P6.1 Peierls instability

The weak interactions between electrons and ions can make a spontaneous symmetry breaking in otherwise simple lattice of identical atoms such as the one in the top figure above. If the atoms interact via a smooth potential, the distortion shown in the bottom picture (like any other lattice distortion) costs an energy $E_L$ proportional to $\delta x^2$. Such a distortion also affects the electrons. Rudolf Peierls (http://en.wikipedia.org/wiki/Rudolf_Peierls) noticed that if there is a single nearly-free electron per atom, the distortion above decreases the electron energy by an amount proportional to $\delta x^p$, where the exponent $p \leq 2$. This means that the total energy can be lowered by increasing the distortion from zero, so that the distortion can happen spontaneously. This “Peierls distortion” is seen in certain real three-dimensional solids.

a) When $\delta x$ is nonzero, what is the smallest $K$ that has a nonzero $U_K$, i.e., what is the smallest reciprocal lattice vector in the distorted lattice?

b) If each atom interacts with electrons via a short-range potential $V(x)$ how does this $U_K$ vary in magnitude with $\delta x$ when $\delta x$ is small?

c) What is the Fermi wavevector in this system?

d) How does the energy of an electron at the Fermi surface vary with $U_K$? with $\delta x$?

e) What is the change in the total electron energy $E_e$ per atom as a function of $U_K$ for small $U_K$?

f) How does $E_e$ vary with $\delta x$? What is the exponent $p$?

g) Is Peierls distortion a necessary feature of this lattice?

P6.2 Wannier functions

Wannier functions are an alternative way to specify the electronic states in a band. They are most useful when the electrons are bound tightly to the atoms. The Wannier state $\phi_n(r)$ for a band $n$ is simply the sum over the Bloch states of that band evaluated at $r$: $\phi_n(r) \equiv \int_{BZ} d^3k \psi_{nk}(r)$. Unlike the Bloch states, Wannier states are concentrated near $r = 0$.

a) Find $\phi_0(x)$ for the lowest band in an empty one dimensional lattice of spacing $a$ i.e., where the Bloch wavefunctions are just plane waves.

b) For a general band of Bloch states $\psi_{nk}$ find the inner product of its Wannier wavefunction $\phi_n(r)$ and a lattice-shifted Wannier wavefunction $\phi_n(r + R)$, i.e., $\int d^3r \phi_n^*(r + R)\phi_n(r)$ with $R \neq 0$. This has a simple, general form for arbitrary Bloch functions.