Homework #1 — Phys625 — Spring 2002  
Victor Yakovenko, Associate Professor  
Deadline: Tuesday, February 5, 2002.  
Turn in homework in the class or put it in  
the box on the door of Phys 2314 by 10 a.m.  
Web page: http://www2.physics.umd.edu/~yakovenk/teaching/phys625.spring2002  

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 \( \gamma \):

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

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

\[
m_n = \begin{cases} 
m, & \text{when } n \text{ is even,} \\
M, & \text{when } n \text{ is odd.}
\end{cases}
\]

(a) [4 points] Determine the frequencies \( \omega \) 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

\[
c = \sqrt{\frac{\partial P}{\partial \rho}},
\]

where \( P \) is pressure and \( \rho \) 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:

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

Determine the phonon spectrum \( \omega(k) \) and calculate the ground state energy.
3. **[6 points]** Interaction between phonons

Suppose the springs have small anharmonicity \( \gamma' \), 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 \( t_n \):

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

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: \( \hat{\psi}_n \rightarrow \hat{\psi}_k \), 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:

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

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]**.