

Phys 971 Stat Mech: Final

due: 12/20/2013 at 10am

1

(10 points) Consider N identical quantum states (with energy ϵ) in contact with a large reservoir of fermion particles. When the system is at equilibrium, it is observed that $N/4$ of the states are occupied with a single particle. Then a wizard magically transforms the particles into bosons. How many particles occupy the states after equilibrium is restored? Assume that the reservoir is large enough that it is not significantly perturbed by the flux of particles into/out of the states. Also, for this admittedly silly question, assume that both the fermions and bosons are spinless.

2

(20 points) The Peierls theorem showed that one dimensional conductors will spontaneously distort in such a way to open a band gap at the Fermi energy. After this transition, the lack of accessible empty electronic states means that the material becomes a very poor conductor. In this problem we will examine a very simple model of this transition.

The energy of the system is the sum of two terms, the electronic energy and the lattice energy $U = U_{\text{elec}} + U_{\text{lattice}}$. The lattice energy is simply the elastic energy of distorting the atoms away from their equilibrium position

$$U_{\text{lattice}} = \frac{K_s}{2} \sum_{i=1}^N u_i^2 = N \frac{K_s}{2} u_0^2$$

where K_s is the effective spring constant for the bonds, N is the number of atoms in the lattice, and we have assumed that each of the atoms is perturbed from its equilibrium position by an amount $\pm u_0$ (see figure). After the transition the periodicity of the lattice doubles from one atom per unit cell to two atoms. According to band theory, this has the effect of opening a gap in the energy spectrum. We will describe this using the greatly simplified model in the right panel of the figure. In this model the dispersion relation is

$$E(k) = \begin{cases} -\Delta + \frac{E_0 - \Delta}{k_0} k & k < 0 \\ \Delta + \frac{E_0 - \Delta}{k_0} k & k > 0 \end{cases} \quad (1)$$

where k_0 and E_0 are the range of states in k - and E -space that are perturbed by the distortion (for simplicity we will assume these are the only states in the system) and $k = 0$ has been defined to coincide with the Fermi energy $E_F = k_F = 0$ (note that $E(\pm k_0) = \pm E_0$). The density of states in k -space is $\rho(k) = Na/2\pi$, where a is the lattice spacing. The gap parameter is related to the lattice distortion by $\Delta = 4\alpha u_0$, where α is a parameter that relates the electronic coupling (hopping) to the atomic spacing.

a) (15 points) If $k_B T N a k_0 / 2\pi E_0 \ll 1$, minimize U to compute the magnitude of the lattice distortion u_0 .

b) (5 points) Describe qualitatively what happens to the lattice distortion in the opposite limit when $k_B T / \Delta \gg 1$.

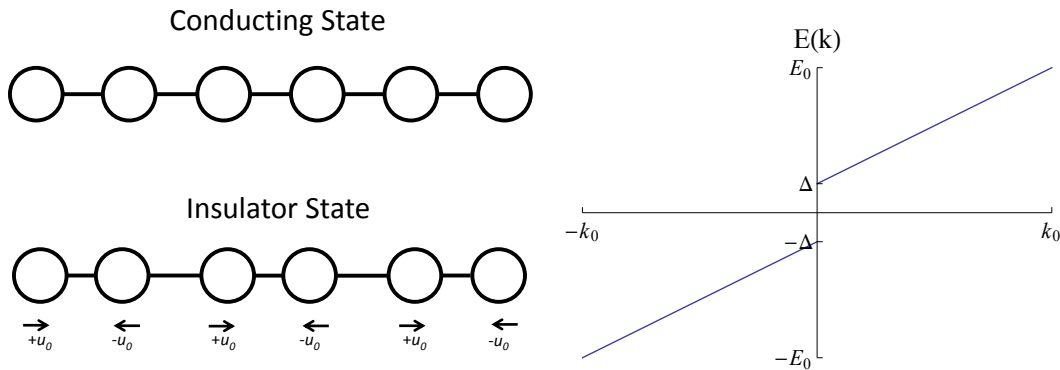


Figure 1: (left) Cartoon of the uniform conducting state and distorted insulator state. (right) Plot of the electronic state energy as a function of the wavenumber k .

3

(25 points) Consider a molecular zipper with N links. Each link has a state in which it is closed with energy $-\epsilon_z$ and a state in which it is open with energy 0. We require that the zipper can unzip only from the right end and that link number s can only open if all links to the right ($s + 1, s + 2, \dots, N$) are already open.

a) Evaluate the partition function of the zipper.

b) Now assume that there are also molecules that can block the zipper. These molecules bind to site M of the zipper with energy $-\epsilon_b$ and prevent sites $s \geq M$ from closing. Treat the blocking molecules as an ideal gas of $N_b \gg 1$ particles in a container of volume V . Compute the probability that the zipper is blocked from closing as a function of the binding site position M and the concentration of blocking molecules $c_b = N_b/V$.

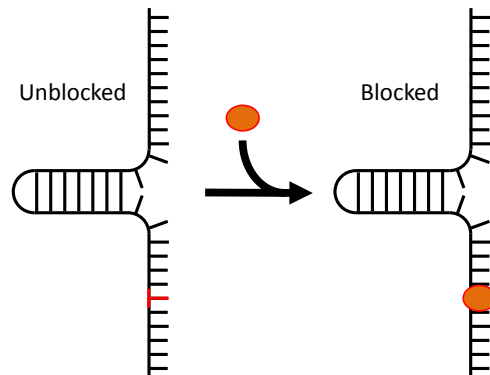


Figure 2: Cartoons of the molecular zipper with (right) and without (left) a blocking molecule bound. The red link indicates the only spot that the blocking molecule can bind to.

4

(25 points) Consider the adsorption of particles to a d -dimensional square lattice from a reservoir of fixed chemical potential μ . Each site on the lattice can accommodate only one particle, but that particle can bind in two different states with energies $-U + \epsilon$ and $-U - \epsilon$, respectively. The Hamiltonian of the system is:

$$H = -U \sum_i n_i - \epsilon \sum_i \sigma_i n_i - \frac{J}{2} \sum_{\{i,j\}} n_i n_j. \quad (2)$$

Here the first term accounts for the average binding energy $-U$ between a particle and the lattice ($n_i = 0, 1$), and the second term describes the energy splitting between the two states ($\sigma_i = \pm 1$). The third term describes an attractive energy between particles on adjacent sites. This energy is $-J$ if both sites are occupied ($n_i = n_j = 1$) and zero if either $n_i = 0$ or $n_j = 0$. The sum on the third term is restricted to nearest neighbor pairs (the coordination number is $q = 2d$ in this case). Develop a mean field theory describing this system. Derive an equation for the density $\theta = \langle n_i \rangle$ order parameter.

5

(20 points) In lecture we analyzed a one-dimensional lattice random walk. Here we will consider the case of a *biased* random walk. At each time step τ the particle has a probability p of hopping to the right and a probability $(1 - p)$ of hopping to the left. Compute the probability $P_N(m)$ that a particle starting at the origin arrives at site m after N steps. Also, compute $\langle m \rangle$ and $\langle m^2 \rangle$.