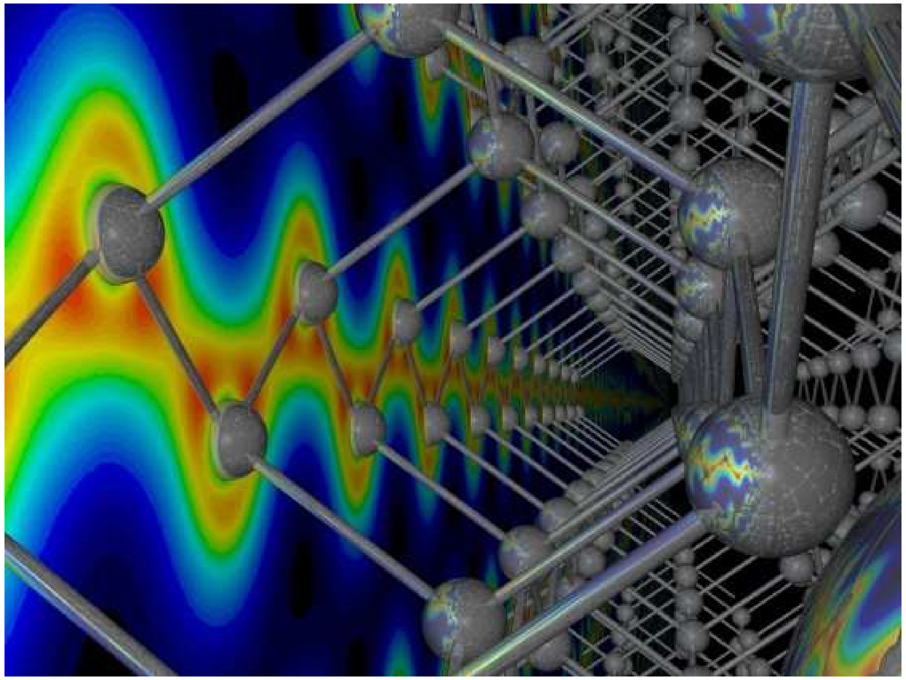
The Fermion Sign Problem

Doing without the fixed-node approximation in quantum Monte Carlo



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The fermion sign problem

• Classical simulations are the most general way of finding out how classical (ordinary objects) behave. But since the microscopic world is really quantum mechanical, chemists, physicists, etc. would like to simulate quantum systems.

• The basic problem is to calculate the properties of a quantum simulation without approximation in a way that scales reasonably as the number of quantum degrees of freedom grows. Simulations can be done for a few quantum problems; chiefly thermodynamic properties of boson systems and of fermion systems in one dimension. But for most many-body quantum systems, the problem is that minus signs come in and when they do the simulation methods become very inefficient because the 'signal' is overwhelmed by the 'noise'. The solution of this problem is one of the most important in all of computational physics.

Numerical solutions of the many-body Schrödinger equation

$$\hat{H}\Psi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N) = E\Psi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N)$$

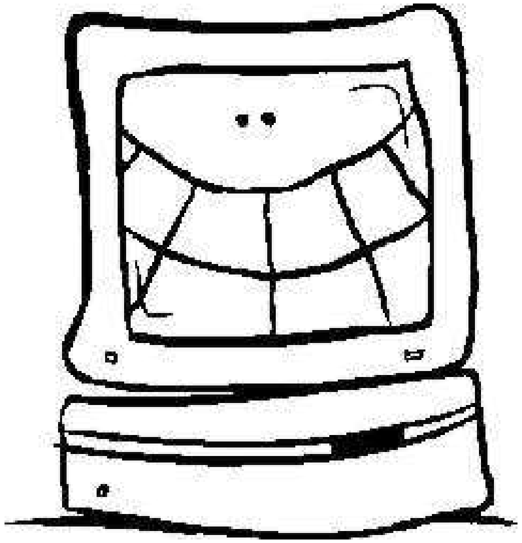
- Monte Carlo methods are the most powerful numerical tools for quantum many-body physics.

- Since they deal effectively with many-dimensional quadrature, they allow the use of a potentially fully-correlated wave function or density matrix.

- By minimizing some variational functional of these, one can obtain, for example, an optimal energy within the framework of a given class of trial functions.

- How can a stochastic or Monte Carlo method ever be said to solve a problem exactly, since there is always a statistical error associated with the result? We rely on the central limit theorem to provide an estimate of the probability that the exact results lies with a given interval. If we need to have the error to be less that amount, this implies that the computer time will scale proportional to one over the square of the error.

Why is quantum Monte Carlo a good thing?



- Basis set truncation errors are absent in the QMC formalism.
- Computer time scales with system size roughly as N^3, where N is the number of particles. Recent developments have made possible the approach to linear scaling in certain cases.
- Computer memory requirements are small and grow modestly with system size.
- Monte Carlo numerical efficiency can be arbitrarily increased. QMC calculations have an accuracy dependence of $\sqrt{T}$, where T is the computer time. This enables one to choose an accuracy range and readily estimate the computer time needed for performing a calculation of an observable with an acceptable error bar.
- Comparatively few people do it, and so you have much more chance of being an individual than if you were one of the thousand-strong herd of density functional theorists at your average mega-conference.

Variational methods

Minimize expectation value of trial wave function such as

$$\boxed{\begin{aligned} \Psi_{\mathrm{Trial}} &= \frac{1}{\sqrt{N_e}} \begin{vmatrix} \psi_1(\mathbf{x}_1) & \psi_1(\mathbf{x}_2) & \dots & \psi_1(\mathbf{x}_{N_e}) \\ \psi_2(\mathbf{x}_1) & \psi_2(\mathbf{x}_2) & & \\ \vdots & & \ddots & \\ \psi_{N_e}(\mathbf{x}_1) & & & \psi_{N_e}(\mathbf{x}_{N_e}) \end{vmatrix} \exp\left(\sum_{i \neq j}^{N_e} -U_0(r_{ij}) \right) \\ & U_0(r_{ij}) = \frac{A}{r_{ij}} \left(1 - \exp\left(-\frac{r_{ij}}{F} \right) \right) \end{aligned}}$$

Doesn't suffer from sign problem - treating antisymmetric trial wave functions is not difficult - the problem is rather one of complexity.

