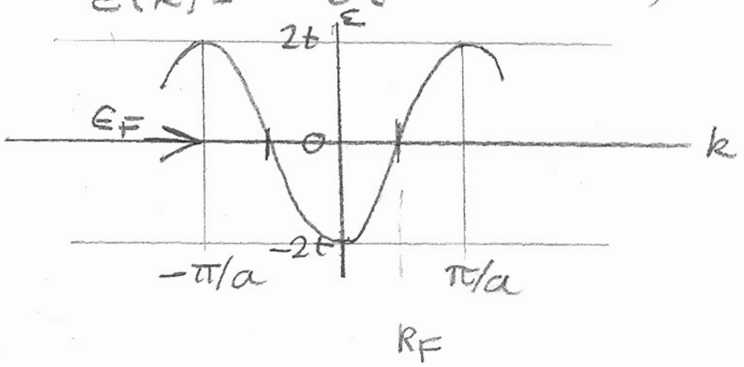
Answers

Physics 555	Fall 2007	HW 6

Due Monday November 12 **Peierls transition, half-filled case**

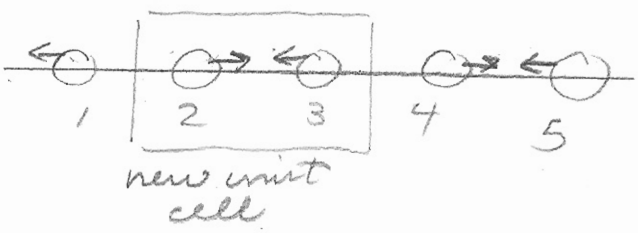
1. Consider a 1-d chain of atoms, with one s-orbital $\psi(x-na)=|n\rangle$ per atom, and one electron per atom (half-filled band). Consider the nearest-neighbor orthogonal tight-binding model ($\langle n|m\rangle=\delta_{mn}$, $\langle n|H|m\rangle=-t$ for nearest neighbors, 0 otherwise. Find $\varepsilon_n(k)$,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

$\psi(x) = |0\rangle$ is the only degree of freedom per unit cell. $|k\rangle = \sqrt{\frac{1}{N}}\sum_n e^{-ikna}|n\rangle$ is a linear combination of Bloch-type with translational symmetry $\hat{T}(a)|k\rangle = \sqrt{\frac{1}{N}}\sum_n e^{-ikna}|n+1\rangle = e^{ika}|k\rangle$. It is also an eigenstate of $\mathcal{H}$, because $\mathcal{H} = -t\left(\hat{T}(a)+\hat{T}(-a)\right)$. 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 $t(1+\delta)$ for hopping the short bond, and $t(1-\delta)$ for hopping the long bond, where t is proportional to δu. Find $\varepsilon_n(k)$, 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

$$|kL\rangle = \sqrt{\tfrac{1}{2N}} \sum_{\ell} e^{-ik(2\ell+1)a} \, |2\ell+1\rangle$$

$$|kR\rangle = \sqrt{\tfrac{1}{2N}} \sum_{\ell} e^{-ik(2\ell)a} \, |2\ell\rangle$$

Both are Bloch states with eigenvalue $e^{ik(2a)}$ for translations $\hat{T}(2a)$. They are not eigenfunctions of

$$\mathcal{H} = -(t+\delta t)\,\hat{T}(2n \leftrightarrow 2n+1) - (t-\delta t)\,\hat{T}(2n+1 \leftrightarrow 2n+2)$$

But

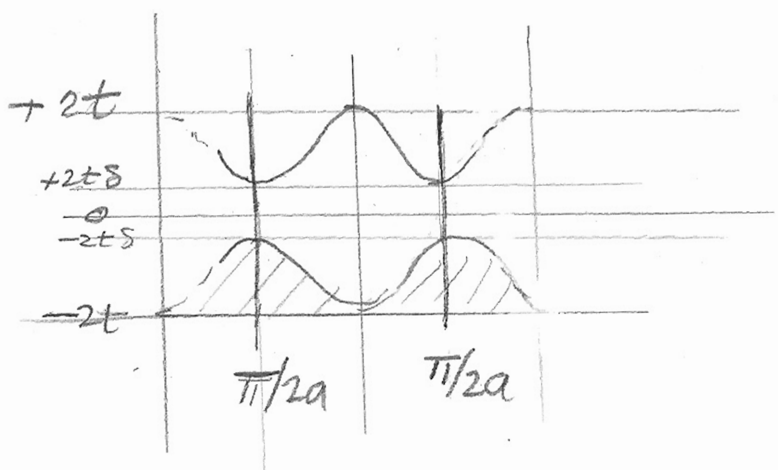
$$\mathcal{H}|kL\rangle = \left[-(t+\delta t)e^{-ika} - (t-\delta)e^{ika}\right]|kR\rangle$$

$$\mathcal{H}|kR\rangle = \left[-(t+\delta t)e^{ika} - (t-\delta)e^{-ika}\right]|kL\rangle$$

Thus these two states are closed under $\hat{\mathcal{H}}$, so the $\mathcal{H}$-matrix is 2×2

$$\hat{\mathcal{H}}(k) = \begin{pmatrix} 0 & -2t\cos ka + 2i\delta t \sin ka \\ -2t\cos ka - 2i\delta t \sin ka & 0 \end{pmatrix}$$

The eigenvalues are $\pm\, 2t\sqrt{\cos^2 ka + \delta^2 \sin^2 ka}$



Gap = $4|t\delta|$

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

$$\epsilon_1(k) - \epsilon_1^0(k) = -2t\left[\sqrt{\cos^2 ka + \delta^2 \sin^2 ka} - |\cos ka|\right]$$

