End-of-Semester Examination

If you are using Julia or Python, we recommend using a jupyter notebook. In WeLearn, you need to submit this file. Please clearly indicate in the markup cells, the number of the question for which you are writing the program. Also, please remember to add documentation through comments in your program.

You may also use scripts and use REPL to evaluate them. In that case, please keep all your files for a particular worksheet in a folder and you may upload the compressed archive of that folder.

Please feel free to ask for help!

Answer (*at least*) one question

1. **Rising Gas Bubble** [30]

A spherical air bubble of initial radius $R_0 = 1.0\,\mathrm{mm}$ is released from rest at the bottom of a vertical water column of height $H = 1.0\,\mathrm{m}$. Assume:

- Water properties: density $\rho_\ell = 10^3\,\mathrm{kg\,m^{-3}}$, viscosity $\mu = 1.0 \times 10^{-3}\,\mathrm{Pa\,s}$.
- Atmospheric pressure at the free surface: $P_a = 1.013 \times 10^5\,\mathrm{Pa}$.
- Hydrostatic pressure profile in the water: $P(y) = P_a + \rho_\ell g\,(H - y)$, where $y(t)$ is the bubble centre's vertical position (measured upward, so $y = 0$ at the bottom and $y = H$ at the surface).
- The bubble contains ideal air at constant temperature $T = 293\,\mathrm{K}$; hence $P\,V = \mathrm{const}$.
- Flow is in the Stokes-drag regime: $F_d = 6\pi\mu R\,v$, where $v = \dot{y}$.
- Added mass: the bubble accelerates an effective mass $m_{\text{eff}} = m_g + \frac{1}{2}\rho_\ell V$ (m_g = mass of the gas, $V = \frac{4}{3}\pi R^3$).
- Gravity $g = 9.81\,\mathrm{m\,s^{-2}}$.

(a) *Modelling:* [6]

(i) Using the ideal-gas law, derive the radius $R(y)$ of the bubble as it rises.

(ii) Show that the gas density is $\rho_g(y) = \rho_{g0}\,P(y)/P_0$ with $P_0 = P_a + \rho_\ell g H$.

(iii) Write the vertical equation of motion for the bubble:

$$m_{\text{eff}}(y)\,\ddot{y} \;=\; \big(\rho_\ell - \rho_g(y)\big)\,g\,V(y) \;-\; 6\pi\mu R(y)\,\dot{y}.$$

Combine this with $\dot{y} = v$ to obtain a first-order system for $\big(y(t),\, v(t)\big)$.

(b) *Dimensionless analysis:* Introduce scales R_0 for length, $g^{-1/2}R_0^{1/2}$ for time, and derive the dimensionless ODEs. Identify all dimensionless groups that govern the motion (e.g. Reynolds number, density ratio, etc.). [4]

(c) *Numerical solution:* Implement a 4th-order Runge–Kutta method with fixed step $h = 1.0 \times 10^{-4}\,\mathrm{s}$ to integrate the original dimensional system from $t = 0$ until the bubble centre reaches the surface ($y = H$). [10]

(d) *Results:* Produce plots of $y(t)$, $v(t)$, and $R(t)$. Report: [6]

- total rise time t_{surf};
- maximum ascent speed;
- bubble radius and volume just before it leaves the liquid.

(e) *Discussion:* Stokes drag is valid when the Reynolds number $\mathrm{Re} = 2\rho_\ell R v/\mu \lesssim 1$. Using your numerical data, comment on whether this assumption remains valid throughout the trajectory. If not, suggest how the model should be modified. [4]

2. **Quantum Particle in a Lennard–Jones–Like Potential** [30]

A spin-zero particle of mass

$$m = 6.63 \times 10^{-26}\,\mathrm{kg} \qquad \text{(approximately one } {}^{40}\text{Ar atom)}$$

moves in the one-dimensional Lennard–Jones (12−6) potential

$$V(x) = 4\varepsilon\big[(\sigma/x)^{12} - (\sigma/x)^{6}\big], \qquad x > 0,$$

with parameters

$$\varepsilon/k_B = 119.8\ \mathrm{K}, \qquad \sigma = 3.40\ \text{Å}.$$

Because $V(x) \to +\infty$ as $x \to 0$ and $V(x) \to 0$ as $x \to \infty$, there is a finite set of bound states $E_n < 0$.

