

Quantum Systems

Stefano Chesi

Beijing Computational Science Research Center

ppt based on:

- Chapter 16 of '*An Introduction to Computer Simulation Methods : Applications to Physical Systems*', H. Gould and J. Tobochnik
- Lecture notes by Hai-Qing Lin (“Quantum Systems”)

Motivation

Quantum systems are **much more challenging** to simulate than classical systems

- ⊕ State of a 1D classical particle: $x(t), p(t)$
- ⊕ Quantum state (wavefunction): $\psi(x, t)$

The problem becomes quickly intractable with N

- ⊕ *Many-body* wavefunction: $\psi(x_1, x_2, x_3, \dots x_N, t)$

However, specialized techniques exists (e.g., QMC)

Topics

- ⊕ Review of quantum mechanical evolution
- ⊕ Time evolution of the wavefunction
- ⊕ Energy eigenstates, shooting method
- ⊕ Variational Quantum Monte Carlo
- ⊕ Diffusion Quantum Monte Carlo

Wavefunction (review)

In coordinate representation, the state is a **complex** function of x : $\Psi(x, t)$

- Spatial distribution (probability density):

$$P(x, t) = |\Psi(x, t)|^2 \quad \text{with} \quad \int dx |\Psi(x, t)|^2 = 1$$

- Expectation values of other observables:

$$\langle A \rangle = \int dx \Psi^*(x, t) A \Psi(x, t)$$

Example (momentum operator): $p = -i\partial/\partial x$

Schroedinger equation

$$i\hbar \frac{\partial \Psi(x, t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi(x, t)}{\partial x^2} + V(x, t)\Psi(x, t)$$

$H\Psi(x, t)$

Two possible strategies of solution:

- ⊕ Direct integration of time-dependence
- ⊕ Expansion in eigenstates of H

Numerical solution of SE

Proceed as usual, discretizing time and space

$$t_n = t_0 + n\Delta t$$

$$x_s = a + s\Delta x$$

Simplest integration scheme (free particle):

$$-i\hbar \frac{\Psi(x_s, t_{n+1}) - \Psi(x_s, t_n)}{\Delta t} = \\ -\frac{\hbar^2}{2m} \frac{\Psi(x_{s+1}, t_n) - 2\Psi(x_s, t_n) + \Psi(x_{s-1}, t_n)}{\Delta x^2}$$

Implicit scheme: $t_n \rightarrow t_{n+1}$ on right-hand side

Visscher's scheme

Consider $\Psi(x, t) = R(x, t) + iI(x, t)$

$$\frac{dR(x, t)}{dt} = HI(x, t)$$

$$\frac{dI(x, t)}{dt} = -HR(x, t)$$

Discretization (half-step method):

$$R(x, t + \Delta t) = R(x, t) + HI(x, t + \frac{1}{2}\Delta t)\Delta t$$

$$I(x, t + \frac{3}{2}\Delta t) = I(x, t + \frac{1}{2}\Delta t) - HR(x, t)\Delta t$$

Visscher's scheme

Important features:

- Explicit
- Stable
- Conserves probability

$$\frac{-2\hbar}{\Delta t} \leq V \leq \frac{2\hbar}{\Delta t} - \frac{2\hbar^2}{(m\Delta x)^2}$$

$$P(x, t) = R(x, t)^2 + I(x, t + \frac{1}{2}\Delta t)I(x, t - \frac{1}{2}\Delta t)$$

$$P(x, t + \frac{1}{2}\Delta t) = R(t + \Delta t)R(x, t) + I(x, t + \frac{1}{2}\Delta t)^2$$

Reference: P. B. Visscher, Computers in Physics **5**, 596 (1991)

Expansion with energy eigenstates

Time-independent Schroedinger equation:

$$\left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right) \phi(x) = E\phi(x)$$

