

Physics 1

You are to solve the time-independent Schrödinger equation for a one-dimensional infinite potential well (particle in a box) numerically. The potential $V(x)$ is defined as:

$$V(x) = \begin{cases} 0 & \text{if } 0 < x < L \\ \infty & \text{otherwise} \end{cases}$$

The Schrödinger equation in this region simplifies to:

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} = E\psi$$

Your tasks are:

1. **Discretize** the spatial domain x from 0 to L into N points.
2. **Construct** the Hamiltonian matrix H using finite difference approximations for the second derivative.
3. **Use** `numpy.linalg.eigh` to find the eigenvalues and eigenvectors of H .
4. **Plot** the first three energy eigenfunctions $\psi_n(x)$ corresponding to the lowest three energy eigenvalues.
5. **Verify** that the numerical energy eigenvalues match the analytical solutions:

$$E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}$$

Assume $\hbar = 1$, $m = 1$, and $L = 1$.

Physics 2

A double pendulum consists of two pendulums attached end to end. The equations of motion for the double pendulum are given by a system of coupled nonlinear ordinary differential equations:

$$\begin{aligned}\frac{d\theta_1}{dt} &= \omega_1 \\ \frac{d\theta_2}{dt} &= \omega_2 \\ \frac{d\omega_1}{dt} &= \left(-g(2m_1 + m_2) \sin \theta_1 - m_2 g \sin(\theta_1 - 2\theta_2) - 2 \sin(\theta_1 - \theta_2) m_2 (\omega_2^2 L_2 + \omega_1^2 L_1 \cos(\theta_1 - \theta_2)) \right) / (L_1(2m_1 + m_2 - m_2 \cos(2\theta_1 - 2\theta_2))) \\ \frac{d\omega_2}{dt} &= \left(2 \sin(\theta_1 - \theta_2) (\omega_1^2 L_1 (m_1 + m_2) + g(m_1 + m_2) \cos \theta_1 + \omega_2^2 L_2 m_2 \cos(\theta_1 - \theta_2)) \right) / (L_2(2m_1 + m_2 - m_2 \cos(2\theta_1 - 2\theta_2)))\end{aligned}$$

Your tasks are:

1. **Define** the equations of motion in a function suitable for use with `scipy.integrate.solve_ivp`.
2. **Set** the initial conditions: $\theta_1(0) = \pi/2$, $\theta_2(0) = \pi/2$, $\omega_1(0) = 0$, $\omega_2(0) = 0$.
3. **Simulate** the motion for t from 0 to 20 seconds.
4. **Plot** the angles $\theta_1(t)$ and $\theta_2(t)$ as functions of time.
5. **Animate** the motion of the double pendulum using `matplotlib`.

Assume $m_1 = m_2 = 1$ kg, $L_1 = L_2 = 1$ m, and $g = 9.81$ m/s².

Physics 3

The quantum harmonic oscillator has energy eigenvalues:

$$E_n = \hbar\omega \left(n + \frac{1}{2} \right)$$

However, we can also find the energy levels numerically by solving the time-independent Schrödinger equation:

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + \frac{1}{2}m\omega^2 x^2 \psi = E\psi$$

Your tasks are:

1. **Discretize** the spatial domain x from $-x_{\max}$ to x_{\max} into N points.
2. **Construct** the Hamiltonian matrix H using finite difference approximations for the second derivative and the potential $V(x)$.
3. **Use** `numpy.linalg.eigh` to find the eigenvalues and eigenvectors of H .
4. **Plot** the first three eigenfunctions $\psi_n(x)$ corresponding to the lowest three energy eigenvalues.
5. **Compare** the numerical energy eigenvalues with the analytical solutions.

Assume $\hbar = m = \omega = 1$ and $x_{\max} = 5$.

Laplace's equation in two dimensions is:

$$\nabla^2 \phi = 0$$

Consider a square region $[0, 1] \times [0, 1]$ with boundary conditions:

- $\phi(x, 0) = 0$
- $\phi(x, 1) = 0$
- $\phi(0, y) = 0$
- $\phi(1, y) = \sin(\pi y)$

Your tasks are:

1. **Discretize** the domain into a grid with $N \times N$ points.
2. **Set up** the finite difference equations for the interior points.
3. **Solve** the resulting linear system using `scipy.sparse.linalg.spsolve`.
4. **Plot** the potential $\phi(x, y)$ using a contour plot.

