Due Monday November 12  Peierls transition, half-filled case

1. Consider a 1-d chain of atoms, with one s-orbital \( \psi(x-na)=|n> \) per atom, and one electron per atom (half-filled band). Consider the nearest-neighbor orthogonal tight-binding model \( \langle n|m\rangle=\delta_{mn}, \langle n|H|m|>\approx-t \) for nearest neighbors, 0 otherwise. Find \( \epsilon_n(k) \), plot, and show where is the Fermi wavevector, the Fermi energy, and the Brillouin zone boundary.

\[ F(k) = 10^2 \text{ is the only degree of freedom per unit cell.} \]

\[ |k> = \sqrt{\frac{1}{N}} \sum_n e^{i kna} |n> \]

is a linear combination of Bloch-type with translational symmetry \( \hat{T}(a)|k> = \sqrt{\frac{1}{N}} \sum_n e^{i kna} |n+1> \)

\[ = e^{ika} |k> \text{ is also an eigenstate of } \hat{H} \]

because \( \hat{H} = -t \left( \hat{T}(a) + \hat{T}(-a) \right) \).
The eigenvalue is \( \epsilon(k) = -t (e^{ika} + e^{ika}) = -2t \cos ka \)

The Brillouin zone boundary is at \( k = \pi/a \). The Fermi wavevector is \( \pi/2a \) and Fermi energy \( = 0 \).

2. Now suppose there is a "dimerization." That is, half the atoms (at \( x=2na \)) move to the right a small amount \( \delta u/2 \), and half the atoms \( (x=(2n+1)a) \) move to the left the same amount. This causes the "hopping matrix element" \( t \) to change to \( t(l+\delta) \) for hopping the short bond, and \( t(l-\delta) \) for hopping the long bond, where \( t \) is proportional to \( \delta u \).

Find \( \epsilon_n(k) \), plot, and show where is the Fermi wavevector, the Fermi energy, and the Brillouin zone boundary.
The new unit cell is twice as large. We can now make two Bloch functions

\[ |kL\rangle = \sqrt{\frac{1}{2N}} \sum_{l} e^{-i k (2l+1) a} |2l+1\rangle \]

\[ |kR\rangle = \sqrt{\frac{1}{2N}} \sum_{l} e^{-i k (2l) a} |2l\rangle \]

Both are Bloch states with eigenvalue \( e^{i k (2a)} \) for translations \( \hat{T}(2a) \). They are not eigenfunctions of \( \hat{H} = -(t+\delta) \hat{T}(2n \leftrightarrow 2n+1) \)

\[ -(t-\delta) \hat{T}(2n+1 \leftrightarrow 2n+2) \]

But

\[ \hat{H} |kL\rangle = \left[ -(t+\delta) e^{-i k a} - (t-\delta) e^{i k a} \right] |kR\rangle \]

\[ \hat{H} |kR\rangle = \left[ -(t+\delta) e^{i k a} - (t-\delta) e^{-i k a} \right] |kL\rangle \]

Thus these two states are closed under \( \hat{H} \), so the \( \hat{H} \)-matrix is \( 2 \times 2 \)

\[ \hat{H}(k) = \begin{pmatrix} 0 & -2t \cos k a + 2i \delta \sin k a \\ -2t \cos k a - 2i \delta \sin k a & 0 \end{pmatrix} \]

The eigenvalues are

\[ \pm 2t \sqrt{\cos^2 k a + \delta^2 \sin^2 k a} \]

\[ \text{Gap} = 4|\delta| \]
3. It is not at all rigorous to say that the total energy is just the sum of the one-electron energies \( \epsilon_k(k) \) of the occupied states, but qualitatively it should give the right type of answer. The dimerization costs energy \( K \delta^2/2 \), for some sensible value of \( K \), but there is a greater energy lowering in the occupied state energy sum \( \sum (\epsilon_0(k) - \epsilon_0^0(k)) \). This sum is proportional, for small \( \delta \), to \( \delta^2 \ln \delta \), which is negative because \( \delta \) is small. Verify this, and find the coefficient.

\[
\epsilon_1(k) - \epsilon_0(k) = -2t \left[ \sqrt{\cos^2 ka + 8^2 \sin^2 ka} - \left| \cos ka \right| \right]
\]

for \( |k| < \pi/2a \). \( |k| > \pi/2a \) is unoccupied in the undistorted structure.

\[
\Delta E = \sum_k \epsilon_1(k) - \epsilon_0(k)
\]

\[
= -\frac{2tL}{2\pi} \int_{-\pi/2a}^{\pi/2a} dk \left[ \sqrt{\cos^2 ka + 8^2 \sin^2 ka} - \left| \cos ka \right| \right]
\]

When \( \cos^2 ka > 8^2 \sin^2 ka \), we can Taylor expand the square root. The answer will be a series in powers of \( \delta^2 \), starting with the \( \delta^2 \)-term. These are negligible compared with \( \delta^2 \ln \delta \).

