Lecture 2: Five problems

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Computational Physics 1
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1. Radioactive decay chains
2. Quantum perturbation theory
3. Cruise-lanes in space
4. Meta-materials
5. Transport in strongly-coupled plasmas

Outline

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Density of radionuclides

Radioactive nuclei transmute from one to another through α emission or β-decay. (γ-decay does not change the nucleus, merely takes it from an excited to a lower state). It turns out that all nuclei in nature belong to one of three decay chains [Decay]. If n_k is the density of the k-th nucleus in a chain, then the time dependence of n_k is given by

$$\frac{dn_k}{dt} = \alpha_{k-1} n_{k-1} - \alpha_k n_k,$$

where $1/\alpha_k$ is the half-life for the decay from the k-th to the $k+1$-st nucleus in the chain, and the unit of time is such that $\alpha_1 = 1$. Then

$$\frac{d\mathbf{n}}{dt} = A\mathbf{n}, \qquad \text{where} \quad A = \begin{pmatrix} -1 & 0 & 0 & \cdots & 0 \\ 1 & -\alpha_2 & 0 & \cdots & 0 \\ 0 & \alpha_2 & -\alpha_3 & \cdots & 0 \\ \vdots & \vdots & \vdots & & \vdots \\ 0 & 0 & 0 & \cdots & -\alpha_N \end{pmatrix}$$

The solution and the problem

These equations can be formally solved by many methods [King et al]:

1. One could simply treat the equations one-by-one to get $n_1(t) = n_1(0)\exp(-\alpha_1 t)$, *etc.*.
2. One could integrate the differential equations numerically.
3. One could formally write $\mathbf{n}(t) = \mathbf{n}(0)\exp(At)$. (One could formally define $\exp A = 1 + A + A^2/2! + \cdots$.)

In any case, to answer any interesting question, (for example, given the concentration of nuclei in the earth's crust, can one estimate the composition of the gas cloud from which the solar system formed?) one has to compute the solutions numerically.
One immediately finds a problem. Some of the half lives are several millions of years. Others are in fractions of seconds. Computing all of them accurately seems difficult. Such a problem is said to be **ill-conditioned**.
We will investigate when the computation of $\exp(At)$ is difficult, and what is a good way to do it even for ill-conditioned problems [van Loan].

Generalization

This is one of a very large class of problems— that of **linear ordinary differential equations with constant coefficients**. They can always be reduced to exponentiating a matrix [Arnold].
Suppose one has a high-order ODE

$$\frac{d^n x}{dt^n} + a_1 \frac{d^{n-1} x}{dt^{n-1}} + \cdots a_n x = 0.$$

One can reduce this to a set of coupled first-order ODEs using the familiar method of writing the Hamiltonian form of Newton's equations. Introduce the variables $y_1 = x$ and $y_k = dy_{k-1}/dt$ for $k = 2$ up to n to reduce this to a set of coupled first-order ODEs. The space of variables $\{y_1, y_2, \cdots, y_n\}$ define the **phase plane** of the problem.
If there are sets of coupled higher order ODES, they can also be reduced simultaneously. After this reduction one can solve them again by exponentiation of a matrix.

The numerical problem

In many modern research problems involving differential equations, the number of variables is very large. For example, molecular dynamics simulations of fluids regularly use as many as 10^6–10^8 variables. Simulations of the evolution of the universe (the N-body gravitational problem) may deal with 10^7–10^9 mass points.
In all these cases there are large hierarchies of time scales. One knows that typical molecular speeds are equal to the speed of sound, c_s. The typical microscopic time is of the order of a/c_s, where a is the average inter-molecular spacing. The typical mesoscopic size scale is of the order of $N^{1/3}a$, and the corresponding time scale is $N^{1/3}a/c_s$. As a result, there is a clear separation of 10^2–10^3 between these time scales. There are sometimes even slower processes, such as diffusion, which may raise the ratio of the small and large time scales to as high as 10^6 or more. Ill-conditioning is then normal in most problems, and methods to alleviate these are important.

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Outline

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5 Transport in strongly-coupled plasmas

Coupled channel computations

The quantum evolution equation for a general system is

$$i\hbar\frac{d\psi}{dt} = H\psi,$$

where ψ is the wavefunction of the system and H its Hamiltonian. It can seldom be solved exactly. However, in many applications, one finds $H = H_0 + H_I$ where H_0 is a solvable Hamiltonian and the remainder, H_I, is small in some sense.

