PH-3205 (Computational Physics), QM Work-Sheet 1 (due: 4 Apr. 2021)

(1) Write a computer program to solve the boundary value problem:

$$\frac{d^2}{dx^2}\left[y(x)\right] = -\frac{\pi^2}{4}\left[y(x)+1\right]$$

with boundaries: $y(x = 0) = 0$ and $y(x = 1) = 1$. Remember, we discussed in the class to turn it into a initial-value problem, and then use root-finding scheme. Use bisection for root-finding, and use Numerov scheme to solve the initial value ODE problem. This, boundary value problem can be solved exactly, so find $y(x)$ numerically in the range between $x = 0$ and $x = 1$ and check your result against the exact one.

(2) Writing a computer program solve the Schrodinger equation to calculate the lowest two eigenvalues and corresponding eigenfunctions for an infinite well, defined as: $V(x) = 0$ for $-2 \leq x \leq 2$, and $V(x) = \infty$ otherwise. Also consider a bump in the potential around $x = 0$ of the form of a Gaussian function $\exp(-x^2/2\sigma^2)$, consider $\sigma^2 = 0.2$ and assume, $m = \hbar = 1$.

(3) Writing a computer program solve the Schrodinger equation to calculate the lowest two eigenvalues and corresponding eigenfunctions for a 1D simple harmonic oscillator: $V(x) = \frac{1}{2}x^2$. Please implement shooting method and Numerov integration for your program. Your program should read in Δ_x, the size of discrete steps for integration along the spatial direction, and then integrate accordingly.

(4) Writing a computer program solve the eigenvalues and eigenvectors of a single free particle on a discrete 2D square lattice of size 20×20 with unit lattice spacing, after turning the problem of solving Schrodinger equation ODE to a matrix diagonalization problem. Please use periodic boundary condition along both spatial directions. Use your favorite diagonalizer to diagonalize the matrix you have constructed. This problem can be solved exactly (analytically). Please carry out the analytical solution and compare your numerical eigenenergies with the exact solution.