Time Evolution of Quantum Systems 2025: Exercise 3

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Symplectic Integrators

H.1 Let $D_H = D_T + D_V$ be the linear operator defining the classical equations of motion $\dot{z} = \{z, H\}$ (via the Poisson-bracket) for some Hamiltonian $H = T(p) + V(q)$ with $z = (q, p)$, i.e. $D_T z = \{z, T\}$ and $D_V z = \{z, V\}$.

(a) Show that $D_T^2 z = D_V^2 z = 0$. (1 P.)

(b) Assume the usual classical kinetic term $T(p) = \frac{p^2}{2m}$. Show that $[D_V, [D_V, [D_V, D_T]]] = 0$. (2 P.)

H.2 Symplectic integrators **preserve the phase space volume**, and are **reversible** (if symmetric), mirroring the time-reversal symmetry of Hamiltonian systems. However, the energy is not exactly conserved by symplectic methods, but a modified energy (the so-called shadow Hamiltonian) is conserved, which leads to bounded energy errors over long simulations, meaning that the error often exhibits oscillatory behaviours. In contrast, Runge-Kutta integrators applied to Hamiltonian systems are non-symplectic methods and generally lead to a drift in the phase space volume over long iterations.

In this exercise, we want to appreciate the difference between the two types of methods. We consider a one-dimensional harmonic oscillator with $m = 1$ and $\omega = 1$, with Hamiltonian

$$H(q, p) = \frac{p^2}{2} + \frac{q^2}{2}$$

where q is the position and p is the momentum. The energy of the system for any initial condition set (q_0, p_0) is $E_0 = \frac{p_0^2}{2} + \frac{q_0^2}{2}$.

(a) Implement the forward Runge-Kutta (RK) method, of arbitrary order, to numerically integrate the equations of motion for this Hamiltonian $\dot{z} = \{z, H(z)\}$, namely

$$\dot{q} = f_q(q, p) = \frac{\partial T}{\partial p} = p$$

$$\dot{p} = f_p(q, p) = -\frac{\partial V}{\partial q} = -q$$

Given a time step Δt, the update rules of the RK of s order are

$$q_{n+1} = q_n + \Delta t \sum_{i=1}^{s} b_i k_{q,i}$$

$$p_{n+1} = p_n + \Delta t \sum_{i=1}^{s} b_i k_{p,i}$$

with

$$k_{q,i} = f_q\left(q_n + \Delta t \sum_{j=1}^{s} a_{ij} k_{q,j}, p_n + \Delta t \sum_{j=1}^{s} a_{ij} k_{p,j}\right)$$
$$k_{p,i} = f_p\left(q_n + \Delta t \sum_{j=1}^{s} a_{ij} k_{q,j}, p_n + \Delta t \sum_{j=1}^{s} a_{ij} k_{p,j}\right).$$

The coefficients a_{ij}, b_i, and c_i (where $c_i = \sum_{j=1}^{s} a_{ij}$) define the specific RK method. (2 P.)

(b) Implement a symplectic integration method for this Hamiltonian. The simplest (Euler) update rules are:

$$p_{n+1} = p_n - \Delta t \; q_n$$
$$q_{n+1} = q_n + \Delta t \; p_{n+1}.$$

(2 P.)

(c) Set the initial position $q_0 = 1.0$ and the initial momentum $p_0 = 0.0$. Select a small time step Δt. Integrate both methods for a total of N time steps, i.e. total time $T = N \times \Delta t$ that is sufficiently large to observe interesting behaviour. (2 P.)

(d) For both methods, calculate numerically the energy E_n at each time step n:

$$E_n = \frac{p_n^2}{2} + \frac{q_n^2}{2}.$$

(1 P.)

(e) Plot the energy E_n as function of time step n for both the forward RK and the symplectic Euler methods. Then, calculate the relative energy error at each n:

$$\epsilon_n = \frac{|E_n - E_0|}{E_0},$$

and plot it as a function of n for both methods. (2 P.)

(f) Describe your observations regarding the energy conservation of the two methods. Which method shows better energy conservation over the long term? (1 P.)

