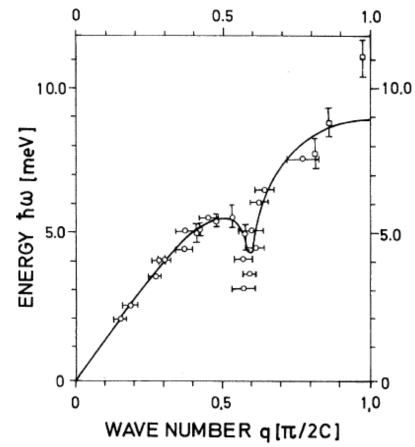
Physics 555	**Fall 2007**		**HW 6**

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.

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.



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

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.

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.