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

$$\Delta E = \sum_k \epsilon_1(k) - \epsilon_1^0(k)$$

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

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

When $\cos^2 ka < \delta^2 \sin^2 ka$, we know $|k|$ is near $\pi/2a$ and can expand in $ka - \pi/2a$

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

$$\approx 1 - \frac{1}{2}\left(ka - \frac{\pi}{2}\right)^2 + \cdots$$

$$\cos\left(\frac{\pi}{2a}a + \left(k - \frac{\pi}{2a}\right)a\right) \approx 0 - \left(k - \frac{\pi}{2a}\right)a \sin\frac{\pi}{2} + \cdots$$

$$\approx -\left(ka - \frac{\pi}{2}\right) + \cdots$$

$$[\,] = \sqrt{\left(ka - \frac{\pi}{2}\right)^2 + \delta^2\left(1 - \frac{1}{2}\left(ka - \frac{\pi}{2}\right)^2\right)^2} - |ka - \pi/2|$$

Let $x = ka - \pi/2$

$$\Delta E \cong -\frac{tL}{\pi a}\int_{-\pi}^{0} dx \left[\sqrt{x^2+\delta^2\left(1-\tfrac{1}{2}x^2\right)^2} - |x|\right]$$

actually we have to cut this off at some cutoff $|x_c| \ll 1$, because the series is invalid. But if $\delta \ll |x_c|$ this will be an accurate answer.

Also we need to expand at the other end, $k \sim -\frac{\pi}{2a} + \left(k+\frac{\pi}{2a}\right)$ for small $k+\frac{\pi}{2a}$.

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

Let $x' = -x$

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

neglect

$$\int_0^{x_c} dx \sqrt{\delta^2+(1-\delta^2)x^2}$$

$$= (1-\delta^2)\int_0^{x_c} dx \sqrt{a^2+x^2} \qquad \text{where } a^2 = \frac{\delta^2}{1-\delta^2}$$

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

Now use $a \ll x_c$

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

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

$$= \frac{x_c^2}{2} + \frac{\delta^2}{2}\log\left(\frac{2x_c}{\delta}\right) + \mathcal{O}(\delta^2)$$

$$\Delta E = -\frac{2tL}{\pi a}\,\frac{\delta^2}{2}\log\left(\frac{2x_c}{\delta}\right) + \mathcal{O}(\delta^2)$$

$$\therefore \boxed{\Delta E = -\frac{Nt}{\pi}\,\delta^2 \log \delta} + \Theta(\delta^2) + \cdots$$

where $N = L/a$.

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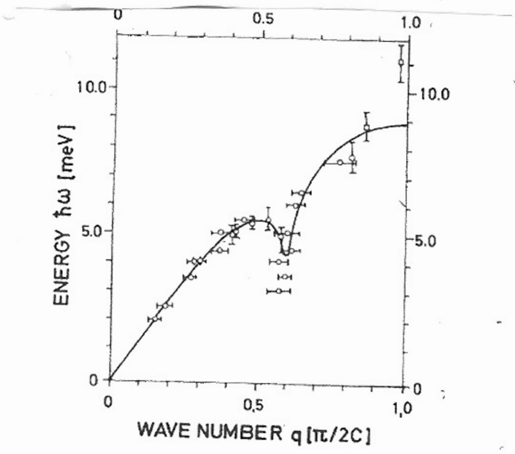
4. The figure is from B. Renker, H. Rietschel, L. Pintschovius, and W. Gläser, P. Brüesch, D. Kuse, and M. J. Rice, "Observation of Giant Kohn Anomaly in the One-Dimensional Conductor $K_2Pt(CN)_4Br_{0.3}\cdot 3H_2O$," Phys. Rev. Lett. 30, 1144 (1973). The wavevector $\sim 0.6(\pi/2c)$ is "incommensurate" 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.

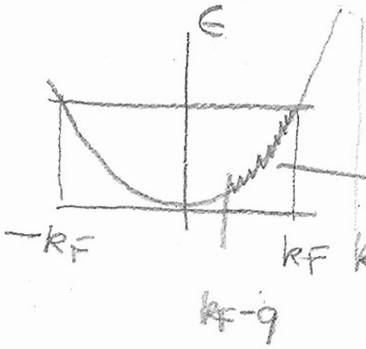


2. LA phonon branch of $K_2Pt(CN)_4Br_{0.3}\cdot 3H_2O$

Sorry if this was obscure! It is sufficient to do free electrons in $d=1$.
use Ziman, eq 5.16 p149

$$\epsilon(q,0) = 1 + \frac{4\pi e^2}{q^2}\sum_k \frac{f(k)-f(k+q)}{\epsilon(k+q)-\epsilon(k)}$$

where $f(k) = \theta(k_F - |k|)$
$\epsilon(k) = \hbar^2 k^2/2m$



states with $k \in (k_F - q, k_F)$ are occupied (assuming $q < 2k_F$) and can make virtual transitions to $k+q$ empty.

$$\epsilon(q,0) = 1 + \frac{4\pi e^2}{q^2}\frac{L}{2\pi}\int_{k_F-q}^{k_F} dk\,\frac{1}{\frac{\hbar^2}{2m}(2kq+q^2)}$$

$$= 1 + \frac{4\pi e^2}{q^2}\frac{L}{2\pi}\frac{m}{\hbar^2 q}\int_{k_F-q}^{k_F}\frac{dk}{k+q/2}$$

$$= 1 + \frac{4\pi e^2}{q^2}\frac{L}{2\pi}\frac{m}{\hbar^2 q}\log\left|\frac{k_F+q/2}{k_F-q/2}\right|$$

This result is also valid for $q > 2k_F$ (check it separately)

The point is, ϵ diverges at $q = 2k_F \Rightarrow$ phonons with $q = 2k_F$ may have weak restoring forces.