1. In class, we discussed the electron-phonon interaction, and how it affects the electrical resistivity. An important quantity in this calculation is the matrix element

\[ \langle n|F_q(r)|n'k' \rangle \] (1)

Here \(|n'k'\rangle\) represents a Bloch state with band index \(n'\) and Bloch vector \(k'\), and

\[ F_q(r) = \sum_i [\nabla_i V(r; r_1, \ldots r_N)]_{r_j = R_i} e^{i q \cdot R_i}. \] (2)

Here \(V(r; r_1, \ldots r_N)\) is the potential acting on an electron at \(r\) when the \(N\) ions are at \(r_1, \ldots r_N\). We write the position of the \(i^{th}\) ion as \(R_i + u_i\), where \(R_i\) is the \(i^{th}\) Bravais lattice vector (we consider a lattice with only one atom per primitive cell), and the subscript means that the gradient is evaluated when the displacements \(u_i = 0\).

Now assume that the potential \(V\) can be written as a sum of atomic potentials in the form

\[ V = \sum_i V_{at}(r - r_i). \] (3)

(a) Show that \(F_q(r)\) can be written

\[ F_q(r) = \sum_i [\nabla_i V_{at}(r - r_i)]_{r_j = R_i} e^{i q \cdot R_i}. \] (4)

(b). If the \(R_i\)’s form a Bravais lattice, show that the function \(F_q(r)e^{-i q \cdot r}\) is periodic on the Bravais lattice. [By definition, a function \(u(r)\) is periodic if it satisfies \(u(r + R_i) = u(r)\) for any Bravais lattice vector.]

(c). Hence, show that the matrix element (1) vanishes unless \(k' = k + q + K\), where \(K\) is a reciprocal lattice vector satisfying \(e^{i K \cdot R_i} = 1\).
for any Bravais lattice vector $i$ (see notes on course web site, or Ashcroft and Mermin). Recall that in $r$-representation, the Bloch state $\langle \mathbf{r}|n\mathbf{k}\rangle = e^{i\mathbf{k} \cdot \mathbf{r}} u_{nk}(\mathbf{r})$, where $u_{nk}(\mathbf{r})$ is a periodic function and $n$ is a band index.

(d). Make the assumption that this matrix element vanishes when $\mathbf{K} = 0$ and $\mathbf{q} = 0$. How would you expect it to depend on $\mathbf{q}$ for $\mathbf{K} = 0$ and small $\mathbf{q}$?

2. As discussed in class, an electromagnetic field can cause an electron to undergo transitions from one state to another. The matrix element of the perturbation between two Bloch states may be written

$$\langle n\mathbf{k}|H'|n'\mathbf{k}'\rangle,$$

where $H'$ is the perturbation Hamiltonian and $|n'\mathbf{k}'\rangle$ is a Bloch state, as described in the previous problem. If the em field is weak, $H'$ takes the form

$$H' = \frac{e}{2mc}(\mathbf{p} \cdot \mathbf{A} + \mathbf{A} \cdot \mathbf{p}),$$

where $\mathbf{A}$ is the vector potential, $\mathbf{p} = -i\hbar \nabla$, and $m$ is electron mass.

(a). Write down a suitable vector potential $\mathbf{A}$ for an electric field $E_0 \dot{x} \cos(kz - \omega t)$.

(b). Show that, if $k$ can be taken as approximately zero, then the matrix element of $H'$ vanishes unless $k = k'$. This means that only so-called vertical transitions are allowed.

(c). If the crystal potential has inversion symmetry, then all the Bloch states have definite parity - that is, they satisfy the relation $\Psi_{nk}(-\mathbf{r}) = \pm \Psi_{nk}(\mathbf{r})$, the plus or minus sign corresponding to states of even or odd parity. Show that $H'$ can produce transitions only between states of opposite parity.

(d). Many semiconductors have an indirect band gap, that is, the minimum energy states of the conduction band do not occur at the same $\mathbf{k}$ as the highest energy states of the valence band. Nonetheless, absorption corresponding to these indirect transitions is observed. Why do you think such transitions can occur, despite your result of part (b)?

