8.512 Theory of Solids II
Spring 2009

**8.512 Theory of Solids**

**Problem Set #1** **Due: February 12, 2004**

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

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

and

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

where $S(q,\omega) = \int d\vec{x}\, dt\, e^{-i\vec{q}-\vec{x}} e^{i\omega x} \left\langle \rho(\vec{x},t)\rho(0,\ ) \right\rangle_T$ and $n_B(\omega) = \left(e^{\beta\omega} - 1\right)^{-1}$ 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 $\vec{k}_i$ to $\vec{k}_f$ is given by $(2\pi b/M_n)^2 S(\vec{Q},\omega)$ where $b$ is the scattering of the nucleus $\vec{Q} = \vec{k}_i - \vec{k}_f$ and

$$S(\vec{Q},\omega) = \int dt\, e^{i\omega t} F(\vec{Q},t)$$

where

$$F(\vec{Q},t) = \sum_{j,e} \left\langle e^{-i\vec{Q}\cdot\vec{r}_j(t)} e^{i\vec{Q}\cdot\vec{r}_l(0)} \right\rangle_T \tag{1}$$

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

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

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

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

where

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

a) Show that

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

Furthermore, for harmonic oscillators, the first factor can be written as

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

b) Using Eqs. (1–4) show that

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

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

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

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

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

$$S(Q,\omega) = N\,V^*\,e^{-2W}\left\{\sum_G \delta\left(\vec{Q}-\vec{G}\right) + \sum_{\vec{q}} \frac{Q^2}{2N\;M\;\omega_q}\left(\left(n_q+1\right)\sum_G \delta\left(\vec{Q}-\vec{q}-\vec{G}\right)\,\delta\left(\omega-\omega_q\right) + n_q\sum_G \delta\left(\vec{Q}+\vec{q}-\vec{G}\right)\delta\left(\omega+\omega_q\right)\right)\right\} \qquad (6)$$

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 $\lambda_\alpha$ of a given mode at energy $\omega_q$?