Exercise 8.1 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. The lattice constant is set to unity. 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

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

Hint: Use a Fourier transform of the electron operators to rewrite the Hamiltonian in k-space. Then use a general Ansatz for a single particle wavefunction in k-space and find the condition for this state to be an eigenstate.

Exercise 8.2 Peierls' Instability in One Dimension

We consider a one-dimensional chain with nearest-neighbor hopping where the position of the atoms 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

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

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 $\alpha = t$.

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