Quantum Monte Carlo methods

1. Variational Quantum Monte Carlo method.

Let us consider a system in the quantum regime :

- System of n particles $\left(R = \left\{ \vec{r}_1, \ldots, \vec{r}_n \right\} \right)$ in n_d dimensions

- Described by Hamiltonian :

$$H = -\frac{\hbar^2}{2\,m} \sum_{i}^{n} \nabla_i{}^2 + \sum_{i<j}^{n} V[r_{ij}]$$

- The ground state behaviour is described by the ground state wave function $\psi_0[R]$
- $\psi_0[R]$ is determined by the Schrödinger equation :

$$H\,\psi_0[R] = E_0\,\psi_0[R]$$

- for atoms, interaction potential has a strongly repulsive short distance behaviour
- Perturbation calculations thus excluded

- Viable alternative : variational approach provides upper bounds to the ground state energy

- Trial or model wave function must incorporate the effect of the hard - core potential

- Common approach : Jastrow type (product of monoparticular orbitals times correlation factors)

- Example : a finite system of bosons :

$$\psi_T = \prod_i \varphi[r_i - R] \prod_{i<j} f[r_{ij}] \qquad R = \text{Center of mass position}$$

- Example : an infinite system of bosons :

$$\psi_T = \prod_{i<j} f[r_{ij}]$$

with $r_i \in$ domain of length L, with periodic boundary conditions

- Example : an infinite system of fermions :

$$\psi_T = \Theta[r_1, \ldots, r_n] \prod_{i<j} f[r_{ij}] \qquad \Theta[r_1, \ldots, r_n] = \text{Slater determinant}$$

- Example : a solid formed by bosons :

$$\psi_T = \prod_i f[r_i - A_i] \prod_{i<j} f[r_{ij}] \qquad A_i = \text{positions of atoms in the crystalline lattice.}$$

- Upper bound energy of the ground state :

$$E_v = \frac{\int \psi^*_T[R]\, H\, \psi_T[R]\, dR}{\int \psi^*_T[R]\, \psi_T[R]\, dR} \geq E_0$$

- provides the exact energy E_0 as ψ_T approaches ψ_0
- requires the wave - function $\psi_T[R]$ to be provided
- allows optimization of parameters in $\psi_T[R, \alpha]$
- Calculations make use of the local energy $E_L[R]$:

$$E_L[R] \equiv \frac{H\, \psi_T[R]}{\psi_T[R]}$$

- $E_L[R]$ is suitable for MC calculations :

$$E_V = \frac{\int \left(\frac{H \psi_T[R]}{\psi_T[R]} \right) \psi^*_T[R] \, \psi_T[R] \, dR}{\int \psi^*_T[R] \, \psi_T[R] \, dR} \equiv \frac{\int E_L[R] \, \psi^*_T[R] \, \psi_T[R] \, dR}{\int \psi^*_T[R] \, \psi_T[R] \, dR}$$

- distribution probability to be used in MC calculations :

$$\psi^*_T[R] \, \psi_T[R] = | \psi_T[R] |^2 = p[R]$$

- Metropolis algorithm can be used to obtain $\{R_i\}$ with a distribution probability

$$p[R] = \psi^*_T[R] \, \psi_T[R] = | \psi_T[R] |^2$$

- Calculation of the energy (or any other property A[R]) :

$$E_V = \frac{1}{N} \sum_i E_L[R_i]$$

$$\epsilon[E_v] = \frac{1}{\sqrt{N-1}} \sqrt{\frac{1}{N} \sum_i E_L[R_i]^2 - E_v^2}$$

with result after N independent samples $\{R_i\}$ $i = 1 \ldots N$

written as $E_v \pm \epsilon[E_v]$

- Reweigthing techniques (using correlated sampling) :

Let us assume that the wave function depends on a set of parameters α : $\psi_T[R, \alpha]$

We are interested in obtaining the optimal value α. We want to compare tue quality of $\psi_T[R, \alpha]$ and $\psi_T[R, \alpha']$ with α and α' very close. $E_v[\alpha]$ and $E_v[\alpha']$ will be very similar and it will be difficult to achieve

$$\epsilon[E_v] < | E_v[\alpha'] - E_v[\alpha] |^2$$

It may be advantageous to sample both $E_v[\alpha]$ and $E_v[\alpha']$ from a single run, writing

$$E_v[\alpha'] = \frac{\int E_L[R, \alpha'] \mid \psi_T[R, \alpha'] \mid^2 dR}{\int \mid \psi_T[R, \alpha'] \mid^2 dR} =$$

$$= \frac{\int E_L[R, \alpha'] \frac{\psi_T[R,\alpha']|^2}{\psi_T[R,\alpha]|^2} \mid \psi_T[R, \alpha] \mid^2 dR}{\int \frac{\psi_T[R,\alpha']|^2}{\psi_T[R,\alpha]|^2} \mid \psi_T[R, \alpha] \mid^2 dR}$$

$$E_v[\alpha'] = \frac{\sum_i E_L[R_i, \alpha'] w[R_i, \alpha']}{\sum_i w[R_i, \alpha']}$$

$$\text{with} \quad w[R_i, \alpha'] = \frac{\psi_T[R_i, \alpha'] \mid^2}{\psi_T[R_i, \alpha] \mid^2}$$

Then tiny differences $E_v[\alpha_2] - E_v[\alpha_1]$ can be computed via

$$E_v[\alpha_2] - E_v[\alpha_1] = \frac{\sum_i E_L[R_i, \alpha_2] w[R_i, \alpha_2]}{\sum_i w[R_i, \alpha_2]} - \frac{\sum_i E_L[R_i, \alpha_1] w[R_i, \alpha_1]}{\sum_i w[R_i, \alpha_1]}$$

with both terms evaluated on the same set of sample points R_i,
thus canceling a large part of the statistical noise.

