One-dimensional Schrödinger equation

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total points: 20

1. Suppose there is a single particle of mass m confined to $0 < x < L$ with potential $V = 0$ bounded by infinite high potential barriers, *i.e.*

$$\begin{aligned} V(x) &= 0 \quad \text{when } 0 < x < L, \\ V(x) &= \infty \quad \text{when } x \geq L; x \leq 0 \end{aligned}$$

   (a) Program Numerov's method for this type of potential. (hint: start with the 1D harmonic oscillator code and update the potential function.) (**2 points**)

   (b) Determine the first three lowest energies and the corresponding wave functions. (**1 points**)

   (c) Compare your results to the exact solution analytically obtained in quantum mechanics. (**1 points**)

$$E_n = \frac{(n\pi\hbar)^2}{2mL^2} \tag{1}$$

$$\begin{aligned} \Psi_n(x) &= \sqrt{\frac{2}{L}}\sin(n\pi x/L) \qquad 0 < x < L \\ &= 0 \qquad\qquad\qquad\qquad x \leq 0, x \geq L \end{aligned} \tag{2}$$

2. Prove the energy of the matrix Schrödinger equation on non-orthogonal basis states satisfies the variational principle as well. (**3 points**)

3. Complete the skeleton program for the matrix diagonalization of the Schrödinger equation for the following potential function and compare this method to the Numerov's approach in terms of the ground state energy accuracy with same $N = 100$ and $x_{max} = 1.0$, where N is the total number of discretized points in $[0, x_{max}]$. (**5 points**)

$$V(x) = 10.0 \text{ for } |x| < 0.5 \text{ and } V(x) = \infty \text{ for } |x| >= 1.0; \text{ otherwise } V(x) = 0.0 \tag{3}$$

4. Double well, quantum tunneling, instantons.
Consider a double well system with the following Hamiltonian,

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{m\omega_0^2}{2}\left[\frac{(x^2 - x_0^2)^2}{4x_0^2} - x^2\right] . \tag{4}$$

   Try to determine the ground state wave function and energy of this system by using both Numerov and matrix diagonalization approaches. (Hint: for the latter, one can take the eigenstates of the harmonic oscillator as basis fucntion) **(8 points)**