8.512 Theory of Solids II
Spring 2009

8.512 Theory of Solids II **Problem Set 1** **Due February**

1. (a) Prove the finite temperature version of the fluctuation dissipation theorem

$$\chi''(q,\omega) = \frac{1}{2}(e^{-\beta\omega} - 1)S(q,\omega) \ ,$$

and

$$S(q,\omega) = -2(n_B(\omega) + 1)\chi''(q,\omega) \ ,$$

where $S(q,\omega) = \int d\mathbf{x}dte^{-i\mathbf{q}-\mathbf{x}}e^{i\omega x}\langle\rho(\mathbf{x},t)\rho(0,0)\rangle_T$ and $n_B(\omega) = (e^{\beta\omega} - 1)^{-1}$ is the Bose occupation factor.

(b) Show that $\chi''(q,\omega) = -\chi''(-q,-\omega)$ and $S(-q,-\omega) = e^{-\beta\omega}S(q,\omega)$. In terms of the scattering probability, show that this is consistent with detailed balance.

2. Neutron scattering by crystals.

We showed in class that the probability of neutron scattering with momentum $\mathbf{k}_i$ to $\mathbf{k}_f$ is given by $(2\pi b/M_n)^2 S(\mathbf{Q},\omega)$ where b is the scattering of the nucleus $\mathbf{Q} = \mathbf{k}_i - \mathbf{k}_f$ and

$$S(\mathbf{Q},\omega) = \int dte^{i\omega t}F(\mathbf{Q},t)$$

where

$$F(\mathbf{Q},t) = \sum_{j,l}\langle e^{-i\mathbf{Q}\cdot\mathbf{r}_j(t)}e^{-i\mathbf{Q}\cdot\mathbf{r}_l(0)}\rangle_T \qquad (1)$$

and $\mathbf{r}_j(t)$ is the instantaneous nucleus position. Write $\mathbf{r}_j = \mathbf{R}_j + \mathbf{u}_j$, where $\mathbf{R}_j$ are the lattice sites, and expand $\mathbf{u}_j$ in terms of phonon modes

$$\mathbf{u}_j = \sum_\alpha\sum_q \boldsymbol{\lambda}_\alpha \frac{1}{\sqrt{2NM\omega_q}}\left(a_{\alpha,q}e^{i(\mathbf{q}\cdot\mathbf{R}_j - \omega_q t)} + c.c.\right) \qquad (2)$$

where $\boldsymbol{\lambda}_\alpha$ are the polarization vectors and α labels the transverse and longitudinal modes. Note that only $\mathbf{Q}\cdot\mathbf{u}_j$ appear in Eq. (1). For simplicity, assume the α modes are degenerate for each $\mathbf{q}$ so that we can always choose one mode with $\boldsymbol{\lambda}_\alpha$ parallel to $\mathbf{Q}$. Henceforth we will drop the α label and $\boldsymbol{\lambda}_\alpha$ and treat $\mathbf{Q}\cdot\mathbf{u}_j$ as scalar products Qu_j. Then

$$F(\mathbf{Q},t) = \sum_{jl} e^{-i\mathbf{Q}\cdot(\mathbf{R}_j - \mathbf{R}_l)}F_{ij}(t)$$

where

$$F_{jl}(t) = \langle e^{-iQu_j(t)}e^{iQu_l(0)}\rangle_T \ .$$

(a) Show that

$$F_{ij}(t) = \langle e^{-iQ(u_j(t)-u_l(0))}\rangle_T e^{\frac{1}{2}[Qu_j(t),Qu_l(0)]} \tag{3}$$

Furthermore, for harmonic oscillators, you may assume without proof that the first factor can be written as

$$\langle e^{-iQ(u_j(t)-u_l(0))}\rangle_T = e^{-\frac{1}{2}Q^2\langle(u_j(t)-u_l(0))^2\rangle_T} \tag{4}$$

(b) Using Eqs. (1–4) show that

$$F_{jl}(t) = e^{-2W}\exp\left\{\frac{Q^2}{2NM}\sum_q \frac{1}{\omega_q}\left((2n_q+1)\cos\theta_{jl} + i\sin\theta_{jl}\right)\right\} \tag{5}$$

where the Debye-Waller factor $2W$ is given by

$$2W = \frac{Q^2}{2NM}\sum_q \frac{1}{\omega_q}(2n_q+1)$$

and $n_q = 1/\left(e^{\beta\omega_q}-1\right)$, $\theta_{jl} = -\omega_q t + \mathbf{q}\cdot(\mathbf{R}_j - \mathbf{R}_l)$

(c) Expand the exp factor in Eq. (5) to lowest order and show that (V^* is the volume of reciprocal lattice unit cell)

$$\begin{aligned} S(Q,\omega) &= NV^* e^{-2W}\left\{\sum_G \delta(\mathbf{Q}-\mathbf{G})\delta(\omega)\right. \\ &+ \sum_{\mathbf{q}} \frac{Q^2}{2NM\omega_q}\left((n_q+1)\sum_G \delta(\mathbf{Q}-\mathbf{q}-\mathbf{G})\delta(\omega-\omega_q)\right. \qquad (6) \\ &+ \left.\left. n_q\sum_G \delta(\mathbf{Q}+\mathbf{q}-\mathbf{G})\delta(\omega+\omega_q)\right)\right\} \qquad (7) \end{aligned}$$

(d) Discuss the interpretation of various terms in Eq. (6) .

(e) Even though we did not compute it explicitly, what experiment would you propose to measure the polarization vector λ_α of a given mode at energy ω_q ?