Assume that $\phi_n(x)$ are eigenfunctions of H_0 with eigenvalue E_n. One can always write any ψ as a superposition of the ϕ_n in the form

$$\psi(x,t) = \sum_n a_n(t)\mathrm{e}^{-iE_nt/\hbar}\phi_n(x).$$

Now taking the matrix elements of the first equation in the basis of ϕ_n, one has

$$i\hbar\frac{d\mathbf{a}}{dt} = H_I\mathbf{a}.$$

The real problem

Once the matrix-elements of H_I,

$$(H_I)_{mn} = \int dx \phi_m^*(x) H_I(x) \phi_n(x),$$

are determined, this is a simple set of coupled first order ODEs. One problem here is that the matrix is infinitely large. The other is that in many cases of interest (for example, atom-light interactions), H_I is time-dependent.

The solution to the second problem is actually pretty straightforward. The first problem is usually solved brutally in quantum perturbation theory. One just truncates the state-space and hopes that nothing goes wrong. The usual treatment of **Rabi oscillations** is one example. When one is close to a **resonance** then this hope actually is borne out. In many other cases it is not. This problem has not been solved satisfactorily till now. (I think I have a general solution based on the renormalization group, but this margin is not large enough to write it down.)

Rabi oscillations

An infinite laser light train is incident on a system with electrons (of charge e), and the laser frequency is tuned to a resonance, *e.g.*, $\omega_{12} = (E_1 - E_0)/\hbar$. Then $H_I = exF\cos\omega_{12}t$. The matrix elements of x vanish between states of equal parity. In particular the diagonal elements vanish. Hence the truncated perturbation equations are

$$i\hbar\frac{d}{dt}\begin{pmatrix} a_0 \\ a_1 \end{pmatrix} = \begin{pmatrix} 0 & V_{12} \\ V_{12}^* & 0 \end{pmatrix}\begin{pmatrix} a_0 \\ a_1 \end{pmatrix}.$$

These equations are easily solved.
However, usually a further approximation is made. When observations are made over a time long compared to $1/\omega$, then the phase factors in V_{12} are averaged over to give a time independent perturbation, $\overline{V}_{12}$. If the initial conditions are $a_0(0) = 1$ and $a_1(0) = 0$, then the solutions are

$$a_0(t) = \cos\Omega t, \quad a_1(t) = \sin\Omega t, \qquad \text{where} \qquad \Omega = \frac{\overline{V}_{12}}{\hbar}.$$

These are the famous Rabi oscillations.

Specific problems

1. Examine the neighbourhood of the Rabi resonance region numerically $\omega_{12}/2 \leq \omega \leq 2\omega_{12}$, keeping successively larger numbers of states (2, 4, 8, 16, *etc.*) and check how many are needed for 1% accuracy in the results. Assume that the electrons are in a quantum dot which can be modelled by a one-dimensional infinitely deep square well. Evaluate the matrix elements of H_I within the program, using symmetries to reduce the computation as far as possible.
2. Laser pulse shaping is modelled by setting $H_I = exf(t)\cos\omega t$ where $f(t)$ is a positive function called the pulse shape. Is it possible to shape the pulse in the neighbourhood of a resonance so that there is multi-state resonance?
3. Apply the coupled channel analysis to the Helium spectrum. H_0 is just the usual central Coulomb potential of the nucleus in which the two electrons move. Take H_I to be the Coulomb interaction between the electrons. Find how the accuracy of the ground state energy of the Helium atom changes as you include more and more channels.

The underlying numerical algorithms

The Helium problem is the prototype of modern ab-initio atomic physics problems. A typical open problem is to compute the spectrum of iron. Apart from the intrinsic interest, it has applications in both chemistry and astrophysics. These computations are currently carried out with 10^6–10^8 basis states. The number of states used is limited only by algorithmic and CPU speeds. There is no convincing evidence that in the near future we will be able to include sufficient number of states to reduce errors to less than one part in 10^3.

The first stage of all three problems above is to compute the large numbers of integrals needed to find the Hamiltonian. Highly efficient methods of computing integrals exist, and we shall study them.

