^3\boldsymbol{k}}{(2\pi)^3}. \tag{1}$$

The Boltzmann equation can be derived from the following intuitive notion:

$$\frac{\mathrm{d}}{\mathrm{d}t} \frac{\Delta V}{V} f_n(\boldsymbol{r}, \boldsymbol{k}, t) = \sum_{\text{initial states}} \Gamma_{\text{initial states} \to n\boldsymbol{k}} - \sum_{\text{final states}} \Gamma_{n, \boldsymbol{k} \to \text{final states}},$$

where we have (according to Fermi golden rule)

$$\Gamma_{1\to 2} = \frac{2\pi}{\hbar} |\langle 2 | H_{\text{int}} | 1 \rangle|^2 \delta() \tag{2}$$

TODO: the real part of the self-energy enters the diffusion part in the equation; the imaginary part contributes to the collision integral. It should be noted that the imaginary part is present with $T = 0$. The physical picture is, the eigenstates of a Coulomb-interactive electron gas are all compositions of Fock states with varying electron distributions, and therefore any single-particle description of the system suffers from the loss of information to 2-electron, 3-electron, etc. subspaces, which is effectively modeled as a finite lifetime of the particle. This doesn't come from any thermal fluctuation. Note that this also means the ground state of the system is "boiling" in the independent-electron picture; we therefore may say "electrons are scattering each other even at the ground state". Note, however, that this scattering rate decreases as $\tau \sim 1/(k - k_{\mathrm{F}})^2$ in RPA, and the single-electron picture at least works good enough for bands near the Fermi surface in systems for which GW works.