Solid State Theory
Exercise 7

Exercise 7.1 Bound and Antibound States in One Dimension

We consider a one-dimensional chain of N atoms with nearest neighbor hopping where one hopping element is different from the others. As we will see, this leads to the formation of a bound state and an antibound state in addition to a continuum of states. This should show that modifications of the hopping elements (as e.g. originating from electron-phonon-coupling) lead to a modification of the energy bands of the electrons.
We describe this by the Hamiltonian

$$\mathcal{H} = -t\sum_j(\hat{c}_j^\dagger\hat{c}_{j+1} + \hat{c}_{j+1}^\dagger\hat{c}_j) - \Delta t(\hat{c}_0^\dagger\hat{c}_1 + \hat{c}_1^\dagger\hat{c}_0), \tag{1}$$

where $t > 0$ and $\Delta t > 0$. Show that the spectrum of this Hamiltonian has a bound state below and an antibound state above the energy band with energies

$$E_{b/ab} = \mp 2t \mp \frac{\Delta t^2}{t + \Delta t}. \tag{2}$$

Exercise 7.2 Peierls' Instability in One Dimension

We consider a one-dimensional chain with nearest-neighbor hopping where the position of the electrons is not fixed. The Hamiltonian is thus given by a (renormalized) hopping and an elastic part:

$$\mathcal{H} = \sum_{i,s}(c_{i+1,s}^\dagger c_{i,s} + h.c.)(-t + \alpha\delta u_i) + \lambda\sum_i \frac{\delta u_i^2}{2} \tag{3}$$

where $\delta u_i = u_{i+1} - u_i$ and u_i is the displacement of the atom at site i from its equilibrium position. $\lambda > 0$ is a measure of the stiffness of the system and $\alpha > 0$ is the coupling constant. We set the lattice constant $a = 1$.
In the following, we consider the half filled case (one electron per site) and make for δu_i the ansatz

$$\delta u_i = u_0\cos(qr_i) \tag{4}$$

a) Calculate for $q = \pi$ the eigenenergies and the eigenstates of the system and the density of states.
Hint: Write the electronic part of the Hamiltonian in the Form

$$\mathcal{H} = \sum_{|k|<\pi/2,s} \boldsymbol{c}_{ks}^\dagger \mathcal{H}_k \boldsymbol{c}_{ks} \tag{5}$$

where $\boldsymbol{c}_{ks}^\dagger = (c_{ks}^\dagger, c_{k+\pi s}^\dagger)$ and $\mathcal{H}_k$ is a 2×2 matrix which can be written in terms of Pauli matrices. The diagonalization is then just a rotation in the space of these matrices. Note that the sum now only runs over a reduced Brillouin zone, $k \in [-\frac{\pi}{2}, \frac{\pi}{2}]$.

b) Show that in this one-dimensional system, there is always a finite u_0 that minimizes the total energy.
Hint: Show it for large λ and small u_0 by using the elliptic integral of the second kind,

$$E(\varphi, k) = \int_0^{\varphi} \sqrt{1 - k^2 \sin^2 \alpha} d\alpha \tag{6}$$

and its series expansion

$$E(\frac{\pi}{2}, \sqrt{1 - k'^2}) = 1 + \frac{1}{2}(\log \frac{4}{k'} - \frac{1}{2})k'^2 + O(k'^4). \tag{7}$$

c) Show that the density of electrons per site, $\rho_i = \sum_s \langle c_{is}^\dagger c_{is} \rangle = 1$ for all i but the bond density, $\tilde{\rho}_i = \sum_s \langle c_{is}^\dagger c_{i+1s} + c_{i+1s}^\dagger c_{is} \rangle$ oscillates with position i. Discuss also the limits $\lambda \to 0$ and $\lambda \to \infty$ for $\alpha = t$.

Office hour:
Monday, April 16th, 2012 - 09:00 to 11:00 am
HIT K 23.3
David Oehri