• Optimization of the trial wave - function $\psi_T[R, \alpha]$:

If the true ground state was known ($\psi_T[R] = \psi_0[R]$) , then

$H\,\psi_T[R] = E_0\,\psi_T[R]$ and the local energy

$$E_L[R] = \frac{H\,\psi_T[R]}{\psi_T[R]} = E_0 = \text{constant}, \quad \text{and} \quad \text{var}[E_L] = 0$$

This is the signature of the exact ground - state.

$\psi_T[R, \alpha]$ will usually not satisfy them exactly, and

we can search the optimal parameters in $\psi_T[R, \alpha]$ by

minimizing either

$$\begin{cases} E_v[\alpha] \\ \\ \text{var}[E_v[\alpha]] \end{cases}$$

and the results (optimal α value) are expected to agree

• Minimization of $E_v[\alpha]$ vs $\text{var}[E_v[\alpha]]$

An example can illustrate the practical equivalence of

both minimizations :

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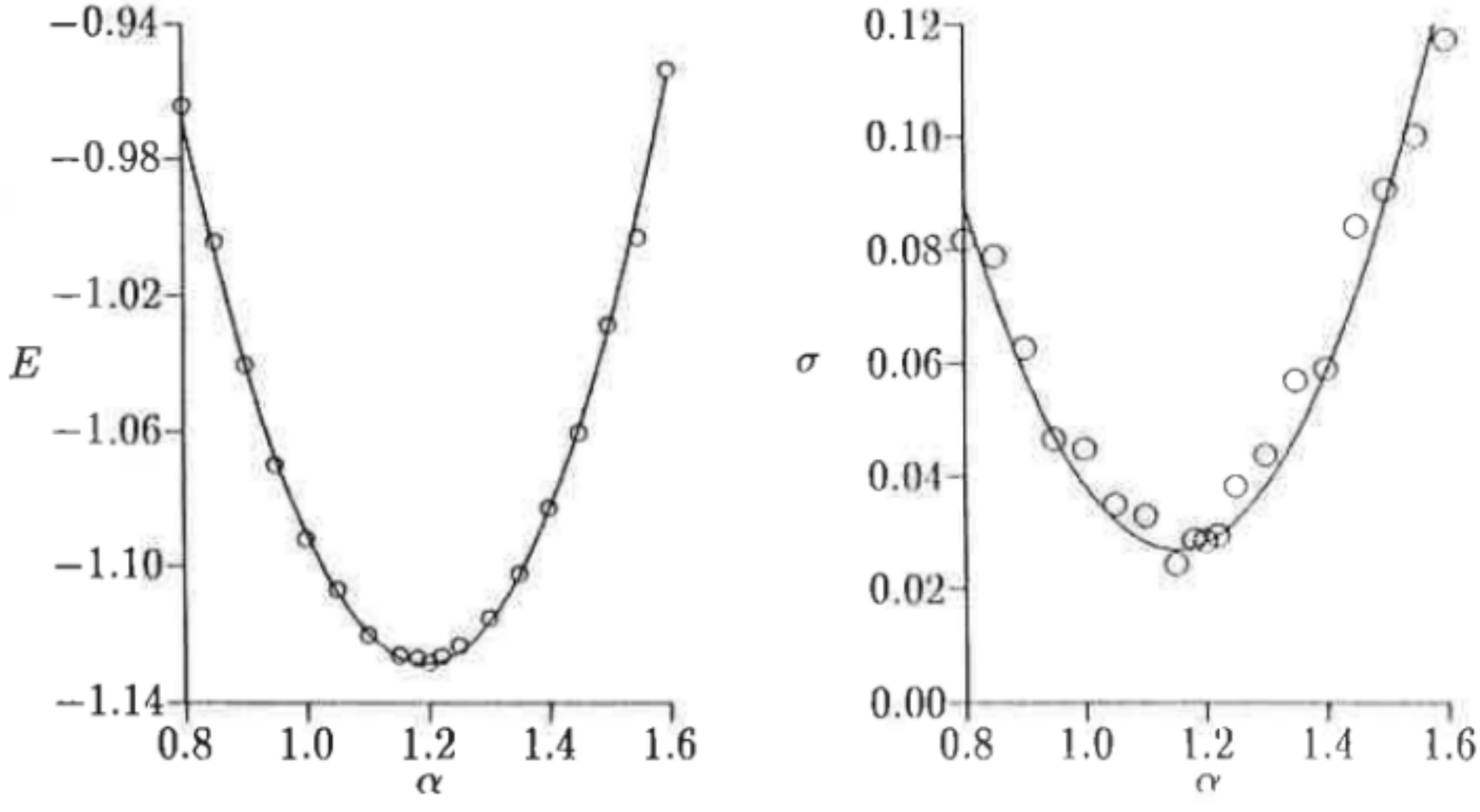
An example can illustrate the practical equivalence of
both minimizations :

for the H_2 molecule (protons A, B, electrons 1, 2) with wave function :

$$\psi_{H_2}[R] = \left(\text{Exp}[-\alpha\, r_{1A}] + \text{Exp}[-\alpha\, r_{1b}]\right) \cdot \left(\text{Exp}[-\alpha\, r_{2A}] + \text{Exp}[-\alpha\, r_{2b}]\right)$$

the dependence of $E_v[\alpha]$ and $\text{var}[E_v[\alpha]]$ on α (figure) makes the difference of the optimal α value hardly distinguishable :

Figure 2.4: Dependence of the variational energy and variance of the local energy on α for the simple H_2 trial function of Eq. 2.5.



