Solid State Physics 240A: Homework #8. Pseudopotentials; Wannier functions.

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Due Monday Nov. 9, 2015

1. Refer to the "handout" on Pseudopotentials by R. M. Martin, posted on the web site under Supplemental Information, for background.

The pseudopotential concept can be illustrated by a 1D square well potential of width s and depth $-V_\circ$. A plane wave (a particle) with energy $\varepsilon > 0$ traveling to the right has a reflection coefficient r and transmission coefficient t. The transmission coefficient is conventionally written as

$$t = |t|e^{i\delta}, \tag{1}$$

where δ is the phase shift.

(a) By matching at the boundaries, derive t and r as a function of $V_\circ$, s, and ε. Demonstrate that δ indeed has the interpretation of a shift of the phase of the wave.

(b) Show that the same transmission coefficient can be found with a different $V_\circ$, or also with a different s, at a chosen energy ε.

2. Again referring to the same handout, derive the transformation from the OPW equation (11.11) to the pseudopotential equation (11.12) for the smooth part of the wavefunction.

3. Suppose the wavefunction for a 1D crystal of lattice constant a is given across the band by

$$\psi_k(x) = \alpha\ cos(kx) + \beta\ sin(2kx), \tag{2}$$

where α, β are constants.

(a) Calculate the Wannier function

$$W(x - X) = \frac{a}{2\pi} \int dk\ e^{ikX}\ \psi_k(x), \tag{3}$$

where X is the reference position of the WF, and the integral runs over the BZ $(-\pi/a, \pi/a)$. Does it have any symmetry?

(b) Plot $W(x)$, *i.e.* set X=0, out to a few lattice constants, for $\alpha = \beta = 1$. Also plot $|W(x)|^2$. Describe briefly how the results differ from the two cases $\alpha = 0$ or β=0.