Homework #1 — Phys625 — Spring 2002 Victor Yakovenko, Associate Professor
Deadline: Tuesday, February 5, 2002. Office: Physics 2314
Turn in homework in the class or put it in the box on the door of Phys 2314 by 10 a.m. Phone: (301)-405-6151
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Do not forget to write your name and the homework number!

Second Quantization

1. *Classical chain of oscillators*

Consider a chain of atoms with masses m_n connected by springs of rigidity γ:

$$\mathcal{H}_{ph} = \sum_{n=-\infty}^{\infty} \frac{p_n^2}{2m_n} + \frac{\gamma}{2}(u_n - u_{n+1})^2, \tag{1}$$

where u_n are the displacements of atoms from their equilibrium positions, and p_n are the corresponding conjugate momenta. Consider the case where

$$m_n = \begin{cases} m, & \text{when } n \text{ is even,} \\ M, & \text{when } n \text{ is odd.} \end{cases} \tag{2}$$

(a) [**4 points**] Determine the frequencies ω of the normal modes of the system. Show that there are two branches: acoustic and optical, and sketch their dispersions $\omega(k)$, where k is the wave vector.

(b) [**2 points**] What is the frequency gap between the optical and acoustic modes? Show that the optical mode almost does not have dispersion in the case $M \gg m$ and explain it qualitatively.

(c) [**4 points**] Determine the sound velocity c. Does it agree with the Laplace formula $c = \sqrt{\partial P/\partial \rho}$, where P is pressure and ρ is density?

2. [**6 points**] *Quantum chain of oscillators*

Consider the same problem in quantum mechanics, i.e. treat $\hat{u}_n$ and $\hat{p}_n$ as operators satisfying the canonical commutation relation $[\hat{p}_n, \hat{u}_{n'}] = -i\hbar\delta_{n,n'}$. For the rest of the homework consider the case $m = M$.

Diagonalize the quantum Hamiltonian (1). In order to do this, first make Fourier transform: $\hat{u}_n \to \hat{u}_k$, $\hat{p}_n \to \hat{p}_k$, and then introduce the creation and destruction operators of phonons $\hat{a}_k^+$ and $\hat{a}_k$ by the following formula:

$$\hat{u}_k = \sqrt{\frac{\hbar}{2m\omega(k)}}(\hat{a}_k + \hat{a}_k^+), \quad \hat{p}_k = -i\sqrt{\frac{\hbar m\omega(k)}{2}}(\hat{a}_k - \hat{a}_k^+). \tag{3}$$

Determine the phonon spectrum $\omega(k)$ and calculate the ground state energy.

3. **[6 points]** *Interaction between phonons*

Suppose the springs have small anharmonicity γ', so the Hamiltonian of the system also has the following term:

$$\mathcal{H}'_{ph} = \sum_{n=-\infty}^{\infty} \gamma'(u_n - u_{n+1})^3. \tag{4}$$

Rewrite Hamiltonian (4) in terms of the phonon operators $\hat{a}_k^+$ and $\hat{a}_k$ introduced in the previous problem. What can you say about momentum conservation for the phonons?

4. *Electron-phonon interaction*

Suppose electrons are also present on the same chain of atoms. Electrons can make transitions between neighboring lattice sites with the amplitude of probability t_n:

$$\mathcal{H}_{el} = \sum_{n=-\infty}^{\infty} t_n \hat{\psi}_{n+1}^+ \hat{\psi}_n + \text{H.c.}, \tag{5}$$

where $\hat{\psi}_n^+$ and $\hat{\psi}_n$ are the fermion operators creating and destroying electrons on the site n.

In the case $t_n = t = \text{const}$, diagonalize Hamiltonian (5) by the Fourier transform: $\hat{\psi}_n \to \hat{\psi}_k$, and determine the spectrum $\varepsilon(k)$ of electronic excitations **[4 points]**.

In general, the amplitude of electron tunneling t_n depends on the relative displacement of the neighboring atoms $u_n - u_{n+1}$. Let us expand $t_n(u_n - u_{n+1})$ to the first order: $t_n = t + (u_n - u_{n+1})t'$. When substituted in Hamiltonian (5), the second term gives the following term in the Hamiltonian:

$$\mathcal{H}_{el-ph} = t' \sum_{n=-\infty}^{\infty} (u_n - u_{n+1}) \hat{\psi}_{n+1}^+ \hat{\psi}_n + \text{H.c.}. \tag{6}$$

Rewrite Hamiltonian (6) in terms of the phonon and electron operators $\hat{a}_k$ and $\hat{\psi}_k$ and their conjugates. Comment on conservation of momentum. Hamiltonian (6) describes electron-phonon interaction **[6 points]**.