The next stage is to actually solve a set of linear first order differential equations. We have met this problem before, and we know that this could be the bottle-neck in the computation. The related problem that we need to solve for the spectrum is to find the eigenvalues and eigenvectors of the matrix. This is also a numerically challenging problem of wide applicability.

Outline

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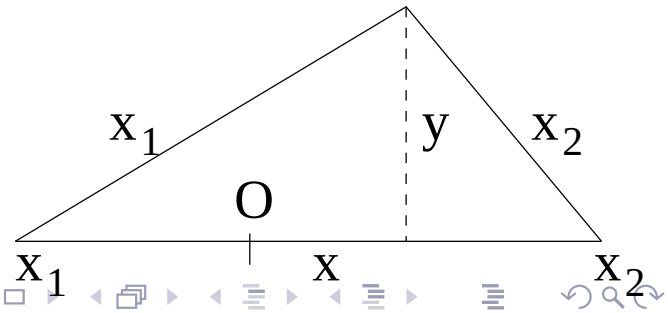
5 Transport in strongly-coupled plasmas

The restricted gravitational three-body problem

Classical gravity is the archetype of non-linear problems and shows all the usual physics associated with it, namely, integrability and chaos. The **circular restricted gravitational three-body problem** (CR3BP) consists of two bodies (which we call the earth and the moon) in circular orbits around each other and a third body (called a satellite) in orbit around them which is so light that the earth and moon do not react to its motion. The heavy masses are $M_1 = M(1-\mu)$ and $M_2 = \mu M$ where $\mu \leq 1/2$. The origin is chosen at the center of mass. Then $\mathbf{r}_1 = -(1-\mu)\mathbf{r}$ and $\mathbf{r}_2 = \mu r$, where $\mathbf{r} = \mathbf{r}_2 - \mathbf{r}_1$ is the relative coordinate. The period of a circular orbit is then $\omega^2 = GM/r^2$. The problem is simplified by choosing units in which sum of the masses $M = 1$, the separation between the two masses $|\mathbf{r}| = 1$ and $G = 1$. Then $\omega = 1$.

Choose the non-inertial coordinates in which the two heavy masses are at rest. The line joining them is the x-axis. The plane of their orbit is the xy plane.



The Jacobi integral

The distance of the satellite from the other two bodies, and its speed are given by the expressions

$$r_i^2 = (x - x_i)^2 + y^2 + z^2, \qquad \text{and} \qquad v^2 = \left(\frac{dx}{dt}\right)^2 + \left(\frac{dy}{dt}\right)^2 + \left(\frac{dz}{dt}\right)^2.$$

Since the reaction of the heavy bodies to the light body is not taken into account, the energy of the system is not conserved. Jacobi constructed an integral of motion [Moulton], C, which is the sum of the kinetic energy and an effective potential

$$C = \frac{1}{2}v^2 + V(r), \quad \text{where} \quad V(r) = -\frac{1}{2}\left(x^2 + y^2\right) - \frac{(1-\mu)}{r_1} - \frac{\mu}{r_2}.$$

This implies that for any C there is a locus of points, $v^2 = 0$, which cannot be crossed by any orbit of the satellite. Analysis of this surface gives the **Lagrange points**.

The Lagrange points

The Lagrange points are those spatial points where the whole orbit has $v = 0$. Therefore these are points with $\nabla V = 0$. One has

$$\frac{\partial V}{\partial z} = z\left[\frac{1-\mu}{r_1^3} + \frac{\mu}{r_2^3}\right] = 0.$$

Therefore, all the Lagrange points lie in the plane $z = 0$. The other two derivatives are

$$\left.\frac{\partial V}{\partial x}\right|_{z=0} = x - (1-\mu)\frac{x-x_1}{r_1^3} - \mu\frac{x-x_2}{r_2^3} = 0, \quad (1)$$

$$\left.\frac{\partial V}{\partial y}\right|_{z=0} = y\left[1 - (1-\mu)\frac{1}{r_1^3} - \mu\frac{1}{r_2^3}\right] = 0. \quad (2)$$

When $y = 0$ there are three values of x where the derivative vanishes. These are called the L1, L2 and L3 points. These are unstable under small perturbations. When $y \neq 0$ the solutions are $r_1 = 1$ and $r_2 = 1$. These are called the L4 and L5 points. These are stable points.

