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PH2140 Mathematics on the Computer — Final Projects

1. **Central force laws**

   Set up the relevant differential equations for a two-body problem in three dimensions, with interacting potential $V(r)$, where r is the magnitude of distance between the two bodies, and use `Mathematica` to analyze the following aspects of such central-force potentials.

   (a) Solve the above differential equations numerically for the Newtonian gravitational potential $V_N(r)$, and plot: (i) $r(\phi)$ (ii) $t(\phi)$.

   (b) For $V_N(r)$, find, by explicit integration, the area ΔA swept by the radius vector between times t and $t+\Delta$. Show, through relevant plots, that this area is independent of t and depends linearly on Δ.

   (c) Plot the orbit $r(\phi)$ for the potential $V = V_N \times (1 + \epsilon\, r^{-2})$ where ϵ is a small parameter. Interpret the result.

   (d) Plot the Laplace-Runge-Lenz vector, $\boldsymbol{A}$, for V_N and V at each point of their respective orbits. From your plots, provide the connection between behaviour of $\boldsymbol{A}$ and your result in (c) above.

   If you have forgotten how this vector is defined, look it up in Goldstein.

   (e) Repeat (a) for a harmonic oscillator potential.

2. **Quantum mechanical tunneling**

   (a) Consider a one-dimensional potential $V(x) = a \exp\left[-(x/0.1)^2\right]$.

   i. Solve the time dependent Schrodinger equation and obtain the time evolution of a wave packet $\psi(t,x)$ which, at $t=0$, has the profile $\psi(0,x) = A \exp\left[-B(x-x_0)^2\right] \exp\left[i5x\right]$ where $x_0 \gg 0.1$. Present your results for an appropriate set of values of the parameters (a, A, B); you will have to justify your choice during the presentation. (You may apply the boundary condition that the wave function vanishes at a sufficiently large x. You may also want to choose A such that $\psi(0,x)$ is normalized: $\int_{-\infty}^{\infty} dx |\psi(0,x)|^2 = 1$.)

ii. Make an appropriate plot of the quantity

$$j(t,x) = \frac{\hbar}{m}\text{Im}\left[\psi^* \frac{\partial \psi}{\partial x}\right]$$

for the above solution, and interpret it's behaviour.

(b) Consider a one-dimensional potential $V(x) = \alpha(x^2 - 1)^2$. Plot this potential. Solve the time dependent Schrodinger equation with initial wave function $\psi(0,x) = A\exp\left[-B(x+1)^2\right]$, which is a gaussian centered at $x = -1$, one of the minima of the potential. Choose α and B such that the initial wave packet is very sharply peaked around $x = -1$. Can you interpret the result?

3. **Classical random walk**

Imagine a drunkard who starts at the origin of a $D = 1$ dimensional space. He then tosses a fair coin to determine whether he will take a unit step forward or backward.

(a) Set up a realization of the above process for $N = 100$ steps by suitably simulating the coin toss by a random process.

(b) Calculate the total distance d_N from the origin travelled by the walker at the end of the process.

(c) Calculate the average value of d_N^2.

(d) Plot d_N^2 as a function of N and find the best fit relation.

(e) Repeat the above exercise for a random walker in $D = 2$ dimensions, assuming that at each time step, the drunkard can only move unit step along $\pm x$ or $\pm y$ directions, with equal probability. (For example, he can toss two independent (and fair) coins to pick one of the four options.)

(f) Repeat all the above steps for the case when the probabilities of moving forward and backward along x axis are unequal.

4. **A study of the undamped simple and double pendulum**

(a) First consider a simple pendulum of length l_1 and a point mass m_1 attached to it. Set up the equation of motion for the angular displacement θ_1. Numerically, solve for the time-period when (a) the initial displacement $\theta_1(0)$ is small, so the small angle approximation $\sin\theta_1 \approx \theta_1$ holds, and, (b) the initial displacement is large so the small angle approximation no longer holds. Produce a table of results, with the calculated time-period versus the initial displacement $\theta_1(0)$. For what values of $\theta_1(0)$ does the time-period differ from $2\pi\sqrt{l/g}$ (g is the acceleration due to gravity) by more than 1? What happens at $\theta_1(0) = \pi$?

(b) Reduce the equation of motion to a pair of coupled first-order differential equations for θ_1 and $\dot{\theta}_1 = d\theta_1/dt$. Hence obtain the *phase plots* for the simple pendulum, that is, for different values of the initial displacement $0 < \theta_1(0) \leq 2\pi$, plot $\dot{\theta}_1(t)$ as a function of $\theta_1(t)$.

(c) Animate the simple pendulum. How different are the trajectories traced out by the point mass ($\theta_1(t)$ vs time) for different initial displacements?

