Statistical Physics & Condensed Matter Theory I: Exercise

The Peierls instability

Consider a simple one-dimensional model of spinful electrons (we implicitly sum over spin),

$$H_0 = -t \sum_{n=1}^{N} \left[c^\dagger_{n\sigma} c_{n+1\sigma} + c^\dagger_{n+1\sigma} c_{n\sigma} \right].$$

In deriving this effective Hamiltonian, is has been assumed that the underlying crystal lattice is fixed, that is the positions R_n of the atoms (and thus of the electronic orbitals) are regularly spaced, $R_n = n$ (we take the lattice spacing to be one).

We can in fact consider a slightly more realistic theory, where small elastic distortions of the lattice are allowed. This will modify the hopping term, and introduce an additional term giving the elastic energy associated to the distortion. Effectively, one gets (Su-Schrieffer-Heeger)

$$H = -t \sum_{n=1}^{N} (1 + u_n) \left[c^\dagger_{n\sigma} c_{n+1\sigma} + \text{h.c.} \right] + \sum_{n=1}^{N} \frac{k_s}{2} (u_{n+1} - u_n)^2,$$

where u_n parametrizes the lattice distortion at site n.

a) Take a periodic lattice with an *even* number of sites. Consider the effects of a distortion $u_n = (-1)^{n+1}\alpha$, that is a distortion in which every odd (even) site gets slightly displaced to the right (left). This is called a **Peierls distortion**, or **dimerization**. It is then better to distinguish between even and odd sites, and to consider a unit cell made up of two sites, one even and one odd.

Let $m = 1, ..., N/2$ label the new unit cells. Let a_m be the fermionic operators on the left of the mth unit cell, and b_m be those on the right. That is, $c_{2m-1\sigma} = a_{m\sigma}$ and $c_{2m\sigma} = b_{m\sigma}$. Show that the Hamiltonian can be rewritten

$$H = -t \sum_{m=1}^{N/2} \left[(1+\alpha)(a^\dagger_{m\sigma} b_{m\sigma} + \text{h.c.}) + (1-\alpha)(b^\dagger_{m\sigma} a_{m+1\sigma} + \text{h.c.}) \right] + 2N k_s \alpha^2.$$

b) Use the Fourier transformation $a_m = \sqrt{\frac{2}{N}} \sum_k e^{2ikm} a_k$ (similarly for b_m) where the momentum k takes $N/2$ values in the interval $[-\pi/2, \pi/2]$ to show that the Hamiltonian can be written as (there is a typo in this equation in CMFT, problem 2.4.3)

$$H = 2N k_s \alpha^2 - \\ -t \sum_k \begin{pmatrix} a^\dagger_{k\sigma} & b^\dagger_{k\sigma} \end{pmatrix} \begin{pmatrix} 0 & (1+\alpha) + (1-\alpha)e^{-2ik} \\ (1+\alpha) + (1-\alpha)e^{2ik} & 0 \end{pmatrix} \begin{pmatrix} a_{k\sigma} \\ b_{k\sigma} \end{pmatrix}.$$

c) Diagonalize this Hamiltonian and show that the single-particle spectrum is given by

$$\varepsilon(k) = \pm 2t \left[1 - (1 - \alpha^2) \sin^2 k \right]^{1/2}.$$

What is the spectrum for $\alpha \to 0$? What happens when $\alpha \to 1$?

d) Specialize now to the half-filled case, that is put one electron per lattice site on average. Write the ground state energy for a finite system as a sum over momentum of single-particle terms. Show that the energy density per site becomes for $N \to \infty$

$$\frac{E_0}{N} = -4t \int_{-\pi/2}^{\pi/2} \frac{dk}{2\pi} (1 - (1-\alpha^2)\sin^2 k)^{1/2} + 2k_s\alpha^2.$$

e) Using the result $\int_{-\pi/2}^{\pi/2} dk (1 - (1-\alpha^2)\sin^2 k)^{1/2} \simeq 2 + (a_1 - b_1 \ln \alpha^2)\alpha^2 + O(\alpha^4 \ln \alpha^2)$ with a_1, b_1 some positive constants, what is the equation giving the value α for which the ground state energy is minimal (don't worry if you get something different from the book...) ? Give your interpretation of this result: is the system unstable to the Peierls distortion ?