- Alternative method to reweigthing technique
  in the search for the minimum of $f[\alpha]$:

It is possible to analytically compute the expressions for $f'[\alpha]$ and $f''[\alpha]$ and sample them. Then from

$$f[\alpha + \delta] = f[\alpha] + f'[\alpha]\,\delta + f''[\alpha]\,\delta^2 / 2$$

the minimum of the function can be searched by iterative application of : $(f'[\alpha + \delta] = 0 \rightarrow \delta = -f'[\alpha] / f''[\alpha])$

$$\rightarrow \quad \alpha_{new} = \alpha_{old} - f'[\alpha_{old}] / f''[\alpha_{old}]$$

- VMC can be used with any model wave function $\psi_T[R, \alpha]$

- VMC provides a starting point for a more powerful method : DMC

2. Diffusion Quantum Monte Carlo (DMC).

Objectives :

- Make use of the trial wave function as a starting point
- to get exact results for the energy of the ground state
- to get exact results for other properties of the ground state

Starting point is the time - dependent Schrodinger equation :

$$i\,\hbar\,\frac{\partial\,\psi}{\partial\,t} \;=\; -\frac{\hbar^2}{2\,m}\sum_i \nabla_i{}^2\,\psi \;+\; \sum_{i<j} V[r_{ij}]\;\psi$$

ψ evolution in time is

$$\psi[t] = \text{Exp}[-i\,H\,t\,/\,\hbar]\;\psi[0]$$

if we compute the evolution towards imaginary time τ

$$(\; t \;=\; -i\,\tau \;,\;\; \tau > 0\;)$$

$$\psi[t = -i\,\tau] = \text{Exp}[-H\,\tau\,/\,\hbar]\;\psi[0]$$

we get the time - dependent Schrodinger equation

in imaginary (or euclidean) time :

$$-\hbar \frac{\partial \psi}{\partial \tau} = -\frac{\hbar^2}{2\,m} \sum_i \nabla_i{}^2 \psi + \sum_{i<j} V[r_{ij}]\, \psi = H\, \psi$$

Defining the diffusion coefficient $D \equiv \frac{\hbar^2}{2\,m}$ and using t for $\tau / \hbar$

the time - dependent Schrodinger equation in imaginary time reads

$$-\frac{\partial \psi}{\partial t} = -D \sum_i \nabla_i{}^2 \psi + \sum_{i<j} V[r_{ij}]\, \psi \qquad \text{Eq 1}$$

Eq 1 makes the evolution of any initial state $\psi[0]$

converge towards the ground state,

as can be seen expanding ψ in the eigenfunctions basis :

$$\psi[0] = \sum_i c_n\, \psi_n[R] \quad \rightarrow \quad \psi[t] = \sum_i c_n\, \text{Exp}[-E_n\, t / \hbar]\, \psi_n[R]$$

$$\Rightarrow \quad \lim_{t\to\infty} \psi[t] \rightarrow c_0\, \psi_0[R]$$

- We will consider a stochastic process for $\left(R = \left\{ \vec{r}_1, \ldots, \vec{r}_n \right\} \right)$ such that the probability distribution p[R, t] evolves in time under Eq 1.

- We introduce importance sampling by defining

$$f[R, t] = \psi_T[R]\, \psi[R, t]$$

where $\psi_T[R]$ is a static (time independent) variational model wave function, and $\psi[R, t]$ time dependence follows Eq 1.

- The goal is that when $t \to \infty$, with $f[R, t \to \infty] = \psi_T[R]\, \psi_0[R]$ we will get information regarding $\psi_0[R]$ via the knowledge of both $\psi_T[R]$ and $f[R, t \to \infty]$

- The evolution of $f[R, t] = \psi_T[R]\, \psi[R, t]$ is dictated by

$$-\frac{\partial \psi}{\partial t} = H \psi$$

which implies for f[R, t] a modified time dependent Schrodinger equation :

$$-\frac{\partial f[R,\,t]}{\partial t} = -D\left(\sum_{i=1}^{n} \nabla_i{}^a\,\nabla_i{}^a\, f[R,\,t]\right) +$$

$$D\sum_{i=1}^{n} \nabla_i{}^a\left(2\,\frac{(\,\nabla_i{}^a\;\Psi t[R]\,)}{\Psi t[R]}\; f[R,\,t]\right) + E_L[R]\; f[R,\,t] \qquad \text{Eq 2}$$

where again we encounter the local energy $E_L[R] \equiv \dfrac{H\,\psi_T[R]}{\psi_T[R]}$.