Can we make arbitrarily accurate wave functions?

No. Can use method of residuals, but unless someone finds out how to go arbitrarily high order it is not a solution.

However, there exists a class of methods (collectively called projector Monte Carlo) which in principle solve quantum problems exactly. Depend upon guessed properties of the many-body wave function only in their computational efficiency, if at all.

Projector methods

First suggestion of Monte Carlo solution of Schrödinger equation dates back to Fermi. Showed that a solution of the stationary state equation,

$$-\frac{1}{2}\nabla^2\Psi(\mathbf{R}) = E\Psi(\mathbf{R}) - V(\mathbf{R})\Psi(R)$$

could be obtained by introducing a time-dependent wave function of the form $\Psi(\mathbf{R},\tau) = \Psi(\mathbf{R})e^{-E\tau}$. This will obey the equation

$$\frac{\partial\Psi(\mathbf{R},\tau)}{\partial\tau} = \frac{1}{2}\nabla^2\Psi(\mathbf{R},\tau) - V(\mathbf{R})\boldsymbol{\Psi}(\mathbf{R},\tau)$$

and in the long time limit, look like the ground state solution to the first equation.

- Ignore 2nd term on RHS, equation is isomorphic with a diffusion equation, which can be simulated by a random walk where random walkers diffuse in an $\mathbf{R}$-dimensional space.

- Ignore 1st term, have first order kinetics equation with position-dependent rate constant $V(\mathbf{R})$ (interpret as stochastic survival prob.).

A numerical simulation in which random walkers diffuse through $\mathbf{R}$-space, reproduce in regions of low potential, and die in regions of high potential leads to a stationary distribution proportional to $\Psi(\mathbf{R})$, from which expectation values can be obtained.

Projector methods

General idea is to project out a state of the Hamiltonian by iteration of a projection operator $\hat{P}$. Assume ground state for simplicity.

$$\lim_{i \longrightarrow \infty} \hat{P}^i |\Psi_T\rangle \approx |\Psi_0\rangle$$

After sufficient iterations i, the contribution of all excited states $|\Psi_i\rangle$ will be filtered out and only the ground state is recovered.

Power method

- Diagonalizable $n \times n$ matrix A i.e. $X^{-1}AX = \text{diag}\,(\lambda_1, \lambda_2, \ldots, \lambda_n)$
- $X = [x_1, x_2, \ldots, x_n]$ matrix of eigenvectors
- $q = (1, 0, 0, 0, \ldots)$ unit norm vector

```
do k = 1,2,...
z(k) = matmul[A,q(k-1)]
q(k) = z(k) / norm[z(k)]
λ(k) = [q(k)]^-1 A q(k)
enddo
```

$$A = \begin{pmatrix} -261 & 209 & -49 \\ -530 & 422 & -98 \\ -800 & 631 & -144 \end{pmatrix} \qquad q(0) = (1, 0, 0) \qquad \lambda(A) = (10, 4, 3)$$

- Only dominant eigenvector survives after large number of iterations.

k	λ(k)
1	13.0606
2	10.7191
3	10.2703
4	10.0633
5	10.0198
6	10.0063
7	10.0020
8	10.0007
9	10.0002

Markov processes and stochastic projection

- For high-dimensional vectors like Ψ need to generalize power method with stochastic implementation.

- In QMC the projection operator is a function of the Hamiltonian operator which is Hermitian by construction, so the eigenvalues are real.

- Stochastic matrix : normalized non-negative matrix, $\sum_i M_{ij} = 1$

- $\mathbf{R}$-space representation of this would be stochastic propagator that satisfies the condition $\int M(\mathbf{R}, \mathbf{R}')d\mathbf{R}' = 1$.

- Can create Markov chain of states $\pi(\mathbf{R}''), \pi(\mathbf{R}'), \pi(\mathbf{R}), \ldots$with transitions from state i to state j with probability related to the stochastic matrix element, M_{ij}, in which the move only depends on the current state, i.

- The propagators for QMC are not generally normalized, therefore not stochastic matrices, but we can represent them in terms of the latter by factoring $\hat{P}_{ij} = M_{ij} w_j$ where the weights w_j are defined by $w_j = \sum_i \hat{P}_{ij}$.

- An MC sampling scheme of $\hat{P}_{ij}|\Psi_T\rangle$ can be generated by performing a random walk, and keeping a weight vector $W(\mathbf{R})$ for the random walkers.

$$\Psi(\mathbf{R}) \equiv \pi(\mathbf{R})W(\mathbf{R}) = \int P(\mathbf{R}, \mathbf{R}')\Psi(\mathbf{R}')d\mathbf{R}' = \int M(\mathbf{R}, \mathbf{R}')B(\mathbf{R})\Psi(\mathbf{R}')d\mathbf{R}'$$

Population Monte Carlo algorithm

Generalized population Monte Carlo stochastic projection algorithm:

1. **INITIALIZE**

Generate set of n random walkers at different positions $(\mathbf{R}_1, \mathbf{R}_2, \ldots, \mathbf{R}_n)$. These points are intended to sample a probability density function $\Phi(\mathbf{R})$.

2. **MOVE**

(a) Each walker j is moved independently from $\mathbf{R}$ to a new position $\mathbf{R}'$, according to the transition probability $T(\mathbf{R} \longrightarrow \mathbf{R}') \equiv M(\mathbf{R}, \mathbf{R}')$.

