Diffusion Monte Carlo

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Diffusion Monte Carlo

The variational wave function can be very accurate, but things can be improved.

The time-dependent Schroedinger equation is ($\hbar = 1$)

$$-i\frac{\partial}{\partial t}\Psi(R,t) = H\,\Psi(R,t)$$

and its solution is given by:

$$\Psi(R,t) = e^{-i\,H\,(t-t_0)}\Psi(R,t_0)$$

we will call $\tau = it$ **imaginary time**.

Projection in imaginary time:

Let's assume that the wave function can be expanded over a set of eigenstates of the Hamiltonian H:

$$\psi = \sum_n \phi_n$$

Then let's apply the evolution operator $\exp[-(H - E_T)\tau]$:

$$\begin{aligned} e^{-(H-E_T)\tau}\psi &= e^{-(H-E_T)\tau}\sum_n \phi_n \\ &= \sum_n e^{-(E_n-E_T)\tau}\phi_n \rightarrow c_0\phi_0 \end{aligned}$$

In this way, in the limit of $\tau \rightarrow \infty$ we can extract the ground-state of H.

Note: E_T is a constant to guarantee a finite normalization.

Diffusion Monte Carlo

Let's represent the wave function as an ensemble of points, i.e. *walkers* in the volume:

$$\langle R|\Psi_T\rangle = \sum_n c_n \delta(R - R_n)$$

then:

$$\langle R'|\Psi_T(\tau)\rangle = \int dR\, G(R, R', \tau)\langle R|\Psi_T(0)\rangle$$

where $G(R, R', \tau)$ is the propagator of the Hamiltonian, and we have used the identity

$$1 = \int dR\, |R\rangle\langle R|$$

Diffusion Monte Carlo

Let's define the propagator in coordinates as the matrix element between two points in the volume:

$$G(R, R', \tau) = \langle R | e^{-(H-E_T)\tau} | R' \rangle$$

The expression above is very difficult to calculate. What easy instead is:

$$G(R, R', t) \approx \prod_n^N G(R_n, R_{n-1}, \delta\tau) \approx \left[\langle R | e^{-T\delta\tau} e^{-V\delta\tau} e^{E_T\delta\tau} | R' \rangle \right]^n$$

where $\delta\tau = \tau/N$, and $\langle R | e^{-T\delta\tau} e^{-V\delta\tau} | R' \rangle$ is easy to sample.

Then we need to iterate the integral in previous slide many times to reach the limit $\tau \to \infty$.

Diffusion Monte Carlo

The kinetic energy is sampled as a diffusion of particles (in 3D):

$$\langle R'|e^{-\frac{\hbar^2}{2m}\nabla^2\delta\tau}|R\rangle = \left(\frac{m}{2\pi\hbar^2\delta\tau}\right)^{3A/2} e^{-m(R-R')^2/2\hbar^2\delta\tau}$$
$$= G_0(R, R', \delta\tau)$$

Note: G_0 is normalized!

The (scalar, local) potential and E_T give the weight of the configuration:

$$\langle R'|e^{-V\delta\tau}e^{E_T\delta\tau}|R\rangle = w\delta_{R,R'}$$

Note: the weight w is basically the normalization of $\exp[-V(R)\delta\tau]$, as the propagator is dependent to the "arrival" (or "starting") point in the diffusion:

$$\int dR\, G(R, R', \delta\tau) = e^{-V(R')\delta\tau}$$

Diffusion Monte Carlo

In summary, the propagation in imaginary time is carried out as

$$
\begin{aligned}
\Psi_T(t) &= \int G(R_n, R_{n-1}, \delta\tau) G(R_{n-1}, R_{n-2}, \delta\tau) \ldots G(R_1, R, \delta\tau) \Psi_T(0) \\
&\times dR_n \, dR_{n-1} \ldots dR_1 \\
&= \int \langle R_n | e^{-\nabla^2 \delta\tau} | R'_{n-1} \rangle \langle R'_{n-1} | e^{-V\delta\tau} | R_{n-1} \rangle \\
&\times \langle R_{n-1} | e^{-\nabla^2 \delta\tau} | R'_{n-2} \rangle \langle R'_{n-2} | e^{-V\delta\tau} | R_{n-2} \rangle \\
&\times \ldots \\
&\times \langle R_2 | e^{-\nabla^2 \delta\tau} | R'_1 \rangle \langle R'_1 | e^{-V\delta\tau} | R_1 \rangle \Psi_T(0) \, dR \\
&= \int e^{-(R_n - R_{n-1})^2 / 2\delta\tau} w_{n-1} e^{-(R_{n-1} - R_{n-2})^2 / 2\delta\tau} w_{n-2} \ldots \\
&\times e^{-(R_2 - R_1)^2 / 2\delta\tau} w_1 \Psi_T(0) \, dR
\end{aligned}
$$

