Homework 6
PHZ 5156
Due Thursday, October 15

1. Consider the time-independent Schrödinger equation,

\[ -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) \phi(x) = E \phi(x) \]

where \( V(x) \) is a periodic potential with periodicity \( L \) such that \( V(x + NL) = V(x) \) where \( N \) is any integer.

Bloch’s theorem shows that the eigenstates of the above equation can be written as,

\[ \phi_{\lambda k}(x) = \frac{1}{\sqrt{L}} \sum_G c_{\lambda k, G} \exp \left[ i (k + G) x \right] \]

where \( G \) are the (one-dimensional in this case) reciprocal lattice vectors given by \( G_n = \frac{2\pi n}{L} \), where \( n \) is an integer.

a) Show that the eigenvalue problem can then be written as,

\[ \sum_{G'} H_{G, G'} c_{\lambda k, G'} = E_{\lambda k} c_{\lambda k, G} \]

and determined an expression for the elements of the matrix \( H_{G, G'} \). Convince yourself that this suggests the need to compute the Fourier transform of \( V(x) \) as,

\[ V_{G, G'} = \frac{1}{L} \int_0^L V(x) \exp \left[ i (G' - G) x \right] dx \]

Also, you should find that the diagonal elements of the matrix depend on \( k \), whereas the off-diagonal elements do not.

b) Write a code to compute \( E_{\lambda k} \) as a function of \( k \), using the potential \( V(x) \) defined on \( 0 < x < L \) as

Use the subroutines four1.f90 and ch.f to compute the Fourier transform and diagonalize the complex Hermitian matrix \( H \) with elements \( H_{G, G'} \). For the potential \( V(x) \), use the Gaussian

\[ V(x) = V_0 \exp \left[ \frac{(x - L/2)^2}{2\sigma^2} \right] \]
Plot a figure which includes only the four lowest eigenvalues for each \( k \) plotted as a function of \( k \). Convince yourself that your figure need only include \(-\pi/\ell < k < \pi/\ell\). Plot data for about 40 uniformly-spaced \( k \) values along this interval. As usual, take \( h = m = 1 \). Also, take \( L = 4 \), \( \sigma = 4 \), and \( V_0 = -10 \). Decide on a suitable discretization \( \Delta x \) for the Fourier transform. Note that as \( \Delta x \) becomes smaller, the computational load goes up very fast. You should choose \( \Delta x < \sigma \), but not dramatically smaller. But remember, for the FFT, the number of discrete points must be an integer power of 2! I chose \( N=64 \), which gives \( \Delta x = 4/64 = 1/16 \). You might get additional insight from an analytical calculation of \( V_{G,G'} \) by taking the integration limits to infinity. In practice, it would be important to test the sensitivity of the results to the chosen value of \( \Delta x \).

For extra credit, plot the probability density for the lowest 5 states at \( k = 0 \).