(b) Ensure detailed balance if $T(\mathbf{R} \longrightarrow \mathbf{R}') \neq T(\mathbf{R}' \longrightarrow \mathbf{R})$ by using a Metropolis acceptance/rejection step.

3. **WEIGHT**

(a) Calculate a weight vector using a weighting function $B(\mathbf{R}_i)$ i.e. $w_i^* = B(\mathbf{R}_i)$. The ideal weight function preserves normalization of $\hat{P}_{ij}(\mathbf{R}, \mathbf{R}')$ and maintains individual weights w_i close to unity.

(b) Update the weight of the walker, multiplying the weight of the previous iteration by the weight of the new iteration $w_i' = w_i^* \times w_i$.

4. **RECONFIGURATION**

Split walkers with large weights into multiple walkers with weights that add up to the original weight. Remove walkers with small weight.

Projection operators or Green's functions

Different projection operators lead to different QMC methods :

- Green's function Monte Carlo

Use resolvent operator

$$\hat{P}(\hat{H}) \equiv \frac{1}{1 + \delta\tau(\hat{H} - E_R)}$$

- Diffusion Monte Carlo

Use imaginary time evolution operator

$$\hat{P}(\hat{H}) \equiv e^{-\delta\tau(\hat{H} - E_R)}$$

Any decreasing function of $\hat{H}$ can serve as a propagator!

Imaginary propagator

$$\left(\hat{H} - E_T\right)\Psi(\mathbf{R}, t) = -\frac{\partial\Psi(\mathbf{R}, t)}{i\partial t} = -\frac{\partial\Psi(\mathbf{R}, t)}{\partial\tau}$$

Can cast the above equation into integral form,

$$\Psi(\mathbf{R}, \tau + \delta\tau) = \lambda_\tau \int G(\mathbf{R}, \mathbf{R}', \delta\tau)\Psi(\mathbf{R}', \tau)d\mathbf{R}'$$

The Green's function $G(\mathbf{R}, \mathbf{R}', \delta\tau)$satisfies the same boundary conditions as the original Schrödinger equation $\frac{\partial}{\partial\tau}G(\mathbf{R}, \mathbf{R}', \delta\tau) = (\hat{H} - E_T)G(\mathbf{R}, \mathbf{R}', \delta\tau)$ with the initial conditions associated with the propagation of a Dirac delta function. The form of G that satisfies this is

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

which can obviously be expanded in eigenfunctions

$$G(\mathbf{R}, \mathbf{R}', \delta\tau) = \sum_n e^{-\tau(E_n-E_T)}\Psi_n^*(\mathbf{R}')\Psi_n(\mathbf{R})$$

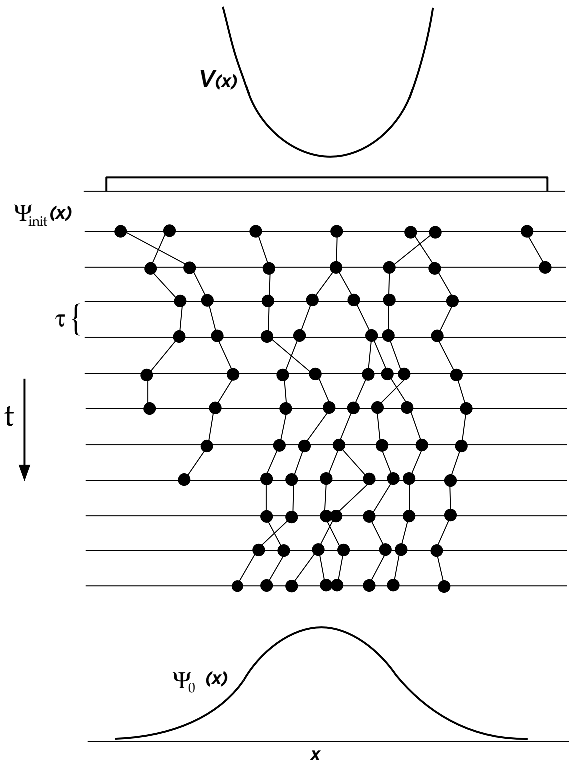
For an arbitrary initial trial function, $\Psi(\mathbf{R})$ in the long time limit

$$\lim_{\tau\longrightarrow\infty} e^{-\tau(\hat{H}-E_T)}\Psi = \lim_{\tau\longrightarrow\infty}\int G(\mathbf{R}, \mathbf{R}', \tau)\Psi(\mathbf{R}')d\mathbf{R}' = \lim_{\tau\longrightarrow\infty}\langle\Psi|\Psi_0\rangle e^{-\tau(E_0-E_T)}\Psi_0$$

Essence of DMC and GFMC

Random walks serve to filter out the higher energy modes of some initial distribution, so that for very large imaginary time, the probability distribution of the random walkers is given by the ground state.

For potentials invariant under particle exchange this is also the symmetric (bosonic) ground state.



Differential form

Consider imaginary time behaviour of time-dependent Schrödinger equation

$$\left(\hat{H} - E_T\right)\Psi(\mathbf{R},t) = -\frac{\partial\Psi(\mathbf{R},t)}{i\partial t}$$

For eigenstate, general solution is clearly

$$\phi(\mathbf{R},t) = \phi(\mathbf{R},0)e^{-i(\hat{H}-E_T)t}$$

Then expand arbitrary $\Psi(\mathbf{R},t)$ in eigenfunctions of $\hat{H}$

$$\Psi(\mathbf{R},t) = \sum_{n=0}^{\infty} c_n\phi_n(\mathbf{R})e^{-i(E_n-E_T)t}$$

Substitute $it \to \tau$ (imaginary time). Oscillatory behaviour becomes exponential.

$$\Psi(\mathbf{R},\tau) = \sum_{n=0}^{\infty} c_n\phi_n(\mathbf{R})e^{-(E_n-E_T)\tau}$$

Get time independence by choosing E_T to be ground state eigenvalue E_0. As $\tau \to \infty$, $\Psi \to$ ground state ϕ_0.