When \( \cos^2 ka < 8^2 \sin^2 ka \), we know \( |k| \) is near \( \pi/2a \) and can expand in \( ka - \pi/2a \).

\[
\sin \left( \frac{\pi}{2a} + (k - \frac{\pi}{2a})a \right) = 1 + (k - \frac{\pi}{2a})a \cos \frac{\pi}{2} - \frac{1}{2}(k - \frac{\pi}{2a})^2 \sin \frac{\pi}{2} \\
\approx 1 - \frac{1}{2}(ka - \frac{\pi}{2})^2 + \ldots
\]

\[
\cos \left( \frac{\pi}{2a} + (k - \frac{\pi}{2a})a \right) \approx 0 - (k - \frac{\pi}{2a})a \sin \frac{\pi}{2} + \ldots
\]

\[
\approx -(ka - \frac{\pi}{2}) + \ldots
\]

\[
\left[ \right] = \sqrt{(ka - \frac{\pi}{2})^2 + \delta^2 \left( 1 - \frac{1}{2}(ka - \frac{\pi}{2})^2 \right)^2} - \left| ka - \frac{\pi}{2} \right|
\]
Let \( x = 2a - \frac{\pi}{2} \).

\[
\Delta E \approx -\frac{tL}{\pi a} \int dx \sqrt{x^2 + s^2 (1 - \frac{1}{2}x^2)^2} - 1x
\]

Actually we have to cut this off at some cutoff \( |x_c| \ll |x| \) because the series is invalid. But if \( s \ll |x_c| \) this will be an accurate answer.

Also we need to expand at the other end,

\[
k \approx -\frac{\pi}{2a} + \left(k + \frac{\pi}{2a}\right)
\]

for small \( k + \frac{\pi}{2a} \).

This will give the same integral, i.e., a factor of 2.

Let \( x' = -x \)

\[
\Delta E = \frac{tL}{\pi a} \int_0^{x_c} dx' \left\{ x' - \sqrt{x'^2 + s^2 (1 + x'^2 + x'^4/4)} \right\}
\]

\[
= (1-s^2) \int_0^{\frac{x_c}{\sqrt{a^2 + x^2}}} dx' \sqrt{a^2 + x'^2}
\]

\[
= (1-s^2) \left[ \frac{x_c}{2} \sqrt{x_c^2 + a^2} + \frac{a^2}{2} \log \frac{x_c + \sqrt{x_c^2 + a^2}}{\sqrt{a^2 + x_c^2}} \right]
\]

Now use \( \alpha \ll x_c \)

\[
= (1-s^2) \left[ \frac{x_c}{2} \left(1 + \frac{a^2}{2x_c^2} + \cdots\right) + \frac{a^2}{2} \log \frac{2x_c}{a} \right]
\]

\[
= \frac{x_c^2}{2} \left[ (1-s^2) + \frac{1}{4} s^2 \right] + \frac{s^2}{2} \log \left(\frac{2x_c}{s} \sqrt{1-s^2} \right)
\]

\[
= \frac{x_c^2}{2} + \frac{s^2}{2} \log \left(\frac{2x_c}{s} \right) + O(s^2)
\]

\[
\Delta E = -\frac{2tL}{\pi a} \frac{s^2}{2} \log \left(\frac{2x_c}{s} \right) + O(s^2)
\]
\[
\Delta E = -\frac{N}{\pi} S^2 \log S + \mathcal{O}(S^2) + \ldots 
\]

where \(N = L/a\).

4. The figure is from B. Renker, H. Rietschel, L. Pintschovius, and W. Gläser, P. Brüesch, D. Kuse, and M. J. Rice, "Observation of Giant Kohn Anomaly in the One-Dimensional Conductor K$_2$Pt(CN)$_6$Br$_{1.7}$·3H$_2$O," Phys. Rev. Lett. 30, 1144 (1973). The wavevector \(\approx 0.6(\pi/2c)\) is "incommensurate" with the underlying lattice spacing \(c\), presumably because the number of acceptor Br$^-$ ions is non-integer. The rapid \(q\)-dependence can be related to the dielectric screening function \(\varepsilon(q,\omega)\) in one-dimension, at \(\omega=0\). Evaluate \(\varepsilon(q,0)\), and give a brief argument why that might cause the observed behavior.