Nuclear Talent course: Computational Many-body Methods for Nuclear Physics

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Lecture slides with exercise for Tuesday 3 2012

Quantum Mechanics in Imaginary Time

- Time dependent Schrödinger Equation is still too hard to solve (all variances are infinite in standard integral formalism.)

$$H|\phi(t_r)\rangle = -\frac{\hbar}{i}\frac{\partial}{\partial t_r}|\phi(t_r)\rangle$$

- We can find low-lying energy eigenstates, $H|\psi_n\rangle = E_n|\psi_n$, with imaginary time equation

$$H|\psi(t)\rangle = -\frac{\partial}{\partial t}|\psi(t)\rangle$$

$t = it_r/\hbar$.

- Write $|\psi(0)\rangle = \sum_n c_n|\psi_n\rangle$,

$$\begin{aligned} |\psi(t)\rangle &= e^{-Ht}|\psi(0)\rangle = \sum_n c_n e^{-E_n t}|\psi_n\rangle \\ &= e^{-E_0 t}\left[c_0|\psi_0\rangle + \sum_{n>0} c_n e^{-(E_n-E_0)t}|\psi_n\rangle\right] \end{aligned}$$

Trotter

- We do not know $\exp[-(H - E_T)t]$.
- Use Trotter Formula: For $\Delta t \to 0$

$$
\begin{aligned}
e^{(A+B)\Delta t} &= e^{A\Delta t} e^{B\Delta t} + O\left([A, B]\Delta t^2\right) \\
e^{(A+B)\Delta t} &= e^{A\Delta t/2} e^{B\Delta t} e^{A\Delta t/2} + O\left(\Delta t^3\right)
\end{aligned}
$$

- $\exp[-(H - E_T)t] = \{\exp[-(H - E_t)\Delta t]\}^M$ with $t = \Delta t M$.
- $\exp\left[-(H - E_T)\Delta t\right] \simeq \exp\left[-\frac{P^2}{2M}\Delta t\right] \exp\left[-V\Delta t\right]$
- $\exp\left[-(H - E_T)\Delta t\right] \simeq \exp\left[-\frac{1}{2}V\Delta t\right] \exp\left[-\frac{P^2}{2M}\Delta t\right] \exp\left[-\frac{1}{2}V\Delta t\right]$

Reversible breakups

- Breakups that are reversible (unitary in real time) have only even order errors.

$$e^{-Ht} \simeq \left[U\left(\frac{t}{N}\right)\right]^N$$

if invariant under $N \to -N$ then errors are even in N, $\to$ even in $\Delta t = t/N$.

- Require:

$$\begin{aligned}\left[U\left(\frac{t}{N}\right)\right]^N &= \left[U\left(-\frac{t}{N}\right)\right]^{-N} \\ U(\Delta t)U(-\Delta t) &= 1\end{aligned}$$

- Useful for Richardson extrapolation.

Imaginary time Schrödinger equation

Imaginary time Schrödinger equation is a diffusion equation with absorption/creation

$$
\begin{aligned}
-D\nabla^2\rho &= -\frac{\partial}{\partial t}\rho \quad \text{Diffusion} \\
\alpha\rho &= -\frac{\partial}{\partial t}\rho \quad \text{absorption} \\
\left[-\frac{\hbar^2}{2m}\nabla_R^2 + v(R)\right]\psi(R,t) &= -\frac{\partial}{\partial t}\psi(R,t)
\end{aligned}
$$

We can simulate this by a diffusion and absorption of a "gas" of "particles" in many dimensions.

The classical diffusion equation is $D\nabla^2\rho(\mathbf{r},t) = \partial_t\rho(\mathbf{r},t)$, D is the diffusion constant. A point source $\rho_0(r,0) = \delta^3(\mathbf{r})$ evolves to

$$
\rho_0(r,t) = \frac{1}{(4\pi Dt)^{3/2}} \exp\left(-\frac{r^2}{4Dt}\right)
$$

Exercise

1-d Harmonic oscillator algorithm

1. Take natural units $\hbar = m = \omega = 1$.

$$H = -\frac{1}{2}\frac{d^2}{dx^2} + \frac{1}{2}x^2$$

   We know the ground state energy is $E_0 = \frac{1}{2}$.

2. We should sample initial walker positions from a variational solution, but any initial sample will work. Distribute positions x_i within roughly ± 2 of the origin for $N_w \simeq 100$ or so walkers each with weight $w_i = 1$.

$$\psi(x,0) = \sum_{1}^{N_w} \delta(x - x_i)$$

Exercise continued

1-d Harmonic oscillator algorithm

3. Write the propagator

$$G(x',x) = \langle x'|e^{-(H-E_T)\Delta t}|x\rangle = \sqrt{\frac{1}{2\pi\Delta t}}e^{-\frac{1}{4}x'^2\Delta t}e^{-\frac{(x'-x)^2}{2\Delta t}}e^{-\frac{1}{4}x^2\Delta t}e^{E_T\Delta t}$$

   Take E_T to be a guess for E_0 (typically from variational calculation) A guess could be $E_T = 1$.