- f[R, t] is more suited than ψ[R, t] for being used as distribution probability.
- f[R, t] is similar to ψ^2
- $E_L[R]$ is more well behavied than V[R]. Actually for a good ψ_T[R]

  $E_L[R] \to E_0$ = constant (or at least much smoother than V[R])
- Formally, eq 2 can be written :

$$-\frac{\partial f[R,\,t]}{\partial t} = (\,A_1 + A_2 + A_3\,)\, f[R,\,t] \qquad \text{Eq 3}$$

with $A_1 f[R, t] = - D \left(\sum_{i=1}^{n} \nabla_i{}^a \nabla_i{}^a f[R, t] \right)$

$$A_2 f[R, t] = D \sum_{i=1}^{n} \nabla_i{}^a \left(2 \frac{(\nabla_i{}^a \Psi t[R])}{\Psi t[R]} f[R, t] \right)$$

(in order to simplify the A_2 expression we will introduce the so - called drift force) :

$$F_i{}^a[R] \equiv 2 \frac{\nabla_i{}^a \Psi t[R]}{\Psi t[R]}$$

and

$$A_3 f[R, t] = E_L[R] f[R, t]$$

Let us examine separately the A_i actions on $f[R, t]$:

The formal solution for

$$-\frac{\partial f[R, t]}{\partial t} = A_i f[R, t] \qquad \text{Eq. 4}$$

is

$$f[R, t] = \int G_i[R, R_0, t] f[R_0, t_0 = 0] \, d R_0$$

with $G_i[R, R_0, t]$ being the Green function of A_i which satisfies

$$G_i[R, R_0, t] \equiv \langle R \left| \text{Exp}[- A_i t] \right| R_0 \rangle \quad \Rightarrow$$

$$\Rightarrow \quad \frac{\partial G_i[R, R_0, t]}{\partial t} = -A_i G_i[R, R_0, t]$$

and

$$G_i[R, R_0, t = 0] = \delta[R - R_0]$$

Let us solve Eq. 4 for the various A_i.

$\mathbf{A_1}$:

$$-\frac{\partial f[R, t]}{\partial t} = A_1 f[R, t] = -D\left(\sum_{i=1}^{n} \nabla_i{}^a \nabla_i{}^a f[R, t]\right)$$

The Green function $G_1[R, R_0, t]$ satisfying

$$\frac{G_1[R, R_0, t]}{\partial t} = -A_1 G_1[R, R_0, t] \quad \text{is}$$

$$G_1[R, R_0, t] = (4 \pi D t)^{-3 N/2} \operatorname{Exp}\left[-\frac{(R - R_0)^2}{4 D t}\right]$$

so the solution of $-\frac{\partial f[R, t]}{\partial t} = A_1 f[R, t]$ is

$$f[R, t] = (4 \pi D t)^{-3 N/2} \int \operatorname{Exp}\left[-\frac{(R - R_0)^2}{4 D t}\right] f[R_0, t_0 = 0] \, dR_0$$

$$\mathbf{A_2}\ :$$

$$-\frac{\partial f[R,\,t]}{\partial t} \;=\; A_2\, f[R,\,t] \;=$$

$$D\sum_{i=1}^{n} \nabla_i{}^a \left(2\,\frac{\nabla_i{}^a\,\Psi t[R]}{\Psi t[R]}\; f[R,\,t]\;\right) \equiv D\sum_{i=1}^{n}\; \nabla_i{}^a\;\left(\,F_i{}^a[R]\; f[R,\,t]\right)$$