$$\Psi(\mathbf{R},\tau) = c_0\phi_0 + \sum_{n=1}^{\infty} c_n\phi_n(\mathbf{R})e^{-(E_n-E_T)\tau}$$

The form of the propagator

- Propagate solution in imaginary time with Green's function

$$\Psi(\mathbf{R},\tau+\delta\tau) = \int G(\mathbf{R},\mathbf{R}',\delta\tau)\Psi(\mathbf{R}',\tau)\,d\mathbf{R}'$$

- How do we find Green's function $G(\mathbf{R},\mathbf{R}',\delta\tau)$? Can't sample previous expression exactly, so consider Schrödinger equation in two parts:

$$\begin{aligned} -\frac{1}{2}\nabla^2_{\mathbf{R}}\Psi &= -\frac{\partial\Psi}{\partial\tau} \quad \text{diffusion equation} \\ V\Psi &= -\frac{\partial\Psi}{\partial\tau} \quad \text{rate equation} \end{aligned}$$

- Green's function for diffusion equation known: $3N$ dimensional Gaussian with variance $\delta\tau$ in each dimension.

$$G(\mathbf{R},\mathbf{R}',\delta\tau) = (2\pi\delta\tau)^{-\frac{3N}{2}} \exp\left(-\frac{|\mathbf{R}-\mathbf{R}'|^2}{2\delta\tau}\right)$$

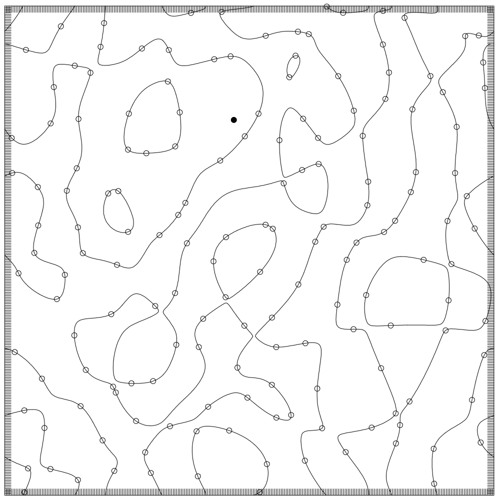
- Extra branching factor from rate equation.

$$\times \exp\left[-\delta\tau\left(\frac{V(\mathbf{R})+V(\mathbf{R}')-2E_{\mathrm{T}}}{2}\right)\right]$$

Importance sampling in DMC

- Problem 1: Ψ is not a probability distribution $\rightarrow$ sign problem.

- Problem 2: Rate equation is poorly behaved.
- Solution: Work with distribution $f(\mathbf{R},\tau) = \Psi(\mathbf{R},\tau)\Phi_T(\mathbf{R})$ and deal with sign problem via fixed-node approximation.



$$\boxed{\begin{aligned} &-\tfrac{1}{2}\nabla^2_{\mathbf{R}} f(\mathbf{R},\tau) + \nabla_{\mathbf{R}} \cdot [\mathbf{F}(\mathbf{R}) f(\mathbf{R},\tau)] \\ &- (E_{\mathrm{L}}(\mathbf{R}) - E_{\mathrm{T}})\, f(\mathbf{R},\tau) = -\frac{\partial f(\mathbf{R},\tau)}{\partial \tau} \end{aligned}}$$

$$\mathbf{F}(\mathbf{R}) \equiv \Phi_T^{-1}\nabla_{\mathbf{R}}\Phi_T$$ drift vector

$$f(\mathbf{R},\tau+\delta\tau) = \int G(\mathbf{R}',\mathbf{R},\delta\tau) f(\mathbf{R},\tau)\, d\mathbf{R}'$$

Importance sampling in DMC

In short time approximation G consists of diffusion, drift and branching processes

$$
\begin{aligned}
G(\mathbf{R}', \mathbf{R}, \delta\tau) \;=\; & (2\pi\delta\tau)^{-\frac{3N}{2}} \exp\left[-\left(\frac{\mathbf{R}' - \mathbf{R} - \delta\tau\mathbf{F}(\mathbf{R})}{2\delta\tau}\right)^2\right] \\
& \times \exp\left[-\delta\tau\left(\frac{E_{\mathrm{L}}(\mathbf{R}) + E_{\mathrm{L}}(\mathbf{R}')}{2} - E_{\mathrm{T}}\right)\right]
\end{aligned}
$$

- Drift term enhances density of configurations where Φ_T is large.
- Branching term contains the local energy which fluctuates less than the potential energy
- Lots of algorithmic subtleties. Save those for a rainy day.

