Problem 13: Polarons **(5 points)**

Consider the coupling of a (single) electron with longitudinal optical phonons (one branch only, with frequency ω_{LO}). In addition to the Hamiltonian H_0 of free electrons (with quadratic band dispersion $\epsilon_{\vec{k}}$ with effective mass m) and phonons, the electron-phonon interaction is given by

$$H_1 = \sum_{\vec{k}\vec{q}\sigma} \left[M(\vec{q}) c^\dagger_{\vec{k}+\vec{q},\sigma} c_{\vec{k}\sigma} b_{\vec{q}} + M(-\vec{q}) c^\dagger_{\vec{k}-\vec{q},\sigma} c_{\vec{k}\sigma} b^\dagger_{\vec{q}} \right]$$

(a) As shown in the lecture, such a Hamiltonian can be transformed into an equivalent form by a canonical transformation, i.e. $\tilde{H} = \exp(-iS) H \exp(iS)$ with a Hermitean operator S, leaving all physics unchanged. S can be chosen arbitrarily; if chosen such that $i[H_0, S]_- = -H_1$, $\tilde{H}$ is (up to second order in S) given by $\tilde{H} \approx H_0 + \frac{i}{2}[H_1, S]_-$, i.e. $\tilde{H}_1 \approx \frac{i}{2}[H_1, S]_-$.
Show that this procedure turns the H_1 given above into the form

$$\tilde{H}_1 = \sum_{\vec{k}\vec{q}\sigma} |M(\vec{q})|^2 \frac{1}{\epsilon_{\vec{k}} - \epsilon_{\vec{k}-\vec{q}} - \hbar\omega_{\vec{q}}} c^\dagger_{\vec{k},\sigma} c_{\vec{k}\sigma}$$

In here, inversion symmetry was used: $M(\vec{q}) = M(-\vec{q})$. [Hint: using the notation of the lecture, consider phonon-free states $|n\rangle = |\tilde{n}\rangle$ = electron at $\vec{k}$ with spin σ, i.e. $|n\rangle = |\tilde{n}\rangle = c^\dagger_{\vec{k}\sigma}|0\rangle$ with $|0\rangle$ = vacuum state, consider intermediate states $|m\rangle$ = electron at $\vec{k}'$ combined with a phonon at $\vec{q}$, and argue that $\vec{k}'$ must be equal to $\vec{k} - \vec{q}$.]

(b) While electron-phonon interaction in its original form requires second-order perturbation theory to show an effect, the present technique of a canonical transformation allows to use first-order perturbation theory. Consider a state with an electron at $\vec{k}_0$ and no phonon. Show that for this state, the Hamiltonian $\tilde{H}_1$ of (a) yields an energy correction of

$$\Delta E^{(1)} = \sum_{\vec{q}} \frac{|M(\vec{q})|^2}{\epsilon_{\vec{k}_0} - \epsilon_{\vec{k}_0+\vec{q}} - \hbar\omega_{\vec{q}}}$$

(c) Evaluate the result of (c) further by using the flat phonon dispersion (frequency ω_{LO}) and quadratic dispersion (with effective mass m) for the electron. Assume that $M(\vec{q}) = a/q$, and replace the first-Brillouin-zone sum over $\vec{q}$ by an integration with respect to $\vec{q}$ which covers the entire 3D space. For small k the result can be Taylor-expanded in k, yielding an increase of the effective mass due to coupling to the phonons.

Usefull integral: $$\int_0^\infty \frac{1}{x} \ln\left|\frac{a^2 + 2bx + x^2}{a^2 - 2bx + x^2}\right| dx = 2\pi \arcsin\frac{b}{a} .$$