where $w_i = \exp[-(V(R_i) - E_T)\delta\tau]$.

Diffusion Monte Carlo

Remember that the wave function is represented as a collection of walkers.

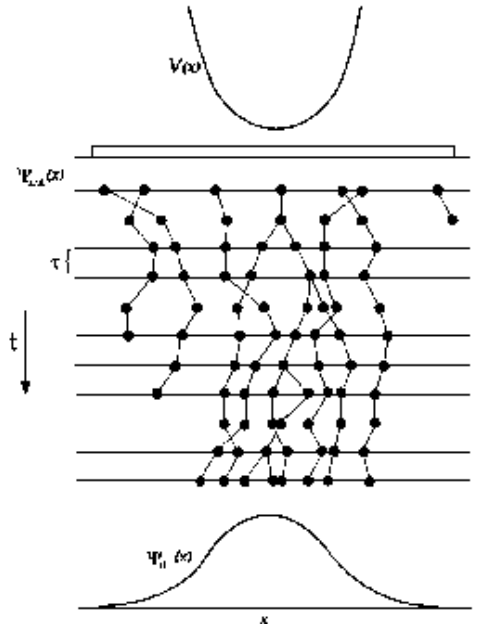
In the previous expression, the product of weights can become very large (or very small) for some of them. For example, consider the case of an infinite potential like repulsive Coulomb. If two particles are sampled to be close, the weight becomes zero, and then that walker will always contribute zero to the observables.

Diffusion Monte Carlo

One possible solution, **the branching** technique: take the weight of a walker and make a number of copies of it according to:

$$\# = int[w_i + \xi]$$

where ξ is a (uniform) random number between 0 and 1.



Importance sampling

The sampling of $G(R, R', \delta\tau)$ can be very noisy. Assume that we know a wave function Ψ_G that describes reasonably the system (i.e. in most of the cases the variational wave function). Then, it is very efficient to "project" our sampling over the "good guess":

$$\begin{aligned}
\langle \Psi_G | R' \rangle \langle R' | \Psi_T(\tau) \rangle &= \int dR\, G(R, R', \tau) \langle \Psi_G | R' \rangle \langle R | \Psi_T(0) \rangle \\
&= \int dR\, G(R, R', \tau) \frac{\langle \Psi_G | R' \rangle}{\langle \Psi_G | R \rangle} \langle \Psi_G | R \rangle \langle R | \Psi_T(0) \rangle \\
&= f(R', \tau)
\end{aligned}$$

In this way we are sampling a different distribution $f(R', \tau)$ whose variance is much improved from before!

Importance sampling

Let's see how to sample the quantity $G(R, R', \tau)\frac{\langle R'|\Psi_G\rangle}{\langle R|\Psi_G\rangle}$ (notation $\Psi_G(R) = \langle R|\Psi_G\rangle$).

The first thing to note is that the normalization of the modified propagator is now dependent to the "arrival" point in the diffusion.

Before:

$$N(R') = \int dR\, G(R, R', \delta\tau) = e^{-[V(R')-E_T]\delta\tau}$$

Now:

$$N(R') = \int dR\, G(R, R', \delta\tau)\frac{\Psi_G(R')}{\Psi_G(R)}$$

Importance sampling

In the limit of small $\delta\tau$ (small $|R - R'|$) we can expand

$$\frac{\Psi_G^*(R)}{\Psi_G^*(R)}\frac{\Psi_G(R')}{\Psi_G(R)} \approx 1 + \frac{\Psi_G^*(R)}{\Psi_G^*(R)}\frac{1}{\Psi_G(R)}\frac{\partial}{\partial x_i}\Psi_G(R)\,(x_i - x_i') + \frac{1}{2}\frac{\Psi_G^*(R)}{\Psi_G^*(R)}\Psi_G(R)\frac{\partial^2}{\partial x_i \partial x_j}\Psi_G(R)\,(x_i - x_i')(x_j - x_j') + \ldots$$

