Methods of Fermion Monte Carlo

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The Challenge

Solve the N-body Schrödinger equation

Antisymmetric solution– a highly excited mode

Diffusion Monte Carlo naturally gives ground state

Antisymmetric state decays exponentially fast

Pauli Principle is non-local; diffusion is local

"Fixed-node approximation" gives upper bound

BUT

Challenge, continued

- ***We want a solution with no uncontrolled approximations***
  - ***Error estimate computable internally***
  - ***Error can be reduced in polynomial computing time***

Is a "fixed node" an uncontrolled approximation?
Often guided by knowledge of experimental result
Yes, unless exact node known, or a sequence can converge to exact node, adding only polynomial complexity
Can one find exact or tractably improvable nodes?

We seek a method based on Monte Carlo variance reduction methods: correlation, importance sampling, non-local moves.

Is this possible?
Many people think not.
But not all "sign problems" are the same!
Some are intractable, some are hard, some are trivial.

Basic ideas

- Ensembles of pairs of plus and minus walkers
- Correlated diffusion to make close pairs
- Cancel close pairs– to control symmetric part of walker distribution
- Make pairs from single walkers– “repairing”
- Break “plus-minus symmetry”
- - Use sign-dependent dynamics
  - Use distinct odd permutations to reconfigure pairs
  - Use asymmetric “second-stage” importance functions

The Schrödinger Equation

One seeks to solve the Schrödinger Equation in imaginary time for an N-body system

$$-\frac{1}{2}\nabla^2\psi(R,\tau) + V(R)\psi(R,\tau) + \frac{\partial\psi(R,\tau)}{\partial\tau} = 0$$

where R stands for the 3N coordinates of the system, τ is i times the physical time, t, and V is the potential energy function.

This is a diffusion equation in a 3N-dimensional Euclidean space, in which the function $V(R)$ governs the birth or death of walkers. This is clear from a short-time expansion:

$$\psi(R,\tau+\delta\tau) = \int \frac{e^{-V(R')\delta\tau-(R-R')^2/(2\delta\tau)}}{(2\pi\delta\tau)^{3N/2}}\psi(R',\tau)\,dR'$$

When $V(R)$ is positive, walkers are removed from the population, and when it is negative, walkers are created.

The eigenfunction expansion

The solution can be written in terms of the eigenvalues and eigenfunctions of the Hamiltonian:

$$-\frac{1}{2}\nabla^2\psi_k(R) + V(R)\psi_k(R) \equiv H\psi_k(R) = E_k\psi_k(R)$$

as

$$\psi(R,\tau) = \sum_k a_k e^{-E_k\tau}\psi_k(R) \xrightarrow[\tau\to\infty]{} a_0 e^{-E_0\tau}\psi_0(R)$$

so that as the imaginary time grows infinitely large, the distribution of walkers approaches the fundamental mode, which is non-negative.

This is a viable way of generating the fundamental mode, except for the fact the the potential *V(R)* can be unbounded from above and from below.

Importance Sampling (1)

These technical difficulties can be overcome by altering the dynamics of the random walk so that the density of walkers is

$$e^{E_T\tau}\psi_T(R)\ \psi(R,\tau)$$

where $\psi_T(R)$ is a trial function that satisfies the Schrödinger equation at singularities of the potential, and E_T is a trial eigenvalue.

For small increments of imaginary time, $\delta\tau$, adding drift and branching to the purely diffusive random walk accomplishes this:

$$R \rightarrow R + \nabla \log\psi_T(R)\delta\tau + U$$

where U is a vector of 3N normal random variables with mean zero and variance $\delta\tau$. Each walker is branched into m walkers where

$$< m(R) >= \exp[\{E_T - H\psi_T(R)/\psi_T(R)\}\delta\tau]$$

Note that if ψ_T were ψ_0 and E_T were E_0, then $< m >$ = 1, and no branching takes place. This is the basis of powerful optimization techniques.

For non-interacting particles, we can take ψ_T = 1 and the dynamics is exact.

Estimating the eigenvalue

A population of walkers is generated using the stochastic dynamics described. The population can be kept close to constant by adjusting the the trial energy, E_T .

Assuming we have generated a random walk that samples $\psi_T(R)\,\psi(R,\tau)$, we can use the trial function $\psi_T(R)$ to project the energy estimator as

$$E = \frac{\sum_k \frac{H\psi_T(R_k)}{\psi_T(R_k)}}{\sum_k 1}$$

where R_k are the configurations of the system in the walk.

Symmetries for identical particles

For a system of identical particles, the potential V is symmetric under the interchange of particle coordinates:

$$V(R) \equiv V(r_1 \ldots r_i \ldots r_j \ldots r_N) = V(r_1 \ldots r_j \ldots r_i \ldots r_N)$$

for every i and j. Then the fundamental mode $\psi_0(R)$, has the same symmetry:

$$\psi_0(R) \equiv \psi_0(r_1 \ldots r_i \ldots r_j \ldots r_N) = \psi_0(r_1 \ldots r_j \ldots r_i \ldots r_N)$$

This is in fact the correct symmetry for wave functions of "bosonic" particles. But for "fermionic" particles, like electrons, wave functions must be "antisymmetric." In the non-relativistic limit, electrons can be thought to have either "spin up" