Field theory for nonequilibrium systems, WS 2016/17

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Sheet 7

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1 Two-temperature model

Consider the coupled kinetic equations for electrons and phonons[1],

$$\frac{\partial n_{\boldsymbol{k}}}{\partial t} = -\frac{2\pi}{N_c}\sum_{\boldsymbol{k}',\boldsymbol{Q}} \delta(\boldsymbol{k}-\boldsymbol{k}'-\boldsymbol{Q})|M_{\boldsymbol{Q}}|^2\{n_{\boldsymbol{k}}(1-n_{\boldsymbol{k}'})[(N_{\boldsymbol{Q}}+1)\delta(\epsilon_{\boldsymbol{k}}-\epsilon_{\boldsymbol{k}'}-\omega_{\boldsymbol{Q}})+N_{\boldsymbol{Q}}\delta(\epsilon_{\boldsymbol{k}}-\epsilon_{\boldsymbol{k}'}+\omega_{\boldsymbol{Q}})] - (1-n_{\boldsymbol{k}})n_{\boldsymbol{k}'}[(N_{\boldsymbol{Q}}+1)\delta(\epsilon_{\boldsymbol{k}}-\epsilon_{\boldsymbol{k}'}+\omega_{\boldsymbol{Q}})+N_{\boldsymbol{Q}}\delta(\epsilon_{\boldsymbol{k}}-\epsilon_{\boldsymbol{k}'}-\omega_{\boldsymbol{Q}})]\}, \tag{1}$$

$$\frac{\partial N_{\boldsymbol{Q}}}{\partial t} = -\frac{4\pi}{N_c}\sum_{\boldsymbol{k},\boldsymbol{k}'} \delta(\boldsymbol{k}-\boldsymbol{k}'-\boldsymbol{Q})|M_{\boldsymbol{Q}}|^2\{n_{\boldsymbol{k}}(1-n_{\boldsymbol{k}'})[N_{\boldsymbol{Q}}\delta(\epsilon_{\boldsymbol{k}}-\epsilon_{\boldsymbol{k}'}+\omega_{\boldsymbol{Q}})-(N_{\boldsymbol{Q}}+1)\delta(\epsilon_{\boldsymbol{k}}-\epsilon_{\boldsymbol{k}'}-\omega_{\boldsymbol{Q}})]\}, \tag{2}$$

with $n_{\boldsymbol{k}}$ the electron occupation at momentum $\boldsymbol{k}$ and energy $\epsilon_{\boldsymbol{k}}$, $N_{\boldsymbol{Q}}$ the phonon occupation at momentum $\boldsymbol{Q}$ and energy $\omega_{\boldsymbol{Q}}$, N_c the number of unit cells ($\boldsymbol{k}$ points), and $M_{\boldsymbol{Q}}$ the matrix element for electron-phonon scattering with momentum transfer $\boldsymbol{k}-\boldsymbol{k}'=\boldsymbol{Q}$. The factor of 2 in Eq. (2) accounts for electron spin degeneracy.

(a) Draw the physical processes (Feynman diagrams and energy dispersion diagrams with arrows for scattering from/to) for the individual terms and give them a physical interpretation.

(b) Show that the kinetic equations fulfill energy conservation within the quasiparticle approximation with energy $E = E_e + E_L = 2\sum_{\boldsymbol{k}} \epsilon_{\boldsymbol{k}} n_{\boldsymbol{k}} + \sum_{\boldsymbol{Q}} \omega_{\boldsymbol{Q}} N_{\boldsymbol{Q}}$, the sum of electronic (e) and lattice (L) contributions.