And we can prove that

$$N(R') = e^{-[\frac{\Psi_G^*(R) H \Psi_G(R')}{\Psi_G^*(R)\Psi_G(R')} - E_T]\delta\tau}$$

At the same time, the modified propagator can be sampled as a shifted Gaussian

$$\exp\left[\frac{-m(R-R')^2}{2\hbar^2\delta\tau}\right] \longrightarrow \exp\left[\frac{-m\left(R - R' + \frac{\Psi_G^*(R)\nabla\Psi_G(R)}{\Psi_G^*(R)\Psi_G(R)}\right)^2}{2\hbar^2\delta\tau}\right]$$

Note: there are other ways to sample the modified propagator.

Calculation of observables

Observables in DMC are calculated:

$$\langle O \rangle = \frac{\sum_i^M \omega_i \frac{\langle \Psi_T | W_i \rangle \langle W_i | \hat{O} | \Psi_T \rangle}{\langle \Psi_G | W_i \rangle \langle W_i | \Psi_T \rangle}}{\sum_i^M \omega_i \frac{\langle \Psi_T | W_i \rangle \langle W_i | \Psi_T \rangle}{\langle \Psi_G | W_i \rangle \langle W_i | \Psi_T \rangle}}$$

But now the weights ω_i contain "information" on the evolution in imaginary time!

Diffusion Monte Carlo

The DMC algorithm can be summarized in the following steps:

1. Generate a set of N walkers randomly or distributed with VMC
2. Loop over the N walkers, and for each i-th walker:
3. Make a step: $R_i' = R_i + \frac{\hbar^2 \delta\tau}{m} \frac{\Psi_T^*(R)\nabla\Psi_G(R)}{\Psi_T(R)\Psi_G(R)} + \xi\sqrt{\hbar^2\delta\tau/m}$
4. Calculate the weight: $w_i = \exp\left[-\left(\frac{\Psi_T(R)H\Psi_G(R')}{\Psi_T(R)\Psi_G(R')} - E_T\right)\delta\tau\right]$
5. Do branching
6. Increase the total imaginary-time by a unit of $\delta\tau$
7. Iterate with 2) until the equilibration is reached, then reset estimators and iterate until the error is small enough