The problem

1. **The Sitnikov problem**: Consider the motion of the satellite in the CR3BP in which the initial conditions are that the satellite starts from rest from some point $x = y = 0$ and $z = z_0$. This motion is one-dimensional and integrable [Sitnikov]. Solve this case analytically. What is the effect of small perturbations orthogonal to the z-axis [Hevia et al]?
2. Consider rockets fired from the earth at an angle ϕ from the x axis in the xy plane with Jacobi integral equal to C. For each pair of initial conditions $\{\phi, C\}$ follow the trajectory

$$\frac{d^2\mathbf{r}}{dt^2} = -\nabla V.$$

   Find the set of trajectories which reach a distance D from the center of mass after a time T.
3. Which set of initial conditions $\{\phi, C\}$ lead to chaotic trajectories?

Difficulties

In both the examples above, the system exhibits chaos. A chaotic system has extreme sensitivity to initial conditions. As a result, small errors in the integration can result in extremely large errors in the trajectories. Control of the numerical solution of the equations is therefore of very high importance.

Note also that the phase space of the systems here have the usual Poisson bracket structure. As a result, Liouville's theorem holds and phase space volume has to be preserved. The methods that are developed for integrating these equations must also be tuned to preserve phase space volume to high accuracy. These are called **symplectic integrators** or **leapfrog** methods.

The second problem is an example of an **embarrassingly parallel** program. Each initial condition can be evolved completely independently of any other part of the computation. In principle, they can even be run on completely different machines.

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Outline

1 Radioactive decay chains

2 Quantum perturbation theory

3 Cruise-lanes in space

4 Meta-materials

5 Transport in strongly-coupled plasmas

Electrodynamics

The Maxwell's equations in vacuum:

$$\nabla \cdot \mathbf{D} = 0, \quad \nabla \cdot \mathbf{B} = 0, \quad \nabla \times \mathbf{H} = \frac{\partial \mathbf{D}}{\partial t}, \quad \nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t},$$

and the constitutive equations, $\mathbf{D} = \epsilon \mathbf{E}$ and $\mathbf{B} = \mu \mathbf{H}$, together are a set of first order linear partial differential equations in six variables. Standard textbook problems involve the study of antennae, waveguides and optical fibers. In all these problems it is useful to Fourier transform and solve algebraic equations in Fourier space.
Typical modern problems are those in which ϵ and μ are engineered to be non-constant. Such is the case for investigation of radar signals incident on stealth aircraft, or the properties of metamaterials which have a negative refractive index [Smith et al]. In this case, Fourier space solutions are less transparent than the numerical solution of the Maxwell equations.

Solving Maxwell's equations

In performing numerical solutions, it is useful to discretize the space and time derivatives and work on a space-time lattice. If the Gauss law (divergence free) conditions are imposed on **D** and **B** at the initial time, then it is possible to define numerical time evolution in such a way that they remain divergence free at all subsequent times. Then the Maxwell's equations become a set of autonomous first order partial differential equations

$$\gamma \frac{\partial \mathbf{F}}{\partial t} + \nabla \times \mathbf{F} = 0, \quad \text{where} \quad \gamma = \begin{pmatrix} \epsilon & 0 \\ 0 & \mu \end{pmatrix}, \quad \mathbf{F} = \begin{pmatrix} \mathbf{E} \\ \mathbf{B} \end{pmatrix}.$$

Numerical solution of these equations can have artificial **dispersion**, if different Fourier modes travel with different phase velocities, **dissipation**, if the evolution equation does not preserve the norm of the signals, and **anisotropy**, since the discretized equations do not have the full rotational symmetry of the original. The numerical problem is to control these effects [Liu].

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Outline

1 Radioactive decay chains

2 Quantum perturbation theory

3 Cruise-lanes in space

4 Meta-materials

5 Transport in strongly-coupled plasmas

Scales in a plasma

A plasma is a fluid with mobile charges which is overall charge neutral. The basic microscopic scales are the charge of each particle, e, its mass, m, and the interparticle separation: $a = n^{-/13}$, where n is the number density of particles in the plasma. The temperature, T is also a microscopic parameter since it is equal to the average energy of each charge carrier. We have used units natural for the classical plasma, *i.e.*, one in which $k_B = 1$ so that T has units of energy, and $4\pi\epsilon_0 = 1$ so that e^2 has units of energy times length.