(c) Assume Fermi-Dirac and Bose-Einstein distributions for the electrons and phonons, respectively. This is the two-temperature ansatz with temperatures T_e and T_L. Compute the rate of energy exchange by considering the electronic energy, $\frac{\partial E_e}{\partial t}$, using Eq. (1). Insert factors of unity of the form $\int d\epsilon \delta(\epsilon_{\boldsymbol{k}}-\epsilon)$, $\int d\epsilon' \delta(\epsilon_{\boldsymbol{k}'}-\epsilon')$, $\int d\Omega \delta(\omega_{\boldsymbol{Q}}-\Omega)$. Introduce the Eliashberg function $\alpha^2F(\epsilon,\epsilon',\Omega) \equiv [2/N_c^2 N(\epsilon_F)]\sum_{\boldsymbol{k},\boldsymbol{k}'} |M_{\boldsymbol{Q}}|^2 \delta(\epsilon_{\boldsymbol{k}}-\epsilon)\delta(\epsilon_{\boldsymbol{k}'}-\epsilon')\delta(\omega_{\boldsymbol{Q}}-\Omega)$ with $N(\epsilon_F)$ the density of states at the Fermi level. Simplify to its average over the Fermi surface (energy ϵ_F), $\alpha^2F(\Omega) \equiv \alpha^2F(\epsilon_F,\epsilon_F,\Omega)$. Result: $\frac{\partial E_e}{\partial t} = 2\pi N_c N(\epsilon_F)\int_0^\infty d\Omega\, \alpha^2F(\Omega)\Omega^2[N_B(\Omega,T_L)-N_B(\Omega,T_e)]$, with $N_B(x,T)$ the Bose-Einstein distribution at energy x and temperature T.

(d) Use a Taylor high-temperature expansion (assume small Ω/k_BT) to obtain a relaxation equation for the electronic temperature using $E_e \approx E_0 + \frac{1}{2}\gamma T_e^2$, with $\gamma = \pi^2 N_c N(\epsilon_F) k_B^2/3$ the linear heat capacity coefficient for the electrons. Also use the moments of the Eliashberg function, $\lambda\langle\omega^n\rangle \equiv 2\int_0^\infty d\Omega\, \frac{\alpha^2F(\Omega)}{\Omega}\Omega^n$. Here λ is the effective electron-phonon coupling known from the theory of superconductivity. What determines the cooling of hot electrons?

[1] P. B. Allen, Phys. Rev. Lett. 59, 1460 (1987)

Tutorial "Two-temperature model"

$$\frac{\partial n_k}{\partial t} = -\frac{2\pi}{N_c} \sum_{k'Q} \delta(k-k'-Q)\,|M_Q|^2 \Big\{ n_k(1-n_{k'})\big[(N_Q+1)\,\delta(\epsilon_k-\epsilon_{k'}-\omega_Q) + N_Q\,\delta(\epsilon_k-\epsilon_{k'}+\omega_Q)\big] - (1-n_k)n_{k'}\big[(N_Q+1)\,\delta(\epsilon_k-\epsilon_{k'}+\omega_Q) + N_Q\,\delta(\epsilon_k-\epsilon_{k'}-\omega_Q)\big]\Big\}$$

N_c: number of unit cells

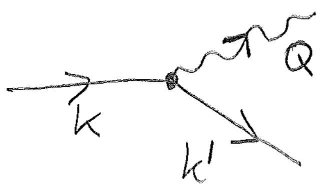
extra factor 2 for electron spin

$$\frac{\partial N_Q}{\partial t} = -\frac{4\pi}{N_c} \sum_{kk'} \delta(k-k'-Q)\,|M_Q|^2\, n_k(1-n_{k'})\big[N_Q\,\delta(\epsilon_k-\epsilon_{k'}+\omega_Q) - (N_Q+1)\,\delta(\epsilon_k-\epsilon_{k'}-\omega_Q)\big]$$

(a) Draw the physical processes.

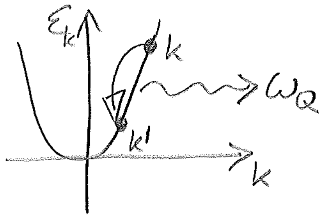
$$n_k(1-n_{k'})\,(N_Q+1)\,\delta(\epsilon_k-\epsilon_{k'}-\omega_Q)$$

Diagram:



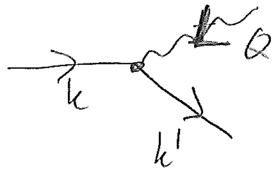
phonon emission (bosonic enhancement)

$$\omega_Q = \epsilon_k - \epsilon_{k'}$$



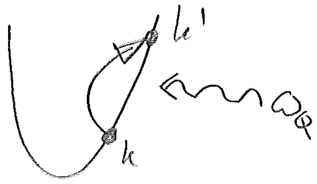
"scattering out to lower state"

$$n_k(1-n_{k'})\,N_Q\,\delta(\epsilon_k-\epsilon_{k'}+\omega_Q)$$



phonon absorption

$$-\omega_Q = \epsilon_k - \epsilon_{k'}$$



"scattering out to higher state"