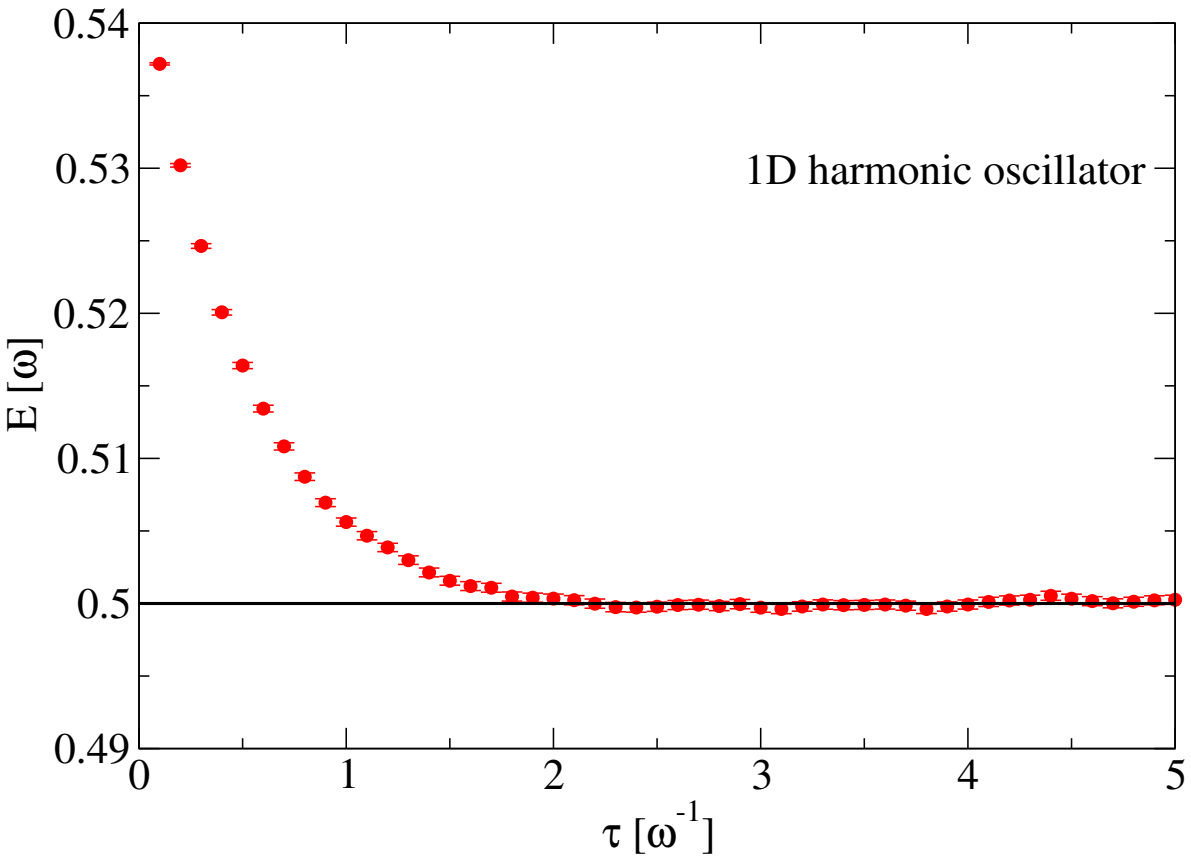
DMC: the first piece of code

Note: here we assume that $\Psi_G = \Psi_T$!

```
...
do j=1,nstep
  nw=0
  do n=1,nwalk
    xtest=xold(n)-sigma**2*alpha*xold(n)+sigma*rgauss(irn)
    eloc=-0.5_r8*((alpha*xtest)**2-alpha)+0.5_r8*omega**2*xtest**2
    weight=exp(-dt*(eloc-etrial))
    call ran(csi,irn)
    iwt=weight+csi
    do k=1,iwt
      nw=nw+1
      xnew(nw)=xtest
    enddo
    tau=tau+dt
  enddo
enddo
...
```

Diffusion Monte Carlo

An example: 1D harmonic oscillator, projection in imaginary time.
Energy as a function of the imaginary time τ:



Ground-state resolved!

Growth energy

In DMC a very nice "diagnostic tool" is the *growth energy*. It can be calculated by measuring the weights of the walkers.

If we had the exact wave function and E_T the exact energy, then the weight of each walker would be 1 independently to the configuration (i.e. $H\Psi/\Psi = E_T$). Then, by averaging over weights, we can define:

$$\omega_i = \exp\left[-(E_G^i - E_T)\delta\tau\right]$$

and we get:

$$\langle E_G \rangle = E_T - \frac{1}{\delta\tau} \log\left(\langle\omega\rangle\right)$$

Note: E_G is very similar to the local energy if $\delta\tau$ is small enough!

Exercise: test it.

Mixed estimates

Note that in DMC we calculate "mixed estimates", i.e.:

$$\langle O \rangle_{\rm mix} = \langle \Psi_T | O | \Phi_0 \rangle$$

where Ψ_T is the variational wave function, and Φ_0 is the DMC (ground state) one. By assuming that

$$|\Psi_T\rangle \simeq |\Phi_0\rangle + \lambda |\delta\Psi\rangle$$

it is easy to show that

$$\langle O \rangle = \langle \Phi_0 | O | \Phi_0 \rangle \simeq 2\langle O \rangle_{\rm mix} - \langle O \rangle_{\rm vmc}$$

where $\langle O \rangle_{\rm vmc} = \langle \Psi_T | O | \Psi_T \rangle$.

Exercise: prove that.

Note: the only exceptions where $\langle O \rangle_{\rm mix}$ is truly the ground state one is for those operators for which $[H, O] = 0$. Can you guess why?

Diffusion Monte Carlo

DMC is a tool to calculate the energy of a many-body system for a given wave function by projecting it in imaginary time.

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... for now :-)