4. The integral $\psi(x', t+\Delta t) = \int dx G(x',x)\psi(x,t)$, gives $\psi(x', t+\Delta t) = \sum_i^{N_w} G(x', x_i)$. Sample from a gaussian of standard deviation 1, for each walker. Call this ζ_i. We then have $x_i' = x_i + \sqrt{\Delta t}\zeta_i$ and

$$\begin{aligned}
\psi(x', t+\Delta t) &= \sum_i^{N_w} w_i'\delta(x - x_i') \\
w_i' &= e^{-\frac{1}{4}(x_i'^2 + x_i^2)\Delta t + E_T\Delta t}
\end{aligned}$$

Exercise continued

1-d Harmonic oscillator algorithm

5. Crude (and biased) population control. Adjust E_T so that $\sum_i w_i' = N_w$, i.e.
$$e^{E_T \Delta t} = \frac{N_w}{\sum_i^{N_w} e^{-\frac{1}{4}(x_i'^2 + x_i^2)\Delta t}}$$
and calculate new w_i'. Less biased would calculate required E_T over many steps and change E_T slowly. Check bias by changing N_w.
6. Crudely change w_i' to integers so that the expected probability is the original weight $n_i = \mathrm{int}(w_i' + \xi_i)$, where ξ_i is a uniform random number between 0 and 1. Take n_i copies of walker i. If $n_i = 0$ drop from simulation. [$\mathrm{int}\, x$ is the largest integer contained in x, e.g. $\mathrm{int}\, 2.8 = 2$, $\mathrm{int}\, 0.3 = 0$]
7. Repeat steps 4 to 6 until it converges. You should get E_T fluctuating around $\frac{1}{2}$.

Importance sampling

We want to calculate

$$
\begin{aligned}
E(t) &= \frac{\langle \psi_T | e^{-\frac{1}{2}(H-E_T)t} H e^{-\frac{1}{2}(H-E_T)t} | \psi_T \rangle}{\langle \psi_T | e^{-\frac{1}{2}(H-E_T)t} e^{-\frac{1}{2}(H-E_T)t} | \psi_T \rangle} = \frac{\langle \psi_T | H e^{-(H-E_T)t} | \psi_T \rangle}{\langle \psi_T | e^{-(H-E_T)t} | \psi_T \rangle} \\
&= \frac{\int dR \langle \psi_T | H | R \rangle \langle R | e^{-(H-E_T)t} | \psi_T \rangle}{\int dR \langle \psi_T | R \rangle \langle R | e^{-(H-E_T)t} | \psi_T \rangle} = \int dR \; E_L(R) P(R,t)
\end{aligned}
$$

where

$$
\begin{aligned}
E_L(R) &= \frac{\langle \psi_T | H | R \rangle}{\langle \psi_T | R \rangle} \\
P(R,t) &= \frac{\langle \psi_T | R \rangle \langle R | e^{-Ht} | \psi_T \rangle}{\int dR \langle \psi_T | R \rangle \langle R | e^{-Ht} | \psi_T \rangle}
\end{aligned}
$$

Small error bars $\Rightarrow$ $E_L(R)$ low variance $\Rightarrow$ $|\psi_T\rangle \sim |\Psi_0\rangle$.
Sample particle positions from a distribution proportional to $\langle \Psi_T | R \rangle \langle R | \psi(t) \rangle$.

Importance sampling continued

- There are many equivalent ways to introduce importance sampling.
- We can rewrite the propagator equation as

$$\langle \Psi_T | R \rangle \langle R | \Psi(t+\Delta t) \rangle$$
$$= \int dR' \frac{\langle \Psi_T | R \rangle}{\langle \Psi_T | R' \rangle} \langle R | e^{-H\Delta T} | R' \rangle \left[\langle \Psi_T | R' \rangle \langle R' | \psi(t) \rangle \right]$$

  and sample $\frac{\langle \Psi_T | R \rangle}{\langle \Psi_T | R' \rangle} \langle R | e^{-H\Delta T} | R' \rangle$ properly normalized.
- We can rewrite the imaginary-time Schrödinger equation.

$$-\partial_t \Psi_T^*(R) \Psi(R,t) = \Psi_T^*(R) \left[-\frac{\hbar^2}{2m} \nabla_R^2 + V(R) \right] \Psi(R,t)$$
$$= \left\{ -\frac{\hbar^2}{2m} \nabla_R \cdot \left[\nabla_R - 2 \frac{\nabla_R \Psi_T(R)}{\Psi_T(R)} \right] + E_L(R) \right\} \Psi_T(R) \Psi(R,t)$$

  as a Fokker-Planck equation with an additional branching term.