(d) Now consider a system of two simple pendulums attached end to end. Say l_1 and l_2 are their respective lengths and m_1, m_2 are the corresponding point-masses attached at the end of each string. If $T(\theta_1, \theta_2)$ is kinetic energy and $V(\theta_1, \theta_2)$ the potential energy of the system at displacements θ_1, θ_2, the equations of motion are given by

$$\frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \dot{\theta}_1}\right) = \frac{\partial \mathcal{L}}{\partial \theta_1}, \quad \frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \dot{\theta}_2}\right) = \frac{\partial \mathcal{L}}{\partial \theta_2},$$

where, $\mathcal{L} = T - V$ is the **Lagrangian** of the system. Solve the equations of motion numerically for some choice of initial conditions and hence plot $\theta_1(t)$ and $\theta_2(t)$ as a function of time t.

(e) In the small angle approximation ($\sin\theta_1 \approx \theta_1, \sin\theta_2 \approx \theta_2$), you can linearize the system of equations, to get the following form:

$$\begin{pmatrix} \ddot{\theta}_1 \\ \ddot{\theta}_2 \end{pmatrix} = \frac{1}{\alpha} M \begin{pmatrix} \theta_1 \\ \theta_2 \end{pmatrix} = \frac{1}{\alpha} \begin{pmatrix} a_1 & a_2 \\ a_3 & a_4 \end{pmatrix} \begin{pmatrix} \theta_1 \\ \theta_2 \end{pmatrix}.$$

Hence obtain the normal modes of the system. Plot the high and low frequency modes, and an arbitrary sum of the two.

(f) A dynamical system is said to be **chaotic** if the dynamics are *sensitive to initial conditions*. By plotting different trajectories ($\theta_1(t), \theta_2(t)$ as a function of time) of the system, show that the double pendulum exhibits chaotic behaviour for large initial displacements. In particular, show that the difference between the displacements $\theta_1^{(1)}(t), \theta_1^{(2)}(t)$ at time t corresponding to two different initial conditions $\theta_1^(1)(0), \theta_1^{(2)}(0)$ can be exponentially large:

$$\begin{aligned} |\theta_1^{(1)}(t) - \theta_1^{(2)}(t)| &\approx e^{\lambda_1 t}|\theta_1^{(1)}(0) - \theta_1^{(2)}(0)|, \\ |\theta_2^{(1)}(t) - \theta_2^{(2)}(t)| &\approx e^{\lambda_2 t}|\theta_2^{(1)}(0) - \theta_2^{(2)}(0)|. \end{aligned}$$

(g) Animate the double pendulum.

5. **Quantum Simple Harmonic Oscillator**

Consider a quantum mechanical particle of mass m subject to the one-dimensional potential $V(x) = \frac{1}{2}m\omega(x - x_0)^2$.

(a) Solve the time-independent Schrödinger equation and hence obtain the possible energy levels $E_n (n = 0, 1, 2, 3, \dots)$ for the particle and the corresponding energy eigenfunctions $\psi_n(x)$, as a function of the position x of the particle. Make sure the eigenfunctions are normalized. Plot the first few energy eigenfunctions, along with the potential $V(x)$.

(b) The energy eigenfunctions can also be visualized as functions of the momentum p of the particle, via the Fourier transform: the Fourier transform of $\psi_n(x)$ gives the n^{th} eigenfunction $\tilde{\psi}_n(p)$ in the momentum-representation. Plot the first few energy eigenfunctions in the momentum representation. How do they compare with the eigenfunctions in the position representation?

(c) Calculate the standard-deviation of position and momentum of the oscillator in the ground state ($n = 0$) and show that it saturates the Heisenberg uncertainty principle. Compute the product of the standard-deviations as a function of n for the higher energy states, and compare with the uncertainty principle.

(d) The **Correspondence Principle** states that in the limit of large quantum numbers (that is, at high enough energies), quantum systems reproduce classical behaviour. Verify this statement for the one-dimensional harmonic oscillator, by plotting (as a function of the position x) the probability density functions for a quantum oscillator for large enough values of n and that of a classical oscillator.

(e) Suppose the system starts out in a **coherent state**, which is a superposition of the energy eigenstates of the form

$$\phi_c(x, 0) = e^{-\frac{|c|^2}{2}} \sum_{n=0}^{\infty} \frac{c^n}{\sqrt{n!}} \psi_n(x), \; c \in \mathbb{C}.$$

Numerically solve the time-dependent Schrödinger equation for this initial state (for some value of c) and hence obtain the expectation values $\langle x(t) \rangle, \langle p(t) \rangle$, the average values of position and momentum at some later time t.