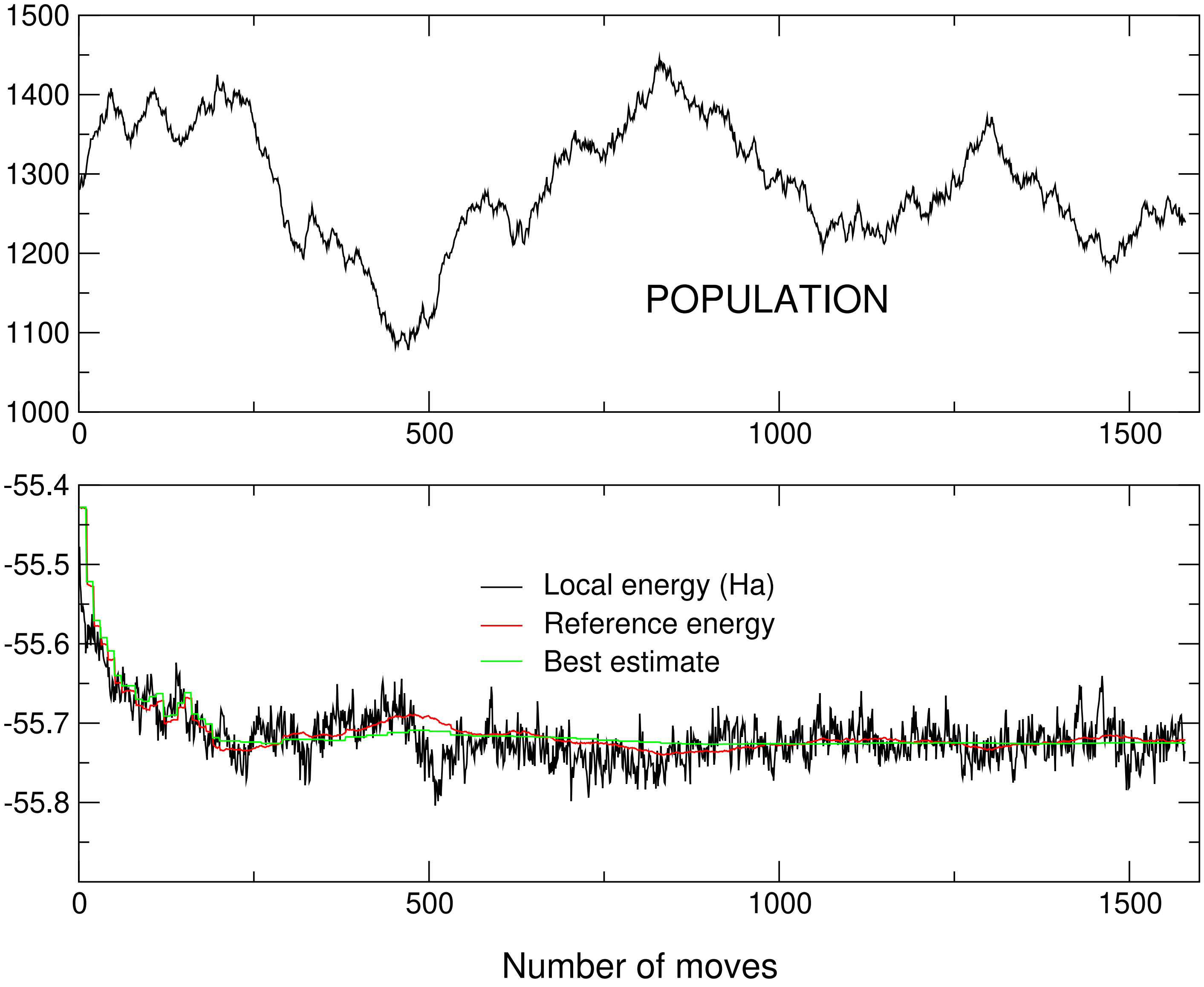
Calculating the energy

Calculate energy from

$$
\begin{aligned}
E_{\mathrm{DMC}} &= \frac{\int \Phi_T \Psi \left(\frac{\hat{H}\Phi_T}{\Phi_T} \right) \, d\mathbf{R}}{\int \Phi_T \Psi \, d\mathbf{R}} \\
&\simeq \frac{1}{M} \sum_i E_{\mathrm{L}}(\mathbf{R}_i)
\end{aligned}
$$

Results of DMC simulation

Antiferromagnetic nickel oxide crystal



Fixed-node approximation

• Fermionic ground state is an excited state in a manifold containing all the fermionic and bosonic states.

Simple DMC

• $\Psi(\mathbf{R})$ contains positive and negative regions (difficult to sample).

Importance sampled DMC

• Initial distribution is positive. Nevertheless, the Green's function can become negative if walker crosses a node.

• If use signs in weights for sampling in either of these case, statistics of the process lead to exponential growth of the variance of any observable.

Simplest approach to avoid exponential growth is to forbid moves in which the product wave function changes sign. This is the defining characteristic of the fixed-node approximation. Fix nodes of sample wave function to be the nodes of the trial function.

Fixed-node energy of the ground state is an upper bound to the exact energy of the system. It is the best solution for that fixed set of nodes. Can be extremely accurate! But it is not a solution to the sign problem.

Exact methods

AIM : *a stable algorithm that can sample the exact wave function without resorting to the fixed-node approximation*.

As FN-DMC is variational, can vary the nodal surface and optimize the energy. However, it's just as difficult to parametrize and vary the nodal surface as it is the wave function. This can be very useful, but it is not a complete solution!

Can therefore use 'exact methods' that impose no additional boundary condition on the wave function, other than the requirements of global antisymmetry. Usually associated with a large increase in computational time. Will discuss two examples :

- Release-node method
- Cancellation method ('Fermion Monte Carlo')

No proper solution is known!

Release-node algorithm

- Application of the evolution operator $e^{-\tau(\hat{H}-E_T)}$ to an arbitrary initial wave function leads to collapse to the ground state bosonic wave function.

- An arbitrary fermion wave function $\Psi(\mathbf{R})$ can be separated into two functions $\Psi^+(\mathbf{R})$ and $\Psi^-(\mathbf{R})$:

$$\Psi^+(\mathbf{R},\tau) \equiv \frac{1}{2}(|\Psi(\mathbf{R},\tau)| + \Psi(\mathbf{R},\tau)) \qquad \Psi^-(\mathbf{R},\tau) \equiv \frac{1}{2}(|\Psi(\mathbf{R},\tau)| - \Psi(\mathbf{R},\tau))$$

Original function recovered as $\Psi(\mathbf{R},\tau) = \Psi^+(\mathbf{R},\tau) - \Psi^-(\mathbf{R},\tau)$

- Release-node algorithm involves two independent DMC calculations, using Ψ^+ and Ψ^- as the wave functions to evolve.

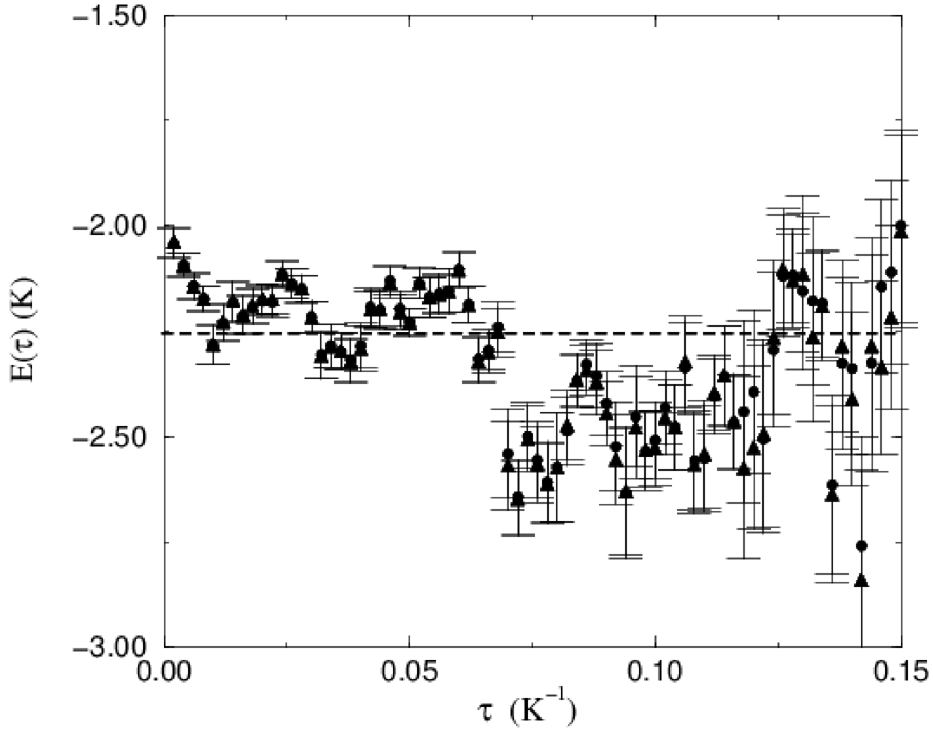
$$\Psi(\mathbf{R},\tau) = \int G(\mathbf{R},\mathbf{R}',\tau)\Psi^+(\mathbf{R}',0)d\mathbf{R}' - \int G(\mathbf{R},\mathbf{R}',\tau)\Psi^-(\mathbf{R}',0)d\mathbf{R}'$$

- The time evolution of the system can be followed from the difference of separate simulations for $\Psi^+(\mathbf{R})$ and $\Psi^-(\mathbf{R})$. Walkers may step through nodes.

- Both distributions are positive during the simulation and both decay to the bosonic ground state. Decay is problematic because the signal-to-noise ratio in this method depends on the difference between the two distributions. Decay of the difference goes roughly as $e^{\tau(E_{fermion}-E_{boson})}$.

Release-node algorithm

• For this method to be practical, one needs to start with the distribution of a good fermion trial function. The distribution will evolve from this starting point to the bosonic ground state at large imaginary time τ. In an intermediate "transient" regime one can collect information on the exact fermion wave function.



$$E = \frac{\int \Psi(\mathbf{R},\tau)\hat{H}\Psi_T(\mathbf{R})d\mathbf{R}}{\int \Psi(\mathbf{R},\tau)\Psi_T(\mathbf{R})d\mathbf{R}}$$

$$= \frac{\int \Psi^+(\mathbf{R},\tau)\hat{H}\Psi_T(\mathbf{R})d\mathbf{R}}{\int \left(\Psi^+(\mathbf{R},\tau) - \Psi^-(\mathbf{R},\tau)\right)\Psi_T(\mathbf{R})d\mathbf{R}} - \frac{\int \Psi^-(\mathbf{R},\tau)\hat{H}\Psi_T(\mathbf{R})d\mathbf{R}}{\int \left(\Psi^+(\mathbf{R},\tau) - \Psi^-(\mathbf{R},\tau)\right)\Psi_T(\mathbf{R})d\mathbf{R}}$$

Fermion Monte Carlo

$$E = \frac{\sum_i \left[\frac{\hat{H}\Psi_T(\mathbf{R}_i^+)}{\Psi_G(\mathbf{R}_i^+)} - \frac{\hat{H}\Psi_T(\mathbf{R}_i^-)}{\Psi_G(\mathbf{R}_i^-)} \right]}{\sum_i \left[\frac{\Psi_T(\mathbf{R}_i^+)}{\Psi_G(\mathbf{R}_i^+)} - \frac{\Psi_T(\mathbf{R}_i^-)}{\Psi_G(\mathbf{R}_i^-)} \right]}$$

- If we have a set of signed walkers that respectively add or subtract their contribution to statistical expectations, and if random walk rules for positive and negative walkers are the same, then they must have the same long term distribution and eigenvalue estimates will be pure noise. Need to avoid this plus-minus symmetry - walkers can no longer move independently - need *correlated walkers*.