Stationary states: $\Psi(x, t) = \phi(x) \text{Exp}[-iEt/\hbar]$

General state: $\Psi(x, t) = \sum_n c_n \phi_n(x) e^{-iE_n t/\hbar}$

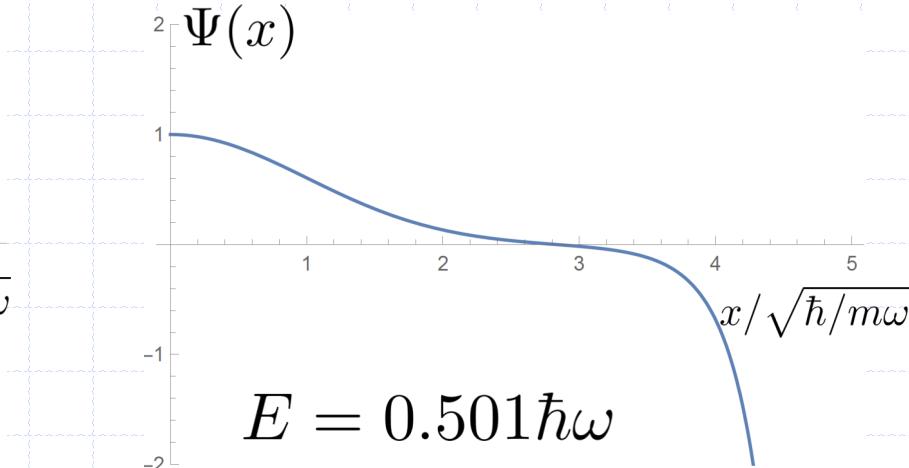
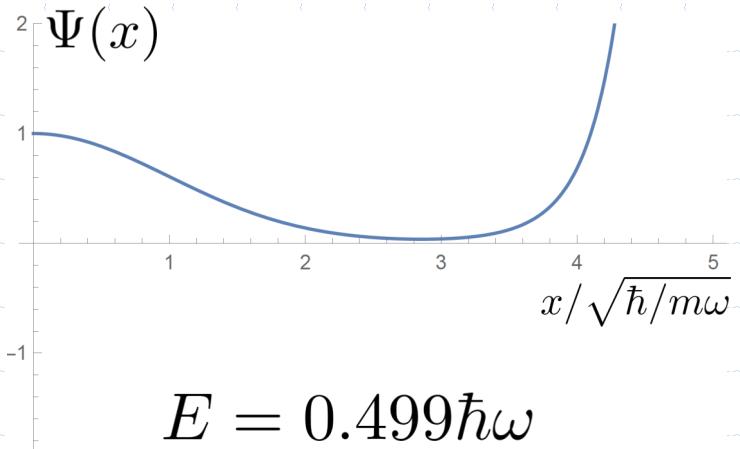
where $c_n = \int dx \phi_n^*(x) \Psi(x, 0)$

Shooting method

Solve the diff equation at generic E :

$$\left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right) \phi(x) = E\phi(x)$$

Example for harmonic oscillator:



Euler-Cromer algorithm

1. Divide $a < x < b$ into intervals of width Δx . Let $x_s = a + s\Delta x$, where s is an integer. Thus $\phi_s = \phi(x_s)$ and $\phi'_s = \phi'(x_s)$.
2. Specify the parity of $\phi(x)$. For even parity, choose $\phi(0) = 1$ and $\phi'(0) = 0$; For odd parity, choose $\phi(0) = 0$ and $\phi'(0) = 1$.
3. Guess a value for E (important, calls for intuition).

Euler-Cromer algorithm

4. Compute ϕ'_{s+1} and ϕ_{s+1} by using the algorithm:

$$\phi'_{s+1} = \phi'_s + \phi''_s \Delta x$$

$$\phi_{s+1} = \phi_s + \phi'_{s+1} \Delta x .$$

5. Iterate $\phi(x)$ with increasing x until it diverges.
6. Vary E and repeat steps (4) & (5). Find E_0 such that
- (i) when $E < E_0$, $\phi(x)$ diverges with decreasing E ;
 - (ii) when $E > E_0$, $\phi(x)$ diverges with increasing E .

Monte-Carlo methods

- ⊕ **Variational Quantum Monte Carlo (QMC)**

based on the variational principle

$$\langle H \rangle = E[\Psi] = \frac{\int dx \Psi^*(x) H \Psi(x)}{\int dx \Psi^*(x) \Psi(x)} \geq E_0$$

- ⊕ **Diffusion or path-integral QMC**

based on imaginary-time evolution

$$e^{-H\tau} |\Psi\rangle = \sum_n c_n e^{-E_n \tau} |\phi_n\rangle \simeq c_0 e^{-E_0 \tau} |\phi_0\rangle$$

Powerful methods to study ground-state $|\phi_0\rangle$

Variational Monte-Carlo

The choice of Ψ depends on your physics insights.

$E[\Psi]$ could have many parameters.

$$E[\Psi] = \frac{\int dx \Psi^2(x) E_L(x)}{\int dx \Psi^2(x)} \quad \text{where: } E_L = \frac{H\Psi(x)}{\Psi(x)} \quad (\text{local energy})$$

$$E[\Psi] = \lim_{n \rightarrow \infty} \sum_{i=1}^n E_L(x_i),$$

where n is the number of times that x is sampled from Ψ^2 .

NOTE: x is a multidimensional space

Metropolis algorithm!