(a) *Parabolic approximation* [6]

(i) Find the equilibrium separation x_0 ($V'(x_0) = 0$).

(ii) Show that near $x = x_0$ $V(x) \approx V_{\min} + \frac{1}{2}m\omega^2(x-x_0)^2$ and derive ω in terms of m, ε, σ.

(b) *Dimensionless Schrödinger equation* [4]

Introduce $y = x/x_0$ and measure energy in units of ε. Show that the TISE becomes

$$-\frac{d^2\psi}{dy^2} \;+\; U(y)\,\psi \;=\; \lambda\,\psi,$$

and write explicit expressions for $U(y)$ and λ.

(c) *Numerical eigenvalues* [10]

Discretise $y \in [0,\, 10]$ with $\Delta y = 0.01$. Impose the boundary conditions $\psi(0) = \psi(10) = 0$ and compute the first three bound energies E_0, E_1, E_2 by shooting with bisection on E.

(d) *Harmonic check* [6]

Using $\hbar\omega$ from part (a) obtain the harmonic-oscillator energies $E_n^{(\mathrm{HO})} = V_{\min} + \hbar\omega\big(n + \frac{1}{2}\big)$. Compute

$$\delta_n = 100\,\frac{|E_n - E_n^{(\mathrm{HO})}|}{|E_n|}$$

for $n = 0, 1, 2$ and state the largest n for which $\delta_n < 5\%$.

(e) *Validity criterion* [4]

Show that the quadratic approximation is valid when $|x - x_0| \ll x_0/3$. Using the harmonic ground-state wavefunction estimate $\langle |x - x_0| \rangle$ and verify that the criterion holds.

Useful constants

$\hbar = 1.055 \times 10^{-34}\,\mathrm{J\,s},\ k_B = 1.381 \times 10^{-23}\,\mathrm{J\,K^{-1}},\ 1\,\text{Å} = 10^{-10}\,\mathrm{m}.$

3. **Planar Random Walk and Its Statistics** [30]

A particle starts at the origin $(0, 0)$ on a frictionless horizontal table. Every $\Delta t = 10$ ms it executes a single *free flight* (step) of fixed length $\ell = 0.05$ mm in a direction θ that is chosen independently and uniformly from $[0, 2\pi)$. After N steps the clock time is $T = N\,\Delta t$ and the Cartesian coordinates are

$$x_N = \sum_{k=1}^{N} \ell \cos\theta_k, \qquad y_N = \sum_{k=1}^{N} \ell \sin\theta_k.$$

For all numerical parts use $N = 200$ steps ($T = 2.0$ s) and $M = 10^5$ independent trajectories.

(a) *Analytic first and second moments* [6]

Show directly from the symmetry of the random angles θ_k that

$$\langle x_N \rangle = \langle y_N \rangle = 0, \qquad \langle x_N^2 \rangle = \langle y_N^2 \rangle = \frac{N\ell^2}{2}.$$

Hence obtain the standard deviations $\sigma_x(N) = \sigma_y(N) = \sqrt{N}\,\ell/\sqrt{2}$.

(b) *Diffusion-constant interpretation* [4]

For very large N the walk approximates Brownian motion with diffusion coefficient $D = \ell^2/(4\Delta t)$. Derive the mean-square displacement $\langle r^2 \rangle = \langle x_N^2 + y_N^2 \rangle = 4D\,T$ and compute its numerical value for $T = 2.0$ s.

(c) *Monte-Carlo test of Cartesian statistics* [8]

Simulate $M = 10^5$ trajectories using the vector update

$$x_{n+1} = x_n + \ell\cos\theta_{n+1}, \qquad y_{n+1} = y_n + \ell\sin\theta_{n+1}.$$

(i) At $T = 2.0$ s plot the normalised histogram of the x coordinates. Overlay the Gaussian $g(x) = \left(2\pi\sigma_x^2\right)^{-1/2} \exp\left[-x^2/(2\sigma_x^2)\right]$ with σ_x from part (a).