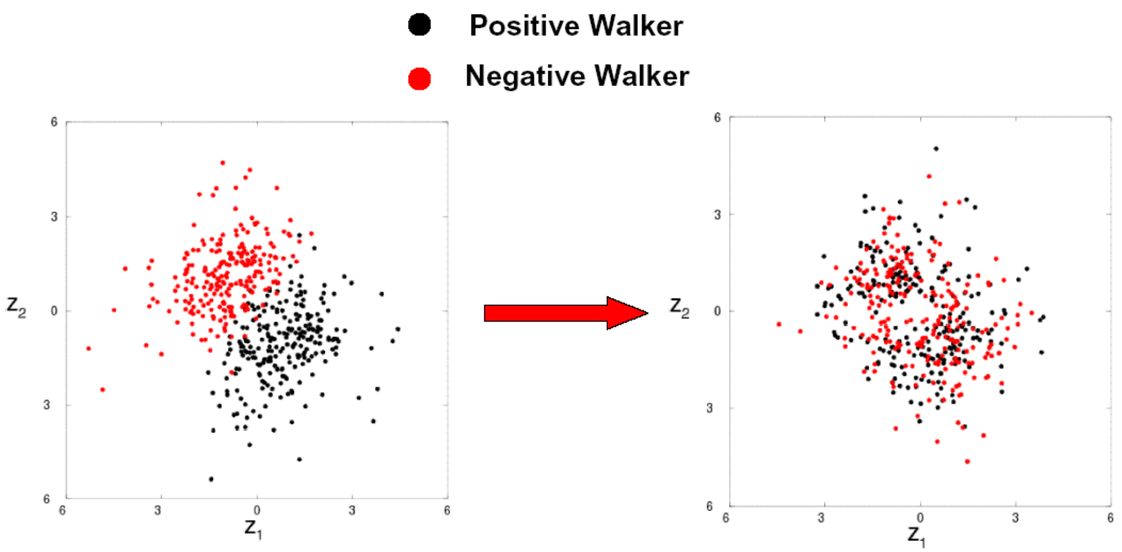
- Note that if two walkers meet, they cancel exactly and we could take them out of the simulation. Turns out this is vital for creating a stable algorithm .

- How do we establish when walkers 'meet'?

- How do we guarantee correct results in spite of the correlation?

- Can use lots of different tricks. All very complicated!

Cancellation (H_2^+ molecule)



• In the absence of cancellation, the two populations spread through the available configuration space, penetrate each other and independently approach the symmetric distribution of the ground state.

• This can be avoided if the growth of the symmetric ground state can be controlled. If positive and negative walkers in close proximity are occasionally allowed to cancel each other, the two populations tend to cancel each other and produce spatially separated distributions.

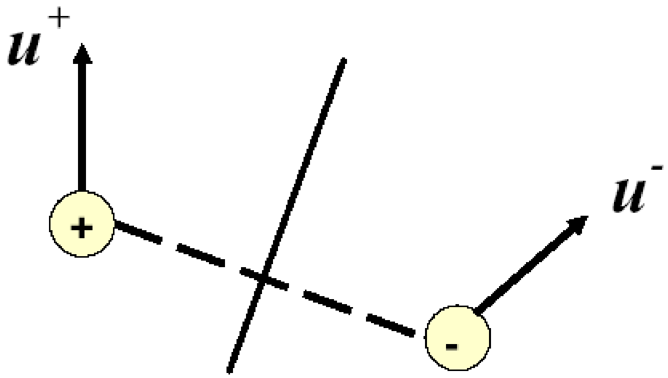
• In order for cancellation to be useful, cancellations need to happen often enough to maintain an adequate ratio of positive to negative walkers in regions where the wave function is positive, and vice versa. Phase space is very large! Need to work out ways of increasing the cancellation rate.

Ingredients for stability of FMC (Kalos/Pederiva)

• Distinct positive guiding functions for positive and negative walkers (drift will then tend to keep the walkers in the corresponding pocket of the antisymmetric function).

$$\Psi_G^{\pm} = \sqrt{\Psi_S^2(\mathbf{R}) + c^2\Psi_A^2(\mathbf{R})} \pm c\Psi_A(\mathbf{R})$$

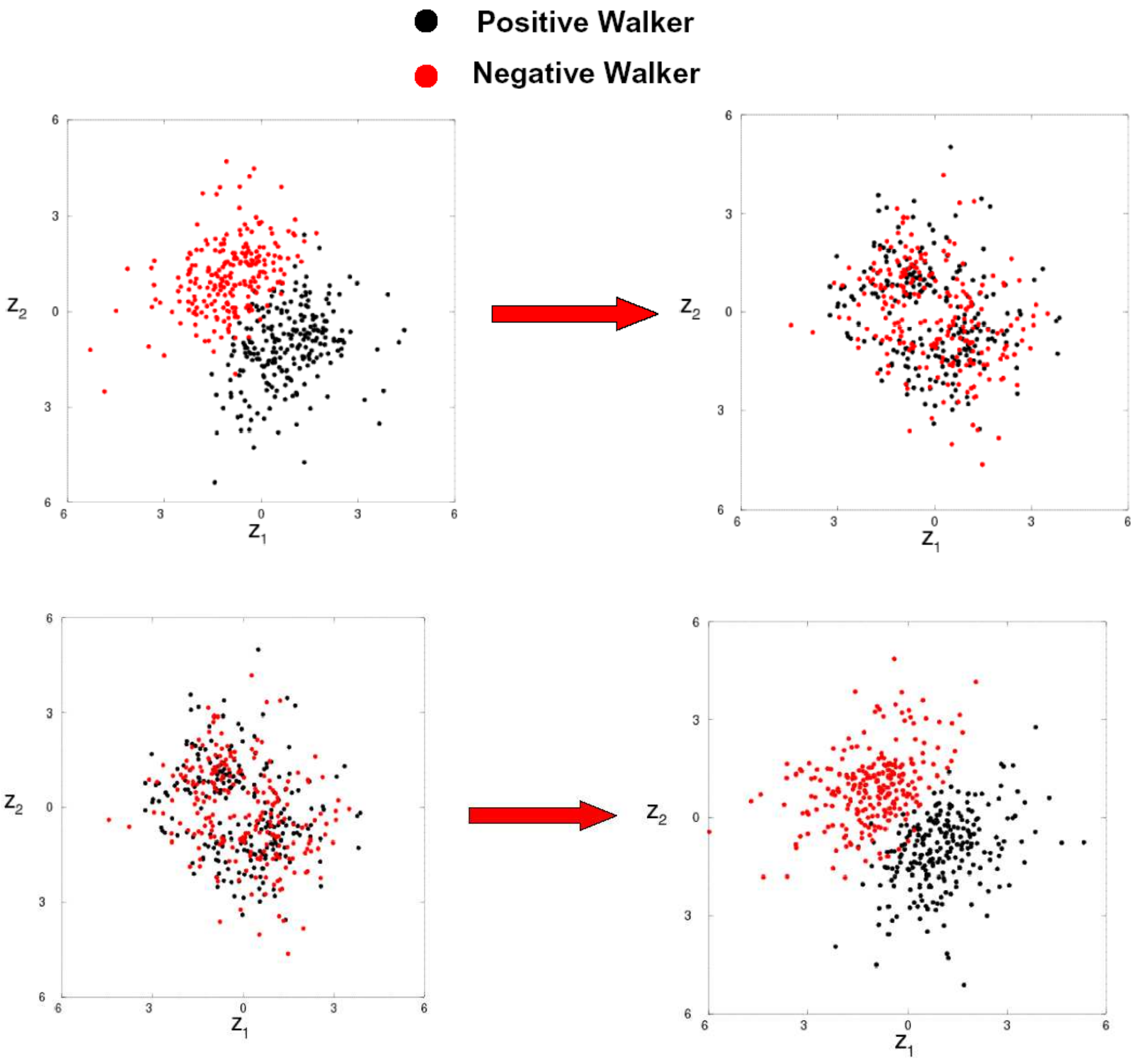
• Positive and negative walkers paired with correlated diffusion. 'Reflected dynamics' guarantees eventual cancellation for a pair in a finite time.