The Green function $G_2[R,\,R_0,\,t]$ satisfying

$$\frac{G_2[R,\,R_0,\,t]}{\partial t} \;=\; -A_2\, G_2[R,\,R_0,\,t]$$

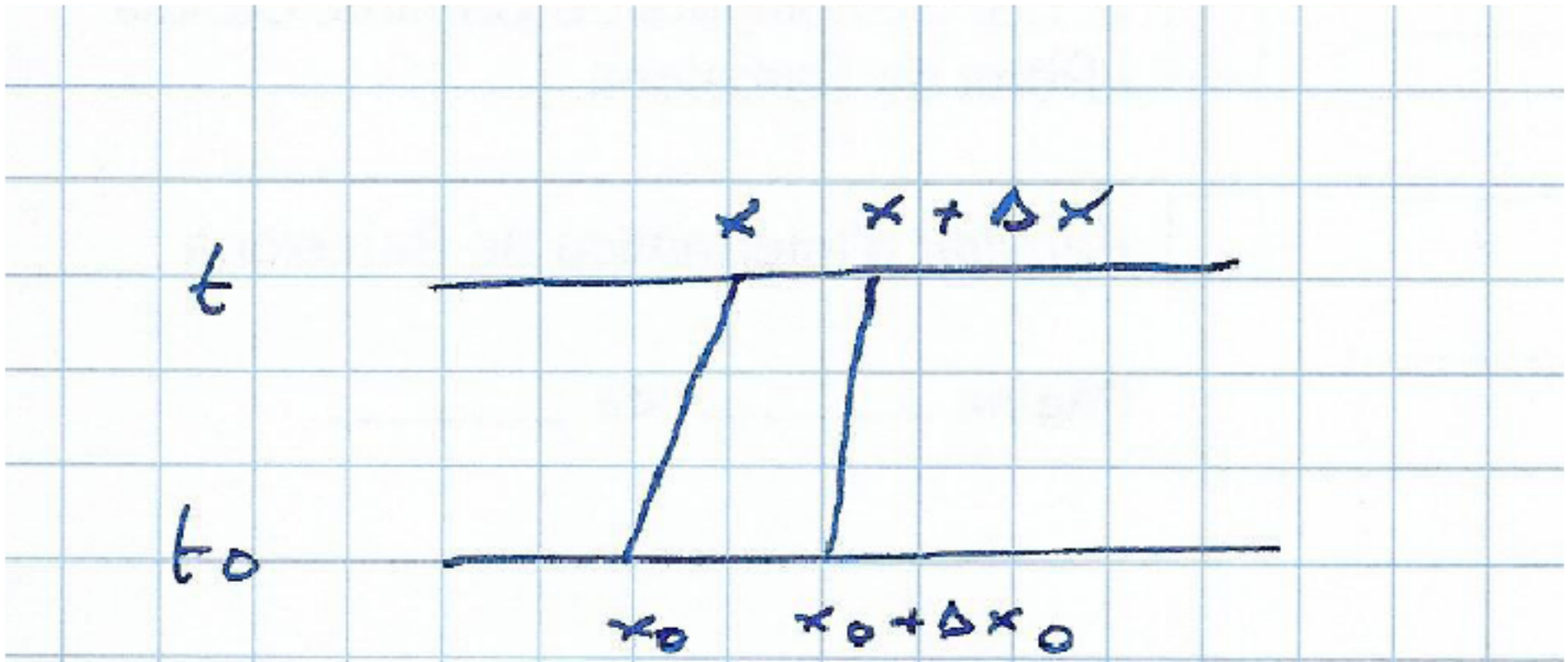
is

$$G_2[R,\,R_0,\,t] = \delta\left[R - \tilde{R}[t]\right]$$

where $\dot{\tilde{R}}_i{}^a[t] \;=\; D\,F_i{}^a[R]$ and $\tilde{R}[t=0] = R_0$

Let us see how this works in 1 D :

$$f[x0, t0]\,\Delta x0 \;=\; f[x, t]\,\Delta x$$



where $x0[t0] \to x[t]$ under evolution dictated by $xd'[t] = D\,F[xd[t]]$

and $(x0 + \Delta x0)[t0] \to (x + \Delta x)[t]$ under evolution dictated by $xd'[t] = D\,F[xd[t]]$

Then, for small $\Delta t = t - t0$:

$$x[t] - x0[t0] \;\equiv\; x - x0$$

$$(x + \Delta x)[t] - (x0 + \Delta x0)[t0] \;\equiv\; (x + \Delta x) - (x0 + \Delta x0)$$

$$x - x0 = D_c\, F[x0]\, \Delta t \qquad \text{(eq 5)}$$

$$(x + \Delta x) - (x0 + \Delta x0) = D_c\, F[x0 + \Delta x0]\, \Delta t \qquad \text{(eq 6)}$$

therefore (eq6 - eq5) :

$$\Delta x - \Delta x0 = D_c\, F[x0 + \Delta x0]\, \Delta t - D_c\, F[x0]\, \Delta t = D_c\, F_x[x0]\, \Delta x0\, \Delta t$$

$$\frac{\Delta x}{\Delta x0} - 1 = D_c\, F_x[x0]\, \Delta t \Rightarrow \frac{\Delta x}{\Delta x0} = 1 + D_c\, F_x[x0]\, \Delta t$$

$$\Rightarrow \boxed{\frac{\Delta x0}{\Delta x} = 1 - D_c\, F_x[x0]\, \Delta t + O[\Delta t]^2}$$

From $f[x0, t0]\, \Delta x0 = f[x, t]\, \Delta x$

we have :

$$f[x, t] = f[x0, t0]\, \frac{\Delta x0}{\Delta x}$$

$$f[x, t] = f[x0, t0] - f[x0, t0]\, D\, F_x[x0]\, \Delta t + O[\Delta t]^2 \qquad \text{(eq 7)}$$

But obviously

$$f[x, t] = f[x0, t0] + f_x (x - x0) + \frac{\partial f}{\partial t} (t - t0) \quad \text{and by eq (5) :}$$

$$f[x, t] = f[x0, t0] + f_x \; D_c F[x0] \, \Delta t + \frac{\partial f}{\partial t} \Delta t + O[\Delta t]^2 \quad \text{(eq 8)}$$

Substracting (eq 7) - (eq 8) :

$$0 = f_x \; D_c F[x0] \, \Delta t + \frac{\partial f}{\partial t} \Delta t + f[x0, t0] \; D_c \; F_x[x0] \, \Delta t + O[\Delta t]^2$$

i.e,

$$-\frac{\partial f}{\partial t} = f_x \; D_c F[x0] + f[x0, t0] \; D_c \; F_x[x0]$$

Finally, omitting the 0 label :

$$-\frac{\partial f}{\partial t} = D_c \nabla_x (F[x] \, f[x, t])$$

or, in the case of n particles :

$$f[x, t] \to f[R, t] \quad \text{and} \quad F[x] \to F_i{}^a[R] = \left(2 \frac{\nabla_i{}^a \Psi_T}{\Psi_T} \right)$$

and

$$-\frac{\partial f}{\partial t} = D \sum_{i=1}^{Np} \nabla_i{}^a \left(F_i{}^a[R] \, f[R, t] \right)$$

is satisfied for

$$G_2[R, R_0, t] = \delta\left[R - \tilde{R}[t]\right] \quad , \quad \dot{\tilde{R}}_i{}^a[t] = D \, F_i{}^a[R] \quad ,$$

$$\text{and} \quad \tilde{R}[t = 0] = R_0 .$$

so the solution of $-\frac{\partial f[R, t]}{\partial t} = A_2 \, f[R, t]$ is

$$f[R, t] = f[R_0, t_0 = 0] \quad \text{with } \tilde{R}[t = 0] = R_0 \text{ such that } \tilde{R}[t] = R$$

