Homework #1 — Phys625 — Spring 2004
Deadline: Wednesday, March 31, 2004.
Turn in homework in the class or put it in the box on the door of Phys 2314 by 3 p.m.

Victor Yakovenko, Associate Professor
Office: Physics 2314
Phone: (301)-405-6151
E-mail: yakovenk@physics.umd.edu
Web page: http://www2.physics.umd.edu/~yakovenk/teaching/phys625.spring2004

Do not forget to write your name and the homework number!

Second Quantization

1. [6 points] *Quantum chain of oscillators*

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

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

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

Consider the problem in quantum mechanics, i.e. treat $\hat{u}_n$ and $\hat{p}_n$ as operators satisfying the canonical commutation relation $[\hat{p}_n, \hat{u}_{n'}] = -i\hbar\delta_{n,n'}$.

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:

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

Write Hamiltonian (1) in terms of $\hat{a}_k^+$ and $\hat{a}_k$ and determine the phonon spectrum $\omega(k)$. Calculate the ground state energy of the system.

2. [6 points] *Interaction between phonons*

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

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

Rewrite Hamiltonian (3) 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 of the phonons in Hamiltonian (3)?

3. *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:

$$\mathcal{H}_{el} = \sum_{n=-\infty}^{\infty} t_n \hat{\psi}_{n+1}^+ \hat{\psi}_n + \text{H.c.}, \tag{4}$$

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 (4) 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 as a function of $(u_n - u_{n+1})$ to the first order: $t_n = t + (u_n - u_{n+1})t'$. When substituted in Hamiltonian (4), the second term gives the following term in the Hamiltonian:

$$\mathcal{H}_{el-ph} = t' \sum_{n=-\infty}^{\infty} (u_n - u_{n+1}) \hat{\psi}_{n+1}^+ \hat{\psi}_n + \text{H.c.}. \tag{5}$$

Rewrite Hamiltonian (5) in terms of the phonon and electron operators $\hat{a}_k$ and $\hat{\psi}_k$ and their conjugates. Comment on conservation of momentum. Hamiltonian (5) describes electron-phonon interaction [**6 points**].