Phys 5870: Modern Computational Methods in Solids
Homework 6

Adrian E. Feiguin

April 3, 2012

Exercise 1:

Consider a potential consisting of a 1D periodic triangular well. The depth of the potential is V_0 and the width $r_0 < a$, where a is the size of the unit cell. The explicit expression is given by:

$$V(x) = \begin{cases} -V_0 - (V_0/r_0)x & \text{if} -r_0 \leq x < 0 \\ -V_0 + (V_0/r_0)x & \text{if } 0 \leq x < r_0 \\ \quad 0 \text{ otherwise} \end{cases} \tag{1}$$

a) Approximate the potential using a Fourier series. For simplicity take $r_0 = a/2$. Plot the series for different numbers of terms kept, 2,4,8,12,24, comparing to the exact potential.

b) Solve numerically the Schrödinger equation using plane waves. Plot the bands in the 1st Brillouin zone, and show the convergence with a number of terms kept in the series.