A dimensionless quantity built from the microscopic scales, called the **plasma parameter**, is related to the ratio of the thermal energy and the Coulomb energy at the mean separation,

$$K = \sqrt{\frac{Ta}{e^2}}.$$

When $K \gg 1$ the plasma is said to be weakly coupled, and when $K \simeq 1$ it is strongly coupled [Gupta].

Length scales in a plasma

The average distance of closest approach between two charges, d, occurs when the Coulomb energy equals the thermal energy,

$$d = \frac{e^2}{T} = a\left(\frac{e^2}{aT}\right) \simeq \frac{a}{K^2}.$$

There is another length called the **Debye screening length** which is equal to

$$\lambda \simeq Ka = \sqrt{\frac{a^3 T}{e^2}}.$$

If a test charge is placed within a plasma, then λ is the distance within which the charge is screened off by an oppositely charged sheath. As a result, particles passing by the test charge at a distance larger than λ do not feel its Coulomb field. For a weakly coupled plasma $\lambda \gg a \gg d$. We will next examine the mean-free path length, ℓ, in terms of a and K [Arnold et al].

The mean-free path length in a plasma

If the mean free path is dominated by close collisions, giving rise to large angle Rutherford scattering, then the cross section $\sigma_l = \pi d^2$. Therefore

$$\ell_l = \frac{1}{n\sigma_l} \simeq aK^4.$$

If distant collisions are important, then the velocity change in a single collision with impact parameter b is $(\Delta v)/v = e^2/(bT)$. Over many collisions, the velocity changes slowly through a random walk in phase space. Therefore for small angle collisions

$$\sigma_s = \int_d^\lambda \left(\frac{\Delta v}{v}\right)^2 2\pi b db \simeq a^2 \frac{\log K}{K^4}, \qquad \ell_s \simeq a\frac{K^4}{\log K}.$$

For a weakly coupled plasma, $\log K \gg 1$, so transport properties depend on ℓ_s. For a strongly coupled plasma large angle scattering dominates. Similar analysis shows that the mean free path increases as the 4th power of the speed of a charge carrier, so that slow particles are the most important for transport [Aarts].

A molecular dynamics simulation of a plasma

Take N particles, and assign them equal masses but charges $\pm e$ at random, making sure that the total charge is exactly zero. Place the particles randomly inside a box with rigid walls. For a fixed N the box size, L, determines the average interparticle spacing: $a = L/N^{1/3}$. Give the particles random velocities drawn from a Maxwellian distribution at temperature T. Tune the parameters so $K = 10$–100.
The simulation [Beck et al] consists of letting the particles evolve under their mutual Coulomb interactions—

$$\frac{d\mathbf{x}_k}{dt} = \mathbf{v}_k, \qquad \frac{d\mathbf{v}_k}{dt} = \left(\frac{e_k}{m}\right) \sum_{j \neq k} \frac{e_j}{|\mathbf{x}_j - \mathbf{x}_k|^2}.$$

Since the paths are not straight lines, computation of the mean free path requires care [Dehnen]. Define it by computing the autocorrelation of the direction of the velocity of a particle. Simultaneously count the number of close approaches [Quinn et al]. Check whether or not the mean-free path is dominated by close encounters.

The difficult bits

A **molecular dynamics** (MD) problem of this kind involves many subtle subproblems. In a classical problem of this kind it is important to satisfy Liouville's theorem; so one has to use symplectic integrators. Next, at each time step, one has to find the force on every particle due to every other, which takes $\mathcal{O}(N^2)$ time. This has to be done carefully in order to save as much time as possible [Dehnen].

Clearly this problem is ill-conditioned [Quinn et al], since the time-step needs to be small when two particles come very close to each other. Otherwise one can have large errors in the trajectory. However, particles which are far from others at the same time can be integrated with a larger time step.

Another problem in MD simulations is to ensure reversibility. Typically, over long times, accumulated errors in the integration of the trajectory will mean that the path cannot be traversed backwards. One has to control errors of this kind.

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