3. **Analytical Properties of Complex Dielectric Function.** In class, I briefly discussed the Kramers-Kronig relations for the complex dielectric function $\epsilon(\omega)$ for a material. To derive these, you need to know
something about the properties of a function of a complex variable, in particular Cauchy’s theorem. This problem does not require knowledge of complex variable theory; however, there is an optional part in which you may, if you wish, apply Cauchy’s theorem to obtain the Kramers-Kronig relations.

Instead of $\epsilon(\omega)$, we will consider the complex susceptibility $\chi(\omega)$, defined in esu by

$$\epsilon(\omega) = 1 + 4\pi\chi(\omega). \tag{6}$$

$\chi(\omega)$ relates the polarization $P(\omega)$ to the electric field $E(\omega)$ by the equation

$$P(\omega) = \chi(\omega)E(\omega). \tag{7}$$

To obtain some of the properties of $\chi(\omega)$ we write down the analogous relation in terms of time rather than frequency:

$$P(t) = \int_{-\infty}^{\infty} \chi(t - t')E(t')dt'. \tag{8}$$

This equation states that $P(t)$ is a linear function of the electric field $E(t')$. Since $P(t)$ can only depend on the electric field at earlier times, we must have $\chi(t - t') = 0$ if $t' > t$. This condition is called causality. Also, the function $\chi(t - t')$ depends only on the difference between $t$ and $t'$, because the absolute time cannot play a role in this equation; only the time differences can enter.

(a). The Fourier transforms are defined by the relations

$$P(\omega) = \int_{-\infty}^{\infty} P(t)e^{i\omega t}dt, \tag{9}$$

with similar relations for $E(\omega)$ and $\chi(\omega)$. Show that in Fourier transform, eq. (8) becomes

$$P(\omega) = \chi(\omega)E(\omega). \tag{10}$$

(b). Since $P(t)$ and $E(t')$ are real, the function $\chi(t - t')$ must also be real. Show that this implies that $\chi(-\omega) = \chi^*(\omega)$, where the star denotes a complex conjugate.
(c). Show that causality implies that $\chi(z)$ is finite for any complex frequency $z$ with a positive imaginary part.

(d). OPTIONAL; not to be turned in. Since $\chi(z)$ is thus analytical in the upper half complex $z$ plane, we can use Cauchy’s theorem:

$$\chi(z) = \frac{1}{2\pi i} \int_C \frac{\chi(z')}{z' - z} \, dz',$$

where integral is taken over any closed counterclockwise contour where $\chi$ is analytic, and including the point $z$.

Now suppose $z$ is on the real axis. We call this value of $z\omega$. We choose the contour $C$ to consist of three parts, $C_1$ consists of an integral along the $z'$ axis, from $-R$ to $+R$, where $R$ is very large, except for an infinitesimal strip of length $2\delta$ centered on $\omega$. $C_2$ consists of a semicircle of radius $\delta$, in the lower half $z'$ plane, centered on $\omega$, around which the integral is taken counterclockwise. $C_3$ consists of a counterclockwise integral around a semicircle of radius $R$ in the upper half plane.

(d1). Explain why the integral over contour $C_3$ vanishes in the limit $R \to \infty$.

(d2). Evaluate the integral over $C_2$ in the limit $\delta \to 0$, taking into account that $\chi(z)$ is analytic near $z = \omega$.

(d3). Hence, use Cauchy’s theorem to obtain the following relations between the real and imaginary parts of the function $\chi(\omega)$ for $\omega$ along the real axis:

$$\chi_1(\omega) = P \int_{-\infty}^{\infty} \frac{d\omega'}{\pi} \frac{\chi_2(\omega')}{(\omega' - \omega)};$$

$$\chi_2(\omega) = -P \int_{-\infty}^{\infty} \frac{d\omega'}{\pi} \frac{\chi_1(\omega')}{(\omega' - \omega)}.$$

Here $P$ denotes “principal part of” and means the limit of the integral over the contour $C_1$ when the length $\delta \to 0$.

Note: Problem set is due by 5PM Friday in either the mailbox of the grader, Wissam Al-Saidi (preferred) or my mailbox.