A_3 :

$$-\frac{\partial f[R,\ t]}{\partial t} = A_3\ f[R,\ t] = E_L[R]\ f[R,\ t]$$

The Green function $G_3[R,\ R_0,\ t]$ satisfying

$$\frac{G_3[R,\ R_0,\ t]}{\partial t} = -A_3\ G_3[R,\ R_0,\ t] = -E_L[R]\ f[R,\ t]$$

is

$$G_3[R,\ R_0,\ t] = \text{Exp}[-E_L[R]\ t]\ \delta[R - R_0]$$

therefore :

$$f[R,\ t] = \text{Exp}[-E_L[R]\ t]\ f[R_0,\ t_0 = 0]$$

The normalization of $G_3[R,\ R_0,\ t]$ is somewhat subtle and will be discussed later. Let us say that we can introduce a shift in the energy origin and write

$$G_3[R,\ R_0,\ t] = \text{Exp}[-E_L[R]\ t]\ \delta[R - R_0]$$

$$f[R,\ t] = \text{Exp}[-E_L[R]\ t]\ f[R_0,\ t_0 = 0]$$

- Complete Green function

$$-\frac{\partial f[R, t]}{\partial t} = (A_1 + A_2 + A_3) f[R, t] = A f[R, t]$$

We have seen exact analytical expressions for the separate A_i

$$G_i[R, R_0, t] = \langle R \mid \mathrm{Exp}[- A_i t] \mid R_0 \rangle$$

even for arbitrary large t. However the combined Green function

$$G[R, R_0, t] = \langle R \mid \mathrm{Exp}[- (A_1 + A_2 + A_3) t] \mid R_0 \rangle$$

can only be worked out for small Δt :

$$\mathrm{Exp}[- (A_1 + A_2 + A_3) \Delta t] =$$

$$= \mathrm{Exp}[-A_1 \Delta t] \mathrm{Exp}[-A_2 \Delta t] \mathrm{Exp}[-A_3 \Delta t] + O[\Delta t]^2 \Rightarrow$$

$$G[R, R_0, \Delta t] = \int dR'' dR' \langle R \mid \mathrm{Exp}[-A_1 \Delta t] \mid R'' \rangle \langle R'' \mid \mathrm{Exp}[-A_2 \Delta t] \mid R' \rangle \langle R' \mid \mathrm{Exp}[-A_3 \Delta t] \mid R_0 \rangle$$

Due to the δ functions in G_2 and G_3 we get simply :

$$G[R, R_0, \Delta t] = G_1\left[R, \tilde{R}_0[\Delta t], \Delta t\right] G_2\left[\tilde{R}_0[\Delta t], R_0, \Delta t\right] G_3[R_0, R_0, \Delta t]$$

which translates to

$$f[R, t + \Delta t] = \qquad \text{Eq (9)}$$

$$= \int dR_0 \left(\text{Exp}\left[- \frac{\left(R - \tilde{R}_0[\Delta t]\right)^2}{4\, D\, \Delta t} \right] \text{Exp}\left[- \left(E_L[R_0] - E_0\right) \Delta t \right] \right) f[R_0, t]\, dR_0$$

The previous equation can be iterated indefinitely, so that the limit $f[R, t \to \infty]$ can eventually be reached.

- When $f[R, t]$ is implemented via Monte Carlo, a set of walkers $\{R_i[t]\}$ distributed following $p[R, t] = f[R, t]$ must evolve according to Eq 3.
- Eq (9) can be readily implemented in a DMC approach
- Note that we have omitted the normalization constant $(4 \pi D \Delta t)^{-3\,N/2}$ in G_1 which is automatically taken care of :

- $f[R_0, t_0 = 0]$ is described by means of N walkers R_i (each one being a set of 3 n coordinates in 3 D)

- The so - called branching term induces a weigth w_i

$$w_i = \mathrm{Exp}[-(E_L[R_0[i]] - E_0)\,\Delta t]$$

to the walker R_i. E_0 is slowly adjusted during the run so that $< w_i > = 1$ on average

- G_1 and G_2 (random Gaussian and drift term respectively) both produce exactly one new walker for each old walker, so the global normalization of Eq. 9 is properly adressed.

Summary of a DMC code :

- Starting from the Hamiltonian H and the trial model wave function ψ_T we will work out the analytical expressions for the local energy and drift force :

$$E_L[R] \equiv \frac{H\,\psi_T[R]}{\psi_T[R]} \qquad\qquad F_i{}^a[R] = 2\,\frac{\nabla_i{}^a\,\psi_T[R]}{\psi_T[R]}$$

Choose the desired number Nw of walkers, the time step Δt and a starting energy reference value E_0 to be used in the DMC code.

Generate the initial configurations R_i {i, 1 …, Nw} , ideally using a VMC code for the same system.

These walkers represent the initial state f[R, t_0] of the system.

