Diffusion to sample more efficiently (reduce rejection rate)

recall FP equation 1d phase space

$$\frac{\partial \rho}{\partial t} = \frac{1}{2}\left[\underbrace{\frac{\partial^2}{\partial x^2}\rho(x,t)}_{\text{diffusion}} - \underbrace{\frac{\partial}{\partial x}\left(F(x)\rho(x,t)\right)}_{\text{drift}}\right]$$

To get the dist ρ_0 we want $F(x) = \frac{1}{\rho_0(x)}\frac{d}{dx}\rho_0(x)$

substitute to find $\frac{d\rho}{dt} = \frac{1}{2} \cdot 0$

Now our walkers become diffusive particles, and have this drift as well as random increments.
$\Rightarrow$ no rejection necessary

Higher accuracy using Green's functions.

consider random walk

This approximates diffusion, ~~discrete time~~ or ⊓ dist, $p_2(x) = \int dy\, \mathrm{block}(y)\, \mathrm{block}(x-y)$

better jump with gaussian dist increments. $\propto \exp\left(-c\frac{x^2}{\Delta t}\right)$

continuous, diff eq $\frac{\partial}{\partial t} = \frac{d^2}{dx^2}\rho$ solution $\rho \propto \exp\left(-c\frac{x^2}{t}\right)$ initial with $\rho(x,0) = \delta(x-x_0)$

solution starting from $\delta(x-x_0)$ is called Green's function, also for ~~that equation~~,

$$G(x, \underbrace{x_0}_{\text{initial}}, t)$$

any solution for initial $\rho(x,0)$

is $\rho(x,t) = \int dy\, \rho(y,0)\, G(x,y,t)$

so, if you do twice, you are still exact.

$$\int dy \exp\left(-c\frac{y^2}{\Delta t}\right)\exp\left(-c\frac{(x-y)^2}{\Delta t}\right)$$

$$= \propto \exp\left(-c\frac{x^2}{2\Delta t}\right)$$

Diffusion MC

No need for trial function. Find GS in general.

SE: $-i\hbar \frac{\partial}{\partial t} \psi = -\frac{1}{2}\frac{\partial^2}{\partial x^2}\psi + V\psi = \mathcal{H}\psi$

time evolution of an eigenfunction ϕ_i

$\exp(-i \cdot E_i t/\hbar)\, \phi_i$

<u>imaginary time</u>: $t \to it$

now we get $\exp(-E_i t/\hbar)\, \phi_i$

the bigger E_i, the faster decay.

$\Rightarrow$ will get us ground state
(and excited states one by one)

im time SE

$-\frac{\partial}{\partial t}\rho = + \quad = -\frac{1}{2}\frac{\partial^2}{\partial x^2}\underset{\psi}{\rho} + V\underset{\psi}{\rho} = E\underset{\psi}{\rho}$ diffusion-ish! 2x12x45 min im time SE

$$\underbrace{-\frac{\partial}{\partial t}\psi = -\frac{1}{2}\frac{\partial^2}{\partial x^2}\psi}_{\text{diffusion eq}} + V\psi = E\psi$$

$$\rho = \psi \exp(+E_T t)$$

$$\frac{\partial}{\partial t}\rho = \left(\frac{\partial}{\partial t}\psi\right)\exp(-E_T t) + \psi E_T \exp(\ldots)$$

$$= \left[\frac{1}{2}\frac{\partial}{\partial x^2}\psi + V\psi\right]\exp(\ldots) - \psi E_T \exp(\ldots)$$

$$\underbrace{\frac{\partial}{\partial t}\rho = \frac{1}{2}\frac{\partial}{\partial x^2}\rho}_{①} + \underbrace{(V - E_T)\rho}_{②}$$

again: randomly placed random walkers

step ① Do diffusion step with proper Green's function $\exp(-\overset{?}{2}\Delta x^2/\Delta t)$

step ② give weight to each walker $\exp\{-\Delta\tau[V(x') - E_T]\} = q$

$\Rightarrow$ correct dist

problem: too much work for irrelevant regions of space

<u>importance sampling trick</u>

replace step ② killing & creating walkers

if $q < 1$ walker survives with prob q, otherwise dies

if $q > 1$ create new walkers at rate $(q-1)$

$\lfloor q \rfloor$ or $\lfloor q-1 \rfloor$ with correct prob.

$\Rightarrow$ correct dist

population might explode / shrink

E_T should control this.

③ Adjust E_T so that population is stable $\Rightarrow$ E_T is gs. energy!

still problem if $V(x)$ diverges somewhere

<u>more importance sampling:</u> Guide function $\psi_T(x)$ that is similar to solution.

$$\rho(x,t) = \psi(R,t)\,\psi_T(R)\,\exp(E_T t)$$

$$\frac{\partial}{\partial t}\rho = \left(\frac{\partial}{\partial t}\psi\right)\psi_T \exp(\,) - \psi\psi_T E_T \exp(\cdot\cdot)$$

$$= \left[\frac{1}{2}\frac{\partial}{\partial x^2}\psi + V\psi\right]\psi_T \exp - E_T\rho$$

$$= \frac{1}{2}\frac{\partial}{\partial x}\left[\frac{\partial}{\partial x} - F\right]\rho - (E_L - E_T)\rho$$

with $F = 2\left(\frac{\partial}{\partial x}\psi_T\right)/\psi_T$ $\quad E_L(x) = \dfrac{-\frac{\partial^2}{\partial x^2}\psi_T/2 + V\psi_T}{\psi_T}$

$\Rightarrow$ same sort of construction.

- useful ψ_T can be gotten from cusp conditions

So far: assumed that $\psi(x)$ always positive.

- ok for bosonic ground state, not for fermions (electrons)

$\Rightarrow$ Thyssen describes some methods for dealing with changes of sign.

Path integral QMC

$$Z = \mathrm{Tr}(\exp(-\beta H)) = \int dR\, \langle R|\exp(-\beta H)|R\rangle$$

$$= \int dR_0\, dR_1 \; \cdots \; R_{M-1}$$

split up in little bits $\Delta\beta$ (small) with β playing role of time

$$\langle R_0|\exp(-\Delta\beta H)|R_1\rangle\langle R_1| \cdots \exp(-\Delta\beta H)|R_0\rangle$$

$$= \frac{1}{(2\pi\Delta\beta)^{3NM/2}} \int dR_0 \cdots dR_{M-1}$$

$$\exp\left\{-\Delta\beta \sum_{m=0}^{M-1}\left[\frac{1}{2}\left(\frac{R_{m+1}-R_m}{\Delta\beta}\right)^2 + V(R_m)\right]\right\}$$

$R_0\, R_1 \ldots R \ldots$ is a path, $\beta \rightarrow$ time

also, can be interpreted as potential

$\Rightarrow$ $N\cdot M$ particles, classical partition function

$\Rightarrow$ use MC to calculate.

Moral of QMC: rewrite SE so that it becomes equivalent to some classical problem and solve that with MC