Strongly Coupled Phonons and Electrons

In this problem, we will use a variational technique to estimate the ground state energy of an electron of mass m and charge $-e$ interacting with phonons in a d dimensional lattice, which turns out to be valid in the limit where the coupling between electrons and phonons is large. For simplicity, we will approximating the noninteracting part of the Hamiltonian to be, if p and x are the momentum/position of the electron, and P_j and Q_j are the momenta and displacements of the ionic lattice vectors at lattice site j:

$$H = \frac{p^2}{2m} + \sum_j \left[\frac{P_j^2}{2M} + \frac{M\omega^2}{2} X_j^2 \right].$$

We will assume that the lattice is a simple cubic lattice with lattice spacing a.

(a) We first need to determine what the proper interaction term in the Hamiltonian is. To do this, use the fact that $H_{\text{int}} = -e\varphi(x)$, with φ the electric potential. Assume that the electric field at each point is given by

$$\mathbf{E}_j = -\lambda \mathbf{X}_j,$$

with λ a positive constant. Fourier transform into a more natural basis for phonons to determine the form of H_{int}. Note that the electron position should enter in the exponentials in the form $\exp[\mathrm{i}\mathbf{k}\cdot\mathbf{x}]$.

(b) To estimate the ground state energy of the electron, we need to determine the effective theory for the electron. To do this, we need to first to estimate what the response of the lattice will be to an electron. The basic idea is that the lattice consists of heavy atoms ($M \gg m$) and therefore, they move in response to how the electron moves. Let's make this more precise. Suppose that the electron wave function is

$$\psi(x) = \frac{1}{(2\pi\sigma^2)^{d/4}} \mathrm{e}^{-x^2/2\sigma^2}.$$

Taking this wave equation as fixed, determine the effective interaction *as seen by the phonons* by computing $\langle\psi|H_{\text{int}}|\psi\rangle$. You should find it is linear in X_j.

(c) Now, since the ions are heavy, let us assume that $X_j \to X_j + \delta_j$, with δ_j chosen to cancel off the linear term in X_j from the previous part. From this, you should see that H decouples into an electron piece and a phonon piece: find the electron piece.

(d) Determine the ground state energy E_0 for the electron by minimizing over the trial ground state energies $E(\sigma)$ in a variational calculation. Feel free to estimate the value of a sum over Fourier modes as an integral. If the integral diverges, think about how you should regulate it.

(e) Comment on how E_0 depends on the value of d. What does it imply about the physical behavior of this system at strong coupling? This has to do with whether or not the phonon-coupling interaction is "irrelevant" or not in higher dimensions.