Solving the Time-Dependent Schrödinger Equation with a Time-Dependent Potential

Consider a quantum particle of mass m in a one-dimensional potential well with a time-dependent potential:

$$V(x, t) = \begin{cases} 0, & \text{if } 0 < x < L \\ \infty, & \text{otherwise} \end{cases}$$

Inside the well ($0 < x < L$), the potential is perturbed by a small time-dependent perturbation:

$$V_{\text{perturb}}(x, t) = V_0 \sin\left(\frac{\pi x}{L}\right) \sin(\omega t)$$

where V_0 is a constant, ω is the angular frequency of the perturbation, and L is the width of the well.

Your tasks are:

1. **Set up** the time-dependent Schrödinger equation (TDSE) for the particle inside the well.
2. **Discretize** the spatial domain using an appropriate grid and apply the Crank-Nicolson method to numerically integrate the TDSE over time.
3. **Initialize** the wavefunction $\psi(x, 0)$ as the ground state of the unperturbed infinite well.
4. **Evolve** the wavefunction over time and **compute** the probability density $|\psi(x, t)|^2$ at each time step.
5. **Calculate** the expectation value of the position $\langle x \rangle$ as a function of time.
6. **Plot** the probability density at different time intervals and the expectation value $\langle x \rangle$ over time.

Assume $\hbar = 1$, $m = 1$, $L = 1$, $V_0 = 0.1$, and $\omega = 5$.

Solving the Gross-Pitaevskii Equation for a Bose-Einstein Condensate

The Gross-Pitaevskii equation (GPE) describes the behavior of a Bose-Einstein condensate (BEC) at zero temperature:

$$i\hbar \frac{\partial \psi(\mathbf{r}, t)}{\partial t} = \left(-\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r}) + g|\psi(\mathbf{r}, t)|^2 \right) \psi(\mathbf{r}, t)$$

where $\psi(\mathbf{r}, t)$ is the condensate wavefunction, $V(\mathbf{r})$ is the trapping potential, $g = \frac{4\pi\hbar^2 a_s}{m}$ is the interaction strength, and a_s is the s-wave scattering length.

Your tasks are:

1. **Set up** the two-dimensional GPE for a BEC in a harmonic oscillator potential $V(x, y) = \frac{1}{2}m\omega^2(x^2 + y^2)$.
2. **Discretize** the spatial domain using a suitable grid and implement the split-step Fourier method to numerically integrate the GPE over time.
3. **Initialize** the wavefunction $\psi(x, y, 0)$ as the ground state of the non-interacting harmonic oscillator.
4. **Evolve** the wavefunction over time and **observe** the effects of interactions on the condensate's density profile.
5. **Plot** the condensate density $|\psi(x, y, t)|^2$ at different time intervals.

Assume $\hbar = m = \omega = 1$, $a_s = 0.005$, and use a grid of 256×256 points over a spatial domain $[-10, 10] \times [-10, 10]$.

Molecular Dynamics Simulation with Lennard-Jones Potential

Perform a molecular dynamics (MD) simulation of N particles in two dimensions interacting via the Lennard-Jones potential:

$$V(r) = 4\epsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right]$$

Your tasks are:

1. **Initialize** $N = 100$ particles in a square box with periodic boundary conditions, with random positions and velocities.
2. **Implement** the Verlet integration algorithm to update the positions and velocities of the particles.
3. **Compute** the forces between particles using the Lennard-Jones potential and account for the minimum image convention due to periodic boundaries.
4. **Simulate** the system for a sufficient number of time steps to reach equilibrium.
5. **Calculate** the radial distribution function $g(r)$ and plot it.
6. **Compute** the pressure and temperature of the system over time.

Physics 8:

Exact Diagonalization of the Heisenberg Spin Chain

Consider a one-dimensional Heisenberg spin- $\frac{1}{2}$ chain with N sites and periodic boundary conditions. The Hamiltonian is:

$$H = J \sum_{i=1}^N \mathbf{S}_i \cdot \mathbf{S}_{i+1}$$

where \mathbf{S}_i are the spin operators at site i , and J is the exchange coupling constant.

Your tasks are:

1. **Construct** the Hamiltonian matrix using the basis of spin configurations in the S^z basis.
2. **Use** `numpy.linalg.eigh` to compute the energy eigenvalues and eigenvectors of the system for $N = 8$ spins.
3. **Calculate** the thermodynamic properties such as the partition function Z and the magnetic susceptibility χ at finite temperature T .
4. **Plot** the specific heat C_V and magnetic susceptibility χ as functions of temperature.