Random walk QMC

Basic principle:

$$\Psi(x, \tau) = \sum_n c_n \phi_n(x) e^{-E_n \tau} \longrightarrow c_0 \phi_0(x) e^{-E_0 \tau}$$

Consider the SE in imaginary time

$$\frac{\partial \Psi(x, \tau)}{\partial \tau} = \frac{\hbar^2}{2m} \frac{\partial^2 \Psi(x, \tau)}{\partial x^2} - V(x) \Psi(x, \tau)$$

diffusion process
(random walk)

$$D = \hbar^2 / 2m$$

branching process

$$\Psi(\tau + \Delta\tau) \simeq e^{-V(x)\Delta\tau} \Psi(\tau)$$

Random walk QMC - remarks

- 1) It is $\Psi \Delta x$ and not $\Psi^2 \Delta x$ which corresponds to the probability distribution of random walkers.

Thus one requires that Ψ be nonnegative!

- 2) The population of walkers goes to **zero** ($E_0 > 0$) or **infinity** ($E_0 < 0$):

$$\Psi(x, \tau) = \sum_n c_n \phi_n(x) e^{-E_n \tau} \longrightarrow c_0 \phi_0(x) e^{-E_0 \tau}$$

Solution: Adjust the reference energy during the simulation, such that the population is approx. constant!

$$V_{ref} = \sum_i V_i / N_0 \simeq E_0$$

Random walk QMC - algorithm

1. Place N_0 walkers at the initial set of positions x_i .
2. Compute the reference energy $V_{ref} = \Sigma_i V_i / N_0$.
3. Randomly move a walker to the right or left by a fixed step length Δs , such that $(\Delta s)^2 = 2D\Delta\tau$. ($D = 1/2$ in units such that $\hbar = m = 1$.)
4. Compute $\Delta V = V(x) - V_{ref}$ and a random number r of $(0,1)$. If $\Delta V > 0$ and $r < \Delta V \Delta\tau$, remove the walker. If $\Delta V < 0$ and $r < -\Delta V \Delta\tau$, add another walker at x . Otherwise, just leave the walker at x .
Assume $\Delta\tau \ll 1$.

Random walk QMC - algorithm

5. Repeat steps 3 and 4 for each of the N_0 walkers and compute the mean potential energy and the actual number of random walkers. The new reference potential is given by

$$V_{ref} = \langle V \rangle - \frac{a}{N_0 \Delta \tau} (N - N_0) ,$$

where N is the new number of random walkers and $\langle V \rangle$ is their mean potential energy.

6. Repeat steps 3-5 until the estimates of the ground state energy $\langle V \rangle$ have reached a steady state value with only random fluctuations.

Alternative view of diffusion/branching

Green's function approach:

$$\Psi(x', \tau) = \int dx G(x', x, \tau) \Psi(x, 0)$$

At short times:

$$G(\Delta\tau) \simeq G_{branch} G_{diff} + O(\Delta\tau^2)$$

where:

$$G_{diff}(x', x, \Delta\tau) = (4\pi D \Delta\tau)^{-1/2} e^{-(x' - x)^2 / 4D\Delta\tau}$$

$$G_{branch} = e^{-\left(\frac{1}{2}[V(x) + V(x')] - V_{ref}\right)\Delta\tau}$$

Diffusion QMC - algorithm

1. Begin with a set of N_0 walkers. Positions of the walkers are continuous. Put more walkers in the region where the wave function is known to be large.
2. Choose one walker and displace it from x to x' . The new position is chosen from a Gaussian distribution with a variance $2D\Delta\tau$ and zero mean. This change corresponds to the diffusion process.
3. Weight the configuration x' by

$$w(x \rightarrow x', \Delta\tau) = e^{-\left(\frac{1}{2}[V(x)+V(x')]-V_{ref}\right)\Delta\tau}.$$

Diffusion QMC - algorithm

make an integer number of copies that is equal on the

average to the number w , e.g., $\text{INT}[w+\text{rand}(0,1)]$, could be 0

4. Repeats steps 2 and 3 for all members of the ensemble, thereby creating a new ensemble at a later time $\Delta\tau$.

One iteration of the ensemble is equivalent to

$$\Psi(x, \tau) = \int dx' G(x, x', \Delta\tau) \Psi(x, \tau - \Delta\tau)$$

5. The quantity of interest $\Psi(x', \tau)$ will be independent of the original ensemble $\Psi(x, 0)$ if a sufficient number of MC steps are taken. We must ensure that $N(\tau)$ is kept close to the desired number N_0 .

Importance sampling

A good approximation $\Psi_T(x)$ can facilitate QMC

Consider $f(x, \tau) = \Psi(x, \tau)\Psi_T(x, \tau)$

Modified SE in imaginary time:

$$\frac{\partial f}{\partial \tau} = D \frac{\partial^2 f}{\partial x^2} - D \frac{\partial [f F(x)]}{\partial x} - [E_L(x) - V_{ref}]f$$

where $F(x) = \frac{2}{\Psi_T} \frac{\partial \Psi_T}{\partial x}$

$$E_L(x) = \frac{H\Psi_T}{\Psi_T}$$

Introduces a **drift** of random walkers
(see textbook for details)

Summary

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