Fokker-Planck generalization

Using the Fokker-Planck method, we see that we simply need to sample from the solution of the Fokker-Planck equation without the $E_L(R)$ term, and then include branching as before using $\exp(-(E_L - E_T)\Delta t)$.

Exercise

- Add the branching step to your variational Monte Carlo calculation to include importance sampling.
- Alternatively, add importance sampling to your harmonic oscillator calculation by adding a drift term to the gaussian sampling, and using $E_L(R)$ instead of $V(R)$ for the branching.

Fermion sign problem

- Quantum Monte Carlo works great for Bosons.
- If the positions of two fermions gets exchanged during the diffusion, the wave function must change sign – Fermion wave functions must change sign.
- The probability of diffusing to an opposite signed region of the wave function becomes 0.5 as time goes on.
- Signal is the average – the signal to statistical noise dies exponentially.

Solutions to fermion sign problem

- Arrange for up spin fermions and down spin fermions to propagate identically. Occurs only in a few special cases. Typically requires a lattice model, attractive interactions, equal numbers of up and down fermions.
- Fixed node approximation – don't allow diffusion into opposite signed region of a trial wave function. Upper bound!
- Transient estimation – ignore problem and stop calculating when errors get too large.

Possible Metropolis step

More Abstract – More General

Ingredients

- Walkers $|W\rangle$ which form a complete or overcomplete basis for our problem.
- A propagator that can be written in terms of operators whose eigenstates are $|W\rangle$, or operators that translate the walker basis:

$$
\begin{aligned}
D|W\rangle &= F(W)|W\rangle \\
T|W\rangle &= G(W)|W'\rangle .
\end{aligned}
$$

Spin 0 bosons DMC

Rewriting standard DMC

- Walkers are positions eigenstates $|R\rangle$ for all the particles.
- The Trotter breakup of the propagator is

$$e^{-H\Delta t} \simeq e^{-\sum_j \frac{p_j^2}{2m}\Delta t} e^{-V\Delta t}$$

- The walkers, $|R\rangle$, are eigenstates of V with eigenvalue $V(R)$.
- The kinetic energy is not diagonal, nor in terms of a translation operator. But

$$e^{-\sum_j \frac{p_j^2}{2m}\Delta t} = \int dX (2\pi)^{-3N/2} e^{-\frac{X^2}{2}} e^{-iP\cdot X\sqrt{\frac{\Delta t}{m}}}$$

Kinetic Energy

- $P \cdot X = \sum_j \mathbf{p}_j \cdot \mathbf{x}_j$
- The space translation operator is

$$e^{-i\mathbf{P}\cdot\mathbf{A}}|R\rangle = |R+A\rangle\,.$$

- The propagator operating on a walker is now

$$\begin{aligned} e^{-H\Delta t}|R\rangle &= \int dX (2\pi)^{-3N/2} e^{-\frac{X^2}{2}} e^{-V(R)\Delta t} e^{-iP\cdot X\sqrt{\frac{\Delta t}{m}}}|R\rangle \\ &= e^{-V(R)\Delta t}\int dX \underbrace{(2\pi)^{-3N/2} e^{-\frac{X^2}{2}}}_{\text{Sample this}} \left| R + X\sqrt{\frac{\Delta t}{m}} \right\rangle \end{aligned}$$

- Sampling X values from gaussians of unit variance reproduces DMC without importance sampling.

Hubbard Stratonovich Transformation

Many Hamiltonian operators are sums of squares of generators of translations i.e. state change operators in some basis

- Nonrelativistic kinetic energy is proportional to square of the momentum – the generator of space translations.
- Shell model Hamiltonian for two-body potential can be written as sum of squares of one-body operators.
- Spin-isospin operators in nucleon-nucleon two-body potential can be written in terms of squares of one-body spin-isospin operators.
- Spin-orbit in nucleon-nucleon potential can be written in terms of squares of operators containing the momentum and spin-isospin operators.

Hubbard Stratonovich continued

Often we want linear operators in exponent. For gaussians:

$$e^{-\frac{O^2}{2}} = \int_{-\infty}^{\infty} dx e^{-\frac{x^2}{2}} \sqrt{2\pi} e^{-iOx}$$

An almost obvious generalization for any function $F(O)$ of the operator O

$$F(O) = \int_{-\infty}^{\infty} dx \tilde{F}(x) e^{-iOx}$$

$$\tilde{F}(x) = \int \frac{dk}{2\pi} e^{ikx} F(k)$$

If $\tilde{F}(x)$ is positive definite, we can identify it as proportional to a probability distribution and sample from $\tilde{F}(x)$ properly normalized. For example, the lowest order kinetic energy from the Fouldy-Wouthesen transformation of the Dirac equation is $\sqrt{p^2+m^2}$ so that

$$e^{-\sqrt{p^2+m^2}\Delta t} = \int d^3x \frac{m^2}{2\pi^2} \frac{\Delta t}{x^2+\Delta t^2} K_2[m\sqrt{x^2+\Delta t^2}] e^{-ipx} .$$