

Numerical Problems on diagonalization

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[1] Consider a quantum pendulum that is described by the Hamiltonian

$$H = \frac{\hbar^2 L^2}{2I} + U(\phi), \quad L = -i \frac{\partial}{\partial \phi}, \quad U(\phi) = Mga(1 - \cos(\phi)),$$

where M is the mass, and a is the distance between the center of mass and the pivot point, I is the moment of inertia, and $\hbar L$ is the quantum-mechanical angular momentum operator for a rotation around a fixed axis by the angle ϕ .

Assume $M = 1$, $a = 1$, $g = 1$ and $I = 300$. Calculate lowest 300 eigenvalues of the Hamiltonian and plot them. Print 1st, 50th and 200th eigenvalues. From which state the eigenvalues are very closed. Give reason whether they will be degenerate (with respect to machine precision).

[2] Assume a potential of the form

$$V(x) = (x^4 - 3)e^{-x^2/2}$$

1. By solving Schroedinger equation numerically calculate the first 5 energy levels within a box of size $L = 10$ in between -5 to 5. (You can solve this potential analytically, and therefore, you can match bound state energy levels to check your program).

2. Assume this potential inside a **periodic** box of size $L = 10$ in between -5 to 5. Plot dispersion relation (energy vs k) and find band gaps near Brillouin zones. Next change the box size from 10 (-5 to 5) to 50 (-25 to 25) (in an increment of 0.5) and calculate the first 20 energy levels for each box size. Then plot these energy levels as a function of box size L . Observe the pattern of third energy level in positive parity. Repeat the solution for negative parity energy levels.