• Cancellation between positive and negative walkers with expected future contributions conserved.

In general, if can generate a stable overlap with an antisymmetric function, and if the behaviour of a walker in a correlated ensemble cannot be distinguished from that of a single free walker ('correct marginal dynamics') then the algorithm will work.

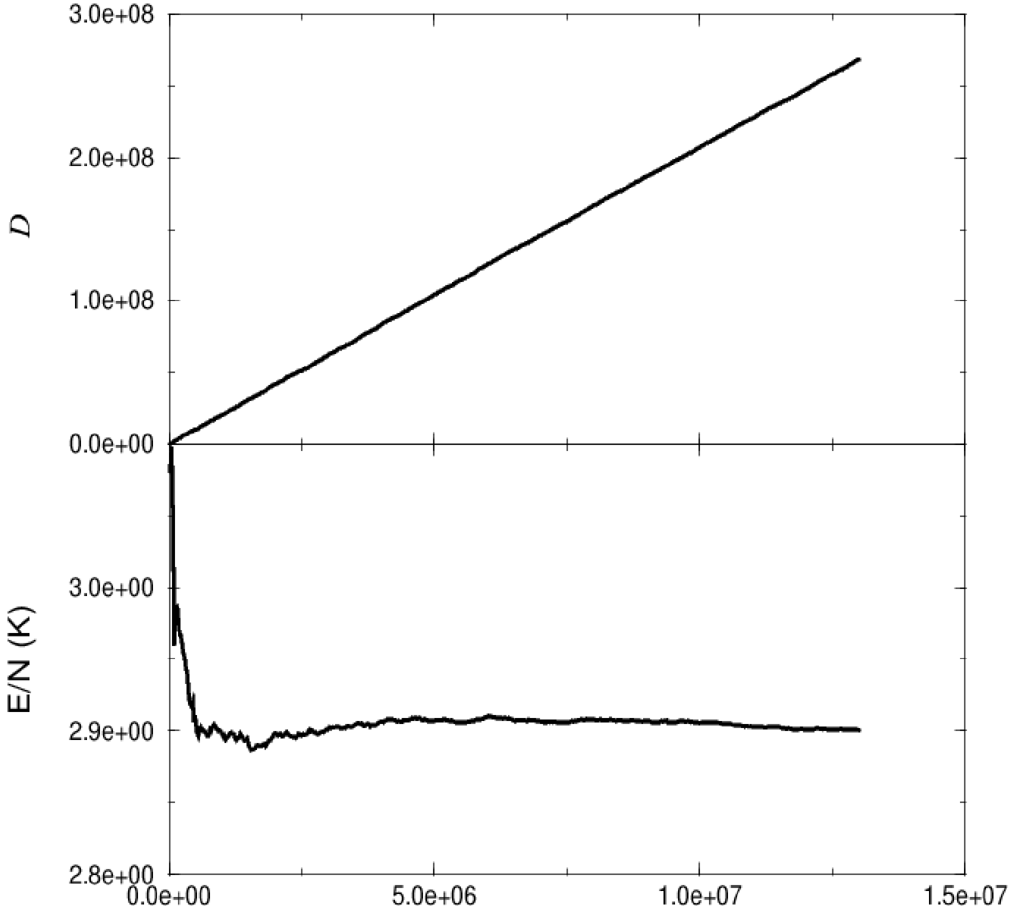
Cancellation (H_2^+ molecule)



(Figures from Kalos/Pederiva)

Kalos/Pederiva results

• Cumulative denominator of energy expression (measure of stable separation of positive and negative walkers) and energy per particle in periodic system of seven free fermions as function of number of time steps :



• Method has been and is being applied to the following systems : free fermions in periodic system, He atom, Be atom, up to 54 He atoms in a periodic system, Li_2 molecule, Be_2 molecule, B_2 molecule, two-dimensional electron gas. Method stable but scales very badly with system size.. More developments required.

Requirements on a solution to the fermion sign problem

Several solutions per year in literature, but all (according to Ceperley) either :

- have a serious error,
- are known not to work ('exact' FN has been discovered at least 3 times),
- work only in special cases (e.g. 1D, certain lattice models, harmonic oscillator),
- cannot scale at large N or low temperature,
- have uncontrolled approximations,
- have not been analyzed enough to know whether they work,

Numerical evidence is nice but not enough, since :

- there are approximation methods that are very accurate in certain problems,
- cancellation of errors is always possible for some limited set of problems.

Scaling must be demonstrated.

Solving this problem would make you happy and popular!