(ii) Estimate $\widehat{\sigma}_x$ from the sample variance and quote the fractional error $|\widehat{\sigma}_x - \sigma_x|/\sigma_x$.

(d) *Radial distribution and moments* [6]

(i) Show that the radial distance $r_N = \sqrt{x_N^2 + y_N^2}$ has mean square $\langle r_N^2 \rangle = N\ell^2$.

(ii) From the same data used in part (c) form $\widehat{\langle r^2 \rangle} = \frac{1}{M}\sum_{k=1}^{M}(x_k^2 + y_k^2)$ at $T = 0.5, 1.0, 2.0$ s and compare with the analytic prediction $4DT$.

(e) *Central-limit convergence* [6]

By grouping the data from part (c) into blocks of size $n = 50$ steps ($T = 0.5$ s), demonstrate numerically that the distribution of the block-averaged displacements $\bar{x} = \frac{1}{n}\sum_{k=1}^{n} \ell\cos\theta_k$ approaches a Gaussian with variance $\ell^2/(2n)$.

4. **Semiclassical Energy Levels of Helium via Bohr–Sommerfeld Quantisation** [30]

A simple "independent–electron" model of the helium atom replaces the true Coulomb–correlated two–electron Hamiltonian by two identical, non-interacting electrons that each move in an effective central potential

$$V_{\text{eff}}(r) = -\frac{Z_{\text{eff}} e^2}{4\pi\varepsilon_0\, r}, \qquad Z_{\text{eff}} = 1.6875,$$

where the constant $Z_{\text{eff}} = 27/16$ reproduces the observed ground-state energy (Slater screening approximation).

Consider one electron with physical mass m_e in this potential. Ignore spin; orbital angular momentum is labelled by the quantum number ℓ.

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For numerical work use atomic units ($m_e = 1,\ \hbar = 1,\ e^2/4\pi\varepsilon_0 = 1$).

(a) *Classical turning points* [8]

For a given energy $E < 0$ and angular momentum ℓ, the classical radial momentum is

$$p_r(r; E, \ell) = \sqrt{2\big[E - V_{\text{eff}}(r)\big] - \frac{\ell(\ell+1)}{r^2}}\,.$$

(i) Derive the equation that determines the two turning points $r_- < r_+$ (roots of the radicand).

(ii) Show that for $\ell = 0$ the inner turning point is $r_- = 0$ and find an analytic expression for $r_+(E)$.

(b) *Bohr–Sommerfeld quantisation* [6]

The radial quantum condition is

$$\int_{r_-}^{r_+} p_r(r; E, \ell)\, dr = \pi\big(n_r + \tfrac{1}{2}\big), \qquad n_r = 0, 1, 2, \ldots$$

for each angular momentum ℓ.

(i) Write the integral explicitly for $\ell = 0$. (Leave it in integral form; exact evaluation is *not* required.)

(ii) Explain why the factor $\frac{1}{2}$ appears in the right-hand side.

(c) *Numerical evaluation and root finding* [10]

Using Simpson's $\frac{1}{3}$ rule with a stepsize $h = 1 \times 10^{-3}\, r_+$, write a program that:

(i) evaluates the action integral $S(E) = \displaystyle\int_0^{r_+(E)} p_r(r; E, 0)\, dr$ for a *given* energy E;

(ii) employs the bisection method to solve $S(E) = \pi(n + \frac{1}{2})$ for E with relative tolerance 10^{-6}.

Tabulate the semiclassical eigenvalues for the three lowest principal quantum numbers $n = 1, 2, 3$ (all with $\ell = 0$).

(d) *Comparison with exact hydrogenic formula* [6]

The hydrogenic (one-electron, unscreened) energy levels would be $E_n^{(\mathrm{H})} = -Z_{\mathrm{eff}}^2/(2n^2)$. Compute the percentage error

$$\delta_n = 100\,\frac{|E_n^{(\mathrm{BS})} - E_n^{(\mathrm{H})}|}{|E_n^{(\mathrm{H})}|}$$

for $n = 1, 2, 3$.