Then, for each walker R_i :

1. Compute the new weigth $w_i = \mathbf{Exp}[-(E_L[R_i] - E_0)\ \Delta t]$

2. Compute the new position originated by the drift term :

$$\tilde{R}_i = R_i + D\ F_i\ \Delta t$$

3. Compute the new position originated by the diffusion term :

$$R_i' = \tilde{R}_i + 2\ D\ \Delta t\ \zeta$$

where ζ is (for each coordinate and dimension) a random gaussian distributed variable :

$$\langle \zeta \rangle = 0 \qquad\qquad \langle \zeta^2 \rangle = 1$$

4. Replicate the walker R_i n_s times,

with $n_s = \mathrm{IntegerPart}\ [w_i + \eta]$

where η is a uniformly [0, 1] distributed random variable,

thus ensuring $\langle w_i \rangle = w_i$

5. Go to point 1 until completion of all walkers.

The procedure described above implements one basic MC iteration (equivalent to advancing from t to $t + \Delta t$ in Eq 9)

- The new configuration is highly correlated with the previous one, so a number of iterations has to be performed (completing what we call a block) until new, truly independent statistical information will be collected.

- At the end of a complete block, the population control parameter E_0 can be adjusted as

$$E_0 \leftarrow E_0 + a\,(Nw - Nw[current]) \qquad \text{Eq[10]}$$

where Nw is the desired number of walkers and a is a proportionality factor.

A higher E_0 term will cause an increase in the number of walkers, a lower E_0 term will reduce it. If the number of configurations changes too quickly, a should be reduced.

- Initially, whilst the steady state has not been reached, more frequent updates of E_0 via Eq[10] will result in a more stable behaviour.

- Once the steady state is reached the DMC code is providing samples of the ground - state wave function (via $p[R] = \psi_T[R]\,\psi[R, t]$).

Some final remarks regarding DMC :

- The expectation value of the local energy estimator provides the exact energy of the ground state, with no need of the exact model wave function :

$$E_0 = \frac{\langle \Psi_0 | H | \Psi_T \rangle}{\langle \Psi_0 | \Psi_T \rangle} = \frac{\langle \Psi_0 | E_L(R) | \Psi_T \rangle}{\langle \Psi_0 | \Psi_T \rangle}$$

- Other observables represented by operators A not commuting with H do not enjoy this property but can be estimated using an auxiliary VMC calculation :

$$A_{var} \equiv \langle \Psi_T | A | \Psi_T \rangle \qquad A_{mixed} \equiv \langle \Psi_T | A | \Psi_0 \rangle$$

$$\Rightarrow \langle A \rangle_{pure} = \langle \Psi_0 | A | \Psi_0 \rangle \simeq 2 A_{mixed} - A_{var}$$

- Pure estimators can be obtained directly from DMC using advanced algorithms.

- Systems with Fermi statistics suffer from the sign problem.

  It is usually imposed the condition that f (R, t) is positive.

  This turns into a kind of variational calculation. It is an open problem to find an algorithm which can circumvent this issue.

- Systems with Boson statistics allow for exact calculations, with the time - step error as the only bias.

- Finite time step error can be made made arbitrarily small.

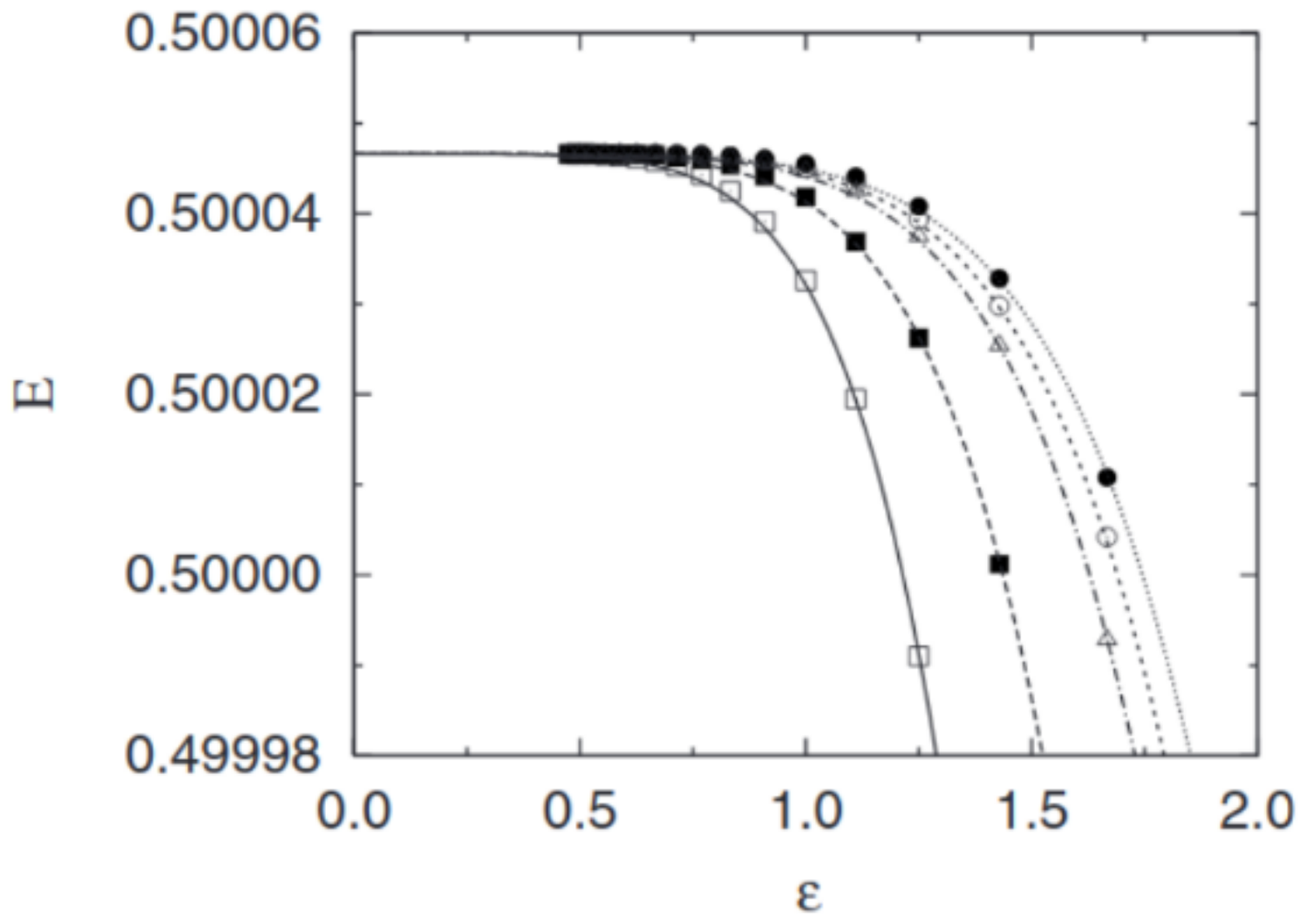
- Other expansion schemes (exact to higher order) can be used : for example

