Statistical Physics & Condensed Matter Theory I: Exercise

The Peierls instability: Solution

a) Writing directly using the index m, and using the mapping $c \to a, b$ gives

$$H = -t \sum_{m=1}^{N/2} \Big[(1+u_{2m-1})(c^\dagger_{2m-1\sigma}c_{2m\sigma} + c^\dagger_{2m\sigma}c_{2m-1\sigma}) + (1+u_{2m})(c^\dagger_{2m\sigma}c_{2m+1\sigma} + c^\dagger_{2m+1\sigma}c_{2m\sigma})\Big] + \frac{k_s}{2}\sum_{n=1}^{N}(u_{n+1}-u_n)^2$$

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

b) Use Fourier $a_m = \sqrt{\frac{2}{N}}\sum_k e^{2ikm}a_k$: hopping part of Hamiltonian

$$H_{hop} = -\frac{2t}{N}\sum_{k,k'}\left[(1+\alpha)(\sum_m e^{-2ikm+2ik'm}a^\dagger_k b_{k'} + \text{h.c.}) + (1-\alpha)(\sum_m e^{-2ikm+2ik'(m+1)}b^\dagger_k a_{k'} + \text{h.c.})\right]$$

$$= -\frac{2t}{N}\sum_{k,k'}\frac{N}{2}\delta_{k,k'}\left[(1+\alpha)(a^\dagger_k b_k + b^\dagger_k a_k) + (1-\alpha)(e^{2ik}b^\dagger_k a_k + e^{-2ik}a^\dagger_k b_k)\right]$$

which gives the equation in the question when written in matrix form. The constant term of course stays the same.

c) Eigenvalues:

$$\begin{vmatrix} -\lambda & -t((1+\alpha)+(1-\alpha)e^{-2ik}) \\ -t((1+\alpha)+(1-\alpha)e^{2ik}) & -\lambda \end{vmatrix} = 0$$

$$\to (\lambda/t)^2 = |(1+\alpha)+(1-\alpha)e^{2ik}|^2 = (1+\alpha)^2 + (1-\alpha)^2 + 2(1-\alpha^2)\cos 2k$$
$$= 2(1+\alpha^2+(1-\alpha^2)(1-2\sin^2 k)) = 4(1-(1-\alpha^2)\sin^2 k)$$

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

For $\alpha \to 0$, the spectrum just becomes the free case $\varepsilon(k) = \pm 2t\cos k$. For $\alpha \to 1$, the system decouples into independent dimers.

d) For the half-filled case, the ground state energy will be obtained by filling in all the negative single particle energy levels, taking into account that we can put both spin up and spin down in each level:

$$E_0 = -2*2t\sum_k\left[1-(1-\alpha^2)\sin^2 k\right]^{1/2} + 2Nk_s\alpha^2 = -4t\sum_{n=1}^{N/2}\left[1-(1-\alpha^2)\sin^2 k_n\right]^{1/2} + 2Nk_s\alpha^2$$

where $k_n = \frac{2\pi}{N}(n - N/4)$, $n = 1, ..., N/2$ so that $k \in]-\pi/2, \pi/2]$. Transforming the sum into an integral using $\sum_n \to \frac{N}{2\pi}\int_{-\pi/2}^{\pi/2} dk$, we get the formula in the question.

e) Using the formula given, we get

$$\frac{E_o}{N} = -\frac{2t}{\pi}(2 + (a_1 - b_1 \ln \alpha^2)\alpha^2 + ...) + 2k_s\alpha^2$$

Varying with respect to α^2 gives the extremum condition

$$0 = \frac{\partial(E_0/N)}{\partial\alpha^2} = -\frac{2t}{\pi}(-b_1 + a_1 - b_1 \ln \alpha^2) + 2k_s \to \alpha^2 = \exp\left(\frac{a_1}{b_1} - 1 - \frac{\pi k_s}{tb_1}\right)$$

The second derivative gives:

$$\frac{\partial^2(E_0/N)}{\partial\alpha^4} = \frac{2tb_1}{\pi\alpha^2} > 0.$$

Therefore, there is always a stable minimal energy point for $\alpha > 0$, so the one-dimensional crystal is *unstable* towards dimerization.