8.512 Theory of Solids II
Spring 2009

8.512 Theory of Solids II **Problem Set 3** **Due** March 2, 2009

1. (a) Consider a one-dimensional chain of hydrogen atoms with lattice spacing a. Using a single $1s$ orbital per atom, construct the tight binding band. You may keep only the nearest-neighbor matrix element $V(a) = \langle \phi(r)|H|\phi(r+a)\rangle$, and ignore the overlap $\langle \phi(r)|\phi(r+a)\rangle$. Assume $V < 0$. Where is the Fermi energy?

   (b) Now assume that the nth atom is displaced by a small amount $(-1)^n\delta$ along the chain direction. For small displacement show that the matrix elements are alternating $V + \Delta$ and $V - \Delta$, where $\Delta = 2\delta\left(\frac{dV}{da}\right)$. What is the new band structure? Is the system a metal or an insulator?

   (c) Calculate the change in the electronic energy upon distortion. Show that it is of the form $\Delta^2 \ln|\Delta/V|$ in the limit $|\Delta| \ll |V|$. Compute the coefficient of this term.

   Hint: Make use of the fact that $|\Delta| \ll |V|$. Then the contributions to the energy change come mainly from momentum states near $k = \pm\pi/2a$, where $\cos ka$ and $\sin ka$ can be expanded to leading order.

   (d) The displacement costs lattice energy which is of the form $b\delta^2$ in the harmonic approximation. Show that the uniform chain is unstable to the distortion assumed in part (b). Similar arguments were put forward by Peierls in 1950 to show that a one-dimensional metal is unstable to distortions which turn it into an insulator.

   (e) Evaluate the polarization function $\Pi_0(q, \omega = 0)$ for a one-dimensional free Fermion gas. Show that a logarithmic singularity appears at $q = 2k_F$.

2. Consider a two-dimensional electron gas (electron motion is confined to the x-y plane). What is the plasmon dispersion $\omega_{pl}(q)$ for small $\mathbf{q}$ in the plane? Show that ω_{pl} is proportional to $|q|^{1/2}$.

   Hint: Note that while the electrons are confined to the plane, the electromagnetic field is not.