$$e^{-(A_1+A_2+A_3)\Delta t} = e^{-A_1 \Delta t/2}\, e^{-A_2 \Delta t/2}\, e^{-A_3 \Delta t} \cdot e^{-A_2 \Delta t/2}\, e^{-A_1 \Delta t/2} + O(\Delta t)^3$$

can be implemented, resulting in a smaller time step error.

- The finite time step error should be controlled by using several time step values.

- A typical time - step dependence of the energy results when using high order expansions has the form :



3. Revisiting VMC :

Let us consider Eq 2 , now neglecting the A_3 term :

$$-\frac{\partial f[R,\,t]}{\partial t} = -D\left(\sum_{i=1}^{n} \nabla_i{}^a\, \nabla_i{}^a\, f[R,\,t]\right) + D\sum_{i=1}^{n} \nabla_i{}^a\,\left(F_i{}^a[R]\;\; f[R,\,t]\right)$$

(Eq. 11)

where $F_i{}^a[R] \equiv 2\,\dfrac{\nabla_i{}^a\,\Psi t[R]}{\Psi t[R]}$

It turns out that it coincides with the Fokker - Plank equation,
but here it comes out of the quantum formalism.

We' ll have a look at it from this point of view.

- We are interested in understanding which would be the steady state

  of this equation. What is the final probability distribution

  $p[R] = f[R,\, t\to\infty]$ $\left(\text{with}\;\; \dfrac{\partial f[R,\,t]}{\partial t} = 0\right)$ we' ll reach?

- We'll see that it is actually $f[R, t \to \infty] = \Psi t[R]^2$
- Indeed, the right hand side of Eq[11] is just

$$D \sum_{i=1}^{n} \nabla_i{}^a \left(F_i{}^a[R] \; f[R, t] - \nabla_i{}^a f[R, t] \right)$$

and for $f[R, t] = \Psi t[R]^2$ we get

$$\nabla_i{}^a f[R, t] = \nabla_i{}^a \Psi t[R]^2 = 2 \Psi t[R] \nabla_i{}^a \Psi t[R]$$

$$\Rightarrow D \sum_{i=1}^{n} \nabla_i{}^a \left(2 \frac{\nabla_i{}^a \Psi t[R]}{\Psi t[R]} \Psi t[R]^2 - 2 \Psi t[R] \nabla_i{}^a \Psi t[R] \right) = 0$$

- So that just omitting the branching term we arrive at a new way to get a variational calculation!
- Also, with no branching term present the population number is strictly constant: a single walker R is enough, (in the spirit of VMC).

- However, there is a finite time step error due to the use of Δt,

  which forces us to examine the time - step dependence,

  just like in the DMC case.

- We note that this dependence can be eliminated by introducing a Metropolis acceptance test :

  if the R walker has been transformed into R' by means of the drift + diffusion term, we compute

$$q\{R', R\} = \frac{G_1\left[R', \tilde{R}[\Delta t], \Delta t\right] G_2\left[\tilde{R}[\Delta t], R, \Delta t\right]}{G_1\left[R, \tilde{R}'[\Delta t], \Delta t\right] G_2\left[\tilde{R}'[\Delta t], R', \Delta t\right]}$$

and use $q\{R', R\}$ to accept the move $\{R' \leftarrow R\}$ with probability

$A[\{R', R\}] = \mathrm{Min}[1, q\{R', R\}]$ (otherwise we keep the old R).

By introducing this additional Metropolis test,

detailed balance is guaranteed and therefore :

- our new VMC is free of any time - step error
- it is more efficient since it contains a drift term which,

  by construction, drives the system towards

  the region where $\Psi t[R]^2$ is maximum.