Other two: scattering in from below/above

(b) Show energy conservation.

$$2 \sum_k \epsilon_k \frac{\partial n_k}{\partial t} + \sum_Q \omega_Q \frac{\partial N_Q}{\partial t} = 0$$

spin

(c) Make effective temperature ansatz for distributions:

$$n_k(t) = \frac{1}{1+e^{\epsilon_k / k_B T_e(t)}} \qquad T_e \equiv \text{electronic temperature}$$

$$N_Q(t) = \frac{1}{e^{\omega_Q / k_B T_L(t)} - 1} \qquad T_L \equiv \text{Lattice temperature}$$

Compute rate of energy exchange

$$E_e = 2 \sum_k \epsilon_k n_k \approx E_0 + \tfrac{1}{2}\gamma T_e^2 \qquad (*)$$

$$E_L = \sum_Q \omega_Q N_Q \approx 3 N_a k_B T_L$$

$$\frac{\partial E_e}{\partial t} = \frac{4\pi}{N_c} \sum_{kk'} \omega_Q |M_Q|^2 \left[(n_k - n_{k'}) N_Q - n_{k'}(1-n_k)\right] \delta(\epsilon_k - \epsilon_{k'} + \omega_Q)$$

linear heat capacity coefficient $\gamma = \pi^2 N_c N(\epsilon_F) k_B^2 / 3$

density of states for both spins per unit cell

Insert 1's: $\int d\epsilon \, \delta(\epsilon_k - \epsilon)$

$\int d\epsilon' \, \delta(\epsilon_{k'} - \epsilon')$

$\int d\Omega \, \delta(\omega_Q - \Omega)$

Eliashberg function

$$\alpha^2 F(\epsilon,\epsilon',\Omega) \equiv [2/N_c^2 N(\epsilon_F)] \sum_{kk'} |M_Q|^2 \delta(\omega_Q-\Omega)\delta(\epsilon_k-\epsilon)\delta(\epsilon_{k'}-\epsilon')$$

Simplify $\alpha^2 F(\Omega) \equiv \alpha^2 F(\epsilon_F,\epsilon_F,\Omega)$

$$\rightarrow \frac{\partial E_e}{\partial t} = 2\pi N_c N(\epsilon_F) \int_0^\infty d\Omega\, \alpha^2 F(\Omega)\, \Omega \int d\epsilon \int d\epsilon' \{[f(\epsilon)-f(\epsilon')] N(\Omega,T_L) - f(\epsilon')[1-f(\epsilon)]\}\delta(\epsilon-\epsilon'+\Omega)$$

$f(\epsilon)$ = Fermi-Dirac dist. at T_e

perform integrals

$N(\Omega,T_L)$ = Bose-Einstein dist. at T_L

$$\rightarrow \frac{\partial E_e}{\partial t} = 2\pi N_c N(\epsilon_F) \int_0^\infty d\Omega\, \alpha^2 F(\Omega)\, \Omega^2 [N(\Omega,T_L) - N(\Omega,T_e)]$$

(d) high-T limit: use moments of $\alpha^2 F$ known from superconductivity theory:

$$\lambda\langle\omega^n\rangle \equiv 2 \int_0^\infty d\Omega\, \frac{\alpha^2 F(\Omega)}{\Omega}\, \Omega^n$$

$\lambda \equiv \lambda\langle\omega^0\rangle$ coupling constant (determines T_c)

Taylor expansion in $\Omega/k_B T$:

$$\frac{\partial E_e}{\partial t} = \pi N_c N(\epsilon_F)\, \lambda \left[\langle\omega^2\rangle - \langle\omega^4\rangle / 12 k_B^2 T_e T_L + \dots\right] k_B (T_L - T_e)$$

$\rightarrow$ temperature relaxation rate via (*)

$$\frac{\partial T_e}{\partial t} = \gamma_T (T_L - T_e)$$

$$\gamma_T \equiv \frac{3\lambda\langle\omega^2\rangle}{\pi k_B T_e}\left(1 - \frac{\langle\omega^4\rangle}{12\langle\omega^2\rangle k_B^2 T_e T_L} + \dots\right)$$

$\longrightarrow$ used to determine $\lambda\langle\omega^2\rangle$ in metals via pump-probe photoemission spectroscopy.

(Cu, Au, W, ...)

Solution for $T_e(t)$?