Physics 556 Spring 2004
Problem Set 1, Due Friday Feb. 13

1. **Einstein Phonon Green's Function**. For nice pedagogical reasons, Doniach and Sondheimer (D&S) derive the harmonic phonon Green's function eq. 1.6.10 in a non-standard way, by first defining a Green's function G_0 for an Einstein lattice and then deriving a series expansion and summing it to get G which includes the effects of inter-atom forces. The definition of G_0, eq. 1.5.2, is used to evaluate it exactly in the time domain, giving the result, eq. 1.5.11, namely

$$G_0(t) = -\frac{i}{2M\Omega_0} e^{-i\Omega_0|t|}. \tag{1}$$

The Fourier transform (pp. 20-22) is used to evaluate $G_0(\omega)$ in eq. 1.6.9, namely

$$G_0(\omega) = \frac{1}{M(\omega^2 - \Omega_0^2 + i\eta)} \tag{2}$$

where the infinitesimal term $i\eta$ is needed to make sense of the original definition.

Let us first think about the Einstein lattice as just equivalent to a single Harmonic oscillator (repeated N times). Suppose we want to solve Newton's laws for the driven oscillator,

$$M\frac{d^2u}{dt^2} + Ku = F(t) \tag{3}$$

where $K/M = \Omega_0^2$ and $F(t)$ is an arbitrary smooth external time-dependent driving force. The solution involves the Green's function G_0. We look for a solution to

$$\left(M\frac{d^2}{dt^2} + K\right) G_0(t-t') = -\delta(t-t') \tag{4}$$

and for convenience we can set t' to zero (a better way to say this is that the new variable t is used in place of $t - t'$.) For $t < 0$, the general solution is

$$G_0(t) = A\cos(\Omega_0 t) + B\sin(\Omega_0 t) \tag{5}$$

while for $t > 0$ it is

$$G_0(t) = C\cos(\Omega_0 t) + D\sin(\Omega_0 t). \tag{6}$$

The coefficients A, B, C, D must be chosen to satisfy the appropriate discontinuity of derivative and continuity in time of G_0 at time $t = 0$ implied by the δ function at time zero. This will give two constraints, leaving two unknown coefficients in the Green's function.

a. Determine the constraints and give the general form of G_0 with two free coefficients.

b. The remaining unknowns are fixed by the physical conditions we demand for a proper solution, which has the form

$$u(t) = -\int_{-\infty}^{\infty} dt' G_0(t-t')F(t') \quad \text{(plus an arbitrary solution of the homogeneous equation).}$$

Specifically, we know that the displacement at time t can only depend on the force $F(t')$ at times t' **earlier** than t. The means that $G_0(t)$ must vanish for $t < 0$. This **condition of causality** provides the missing constraints that fix the Green's function for this problem. Find the required form of $G_0(t)$ and write the general solution for $u(t)$.

c. Compare (A, B, C, D) needed for (**b.**) above with (A, B, C, D) used in eq.(1). Show that eq.(1) also satisfies eq.(4).

d. Find the Fourier transform $G_0(\omega)$ of your $G_0(t)$ and compare with the version 1.6.10 used by D&S. Also compare with 1.6.12.

2. **Harmonic Phonon Green's Function** Now let's derive the final result of Chapter 1, eq. 1.6.10, in the more conventional way, by direct evaluation of the defining eq. 1.4.6 (we can set $\lambda = 1$.) This means, do the analog of the derivation on pp. 16 and 17, between eqs. 1.5.2 and 1.5.11, except for $G_{ij}(t)$ rather than $G_0(t)$. To do this requires solving the harmonic lattice dynamics by Bloch's theorem and then quantizing. This was done in PHY 555 and is done by D&S on pp. 32 and 33. Note the typos on p.32 which are corrected in the typo notes. Also note and derive the equations

$$u_i = \sum_k \sqrt{\frac{\hbar}{2NM\Omega_k}}(b_k + b_{-k}^\dagger)e^{-i\vec{k}\cdot\vec{R}_i},$$

and

$$b_k(t) = b_k e^{-i\Omega_k t}.$$

Note also that the ij to k Fourier transform is given in eq. 1.6.13, and the t to ω Fourier transform is given on p.20.