(f) Draw the phase plots ($\langle x(t) \rangle$ vs $\langle p(t) \rangle$ for coherent states, assuming different values of c. How do these compare with the phase plots of a classical oscillator? Does **Ehrenfest Theorem** (which predicts that the quantum mechanical expectation values satisfy the classical equations of motion) hold for the coherent states of the harmonic oscillator?

(g) Animate the time evolution of a coherent state.

(h) Numerically, evaluate the standard deviations in the position $x(t)$ and momentum $p(t)$ of the oscillator in a coherent state. How does their product evolve with time? Compare with the Heisenberg uncertainty principle.

6. **Electromagnetic fields of a moving charge**

The electric and magnetic fields produced by a point charge moving on a trajectory $\boldsymbol{z}(t)$ are given by standard expressions derived from the *Lienerd-Wiechert* potentials. (For e.g., look up Griffiths or Jackson.)

Consider a point charge on a trajectory described by

$$\boldsymbol{w}(t) = \sqrt{\left(\frac{c^2}{g}\right)^2 + (ct)^2}\,\hat{\boldsymbol{z}}$$

for $-\infty < t < \infty$. (This trajectory describes a uniformly accelerated motion, along $+z$ axis in Special Relativity, with g as the magnitude of acceleration.)

(a) Make appropriate plots for the scalar and vector potential.

(b) Plot the Electric and Magnetic field lines.

(c) Plot the Poynting vector.

7. **Bose-Einstein Condensation** Consider the ideal, non-relativistic, degenerate Bose gas. Let s denote the spin of the particles.

(a) Treating this as a grand-canonical ensemble, obtain (by performing the sum/integral in mathematica) the average occupancy number $\langle n_(\varepsilon)\rangle$ for a given single-particle energy ε, as a function of the chemical potential μ and the temperature T. Analyze this function with suitable plots. What happens to the average occupancy of the ground state (with energy ε_0) when the chemical potential $\mu \to \varepsilon_0$ at some finite temperature $T = T_c$?

(b) In order to compute thermodynamic properties of the system, it is useful to consider the following functions:

$$B(m,z) = \frac{1}{\Gamma(m)} \int_0^\infty \frac{x^{m-1}}{z^{-1}e^x - 1},\ m \geq 0,$$

where $z = e^{\mu/k_BT}$ is a function of the chemical potential, called the *fugacity*, and $\Gamma(m)$ is the gamma function. Plot $B(m,z)$ as function of z for $\frac{1}{2} \leq m \leq \frac{3}{2}$ and $0 \leq z \leq 1$. Observe the behavior of the functions at $z = 1$: in particular, show that (a) for $m \leq 1$ diverge as $z \to 1$, (b) $B(\frac{3}{2}, z)$ is finite for $z = 1$ but with infinite slope, (c) for $m > \frac{3}{2}$, the functions $B(m,z)$ have finite values and finite slopes at $z = 1$. In the limiting case of $m \to \infty$, show that $B(m,z) \to z$.

(c) The total particle number N is obtained by evaluating,

$$N = \int_0^\infty \langle n_\varepsilon \rangle \rho(\varepsilon) d\epsilon,$$

where the single particle energy is $\varepsilon = (\hbar)^2 k^2/2m$ in terms of the momentum k, and the density of states in the momentum space is $\rho(k)d^3k = (2s+1)V\frac{d^3k}{(2\pi)^3}$. Show that the density of excited states of the system is given by

$$n \equiv \frac{N}{V} = \frac{2s+1}{\lambda^3} B(\frac{3}{2}, z), \ \lambda = \sqrt{\frac{2\pi\hbar^2}{mk_BT}}.$$

(λ is called the *thermal wavelength* of the system.)

(d) The phase-transition occurs when the fugacity z reaches its limiting value of 1, so that the density n reaches its maximum value n^*. By inverting the expression, obtain the critical temperature as a function of n and s. For temperatures below the critical temperature, show that there is a macroscopic occupation of the ground state, i.e. Bose-Einstein condensation. Plot n as a function of T and justify the above statement.

(e) Instead of the simple particle-in-a-box potential which is assumed here, suppose the ideal Bose gas was confined by an isotropic harmonic potential of the form

$$V(r) = \frac{1}{2} m w^2 r^2.$$

At high temperatures $k_BT >> \hbar\omega$, it can be shown that the density of states takes the form $\rho(\varepsilon) \propto \varepsilon^2$. Evaluate the constant of proportionality. Use this to obtain the number density of states in the form of an appropriate function $B(m, z)$. Evaluate the critical temperature for Bose-Einstein condensation as a function of N and ω.