Adiabatic Search of the Ground State

H.3 Consider the one-dimensional transverse field Ising model (TFIM) with N spins, governed by the Hamiltonian:

$$H(h) = -J \sum_{i=1}^{N} \sigma_i^z \sigma_{i+1}^z - h \sum_{i=1}^{N} \sigma_i^x,$$

where σ_i^z and σ_i^x are the Pauli matrices acting on site i , $J > 0$ is the coupling constant, h is the transverse magnetic field.

In this exercise, you will study the adiabatic preparation of the ground state of $H(h_f)$ by starting from the ground state of the classical Ising model ($h = 0$) and slowly turning on the transverse field using a time-dependent Hamiltonian.

(a) Write down the ground state of the Hamiltonian $H(0)$, namely with $h = 0$. (1 P.)

(b) Define a time-dependent Hamiltonian $H(t)$ with $t \in [0, T]$ that interpolates linearly $H(0) = -J \sum_i \sigma_i^z \sigma_{i+1}^z$, and $H(T) = -J \sum_i \sigma_i^z \sigma_{i+1}^z - h_f \sum_i \sigma_i^x$, where $h_f > 0$ is the final field strength. Write the explicit form of $H(t)$. (1 P.)

(c) Numerically compute and plot the energy gap (difference between the first excited and ground state energies) of the model for $L = 4$ and $L = 6$ spins as a function of the transverse field strength h (ranging from 0 to $h_f = 2$, with a suitable number of steps), using ED. (2 P.)

(d) The *adiabatic theorem* states that if a quantum system is initialized in the ground state of $H(0)$ and the Hamiltonian changes sufficiently slowly, the system will remain in the instantaneous ground state of $H(t)$ at all times, up to a phase.

For $N = 4$ spins, numerically solve the time-dependent Schrödinger equation for $H(t)$, starting from the ground state of $H(0)$, slowly evolving the state up to time T. Use $J = 1$ and $h_f = 2$. (2 P.)

(e) Plot the exact energy of the instantaneous ground state of $H(t)$ as function of time t and compare it to the energy obtained at the same time t using numerical adiabatic evolution. (1 P.)

(f) Plot the overlap between the instantaneous ground state of $H(t)$ and the evolving quantum state $|\psi(t)\rangle$ as a function of time. (2 P.)

(g) How does the presence of the quantum phase transition at $h_c = J$ (in the thermodynamic limit) affect the adiabatic evolution? (1 P.)

Imaginary Time Evolution

H.4 In this exercise, you will explore how imaginary time evolution can be used to project a generic quantum state onto the ground state of $H(h)$

$$H(h) = -J \sum_{i=1}^{N} \sigma_i^z \sigma_{i+1}^z - h \sum_{i=1}^{N} \sigma_i^x,$$

(a) Write down the imaginary time Schrödinger equation for a state $|\psi(\tau)\rangle$ with $\tau \geq 0$. (1 P.)

(b) Show that, for large τ, the state $|\psi(\tau)\rangle$ approaches the ground state of $H(h)$ (up to normalization), assuming the initial state has non-zero overlap with the ground state. (2 P.)

(c) Explain why it is necessary to periodically renormalize the state during imaginary time evolution. (1 P.)

(d) For $N = 4$ spins, choose a random normalized initial state $|\psi(0)\rangle$. Numerically integrate the imaginary time Schrödinger equation up to a final time $\tau_{\max}$. (2 P.)

(e) In order to monitor the convergence to the ground state in the numerical simulation, at each step, compute the energy expectation value:

$$E(\tau) = \langle \psi(\tau) | H(h) | \psi(\tau) \rangle.$$

As τ increases, $E(\tau)$ should approach the true ground state energy, the convergence is indicated when $E(\tau)$ plateaus within desired precision. Plot $E(\tau)$ as a function of τ. (2 P.)

(f) Check that the final state matches the ground state obtained via direct diagonalization, e.g. by computing the overlap. (1 P.)

(g) Compare the efficiency of imaginary time evolution versus real-time adiabatic evolution for finding the ground state of $H(h)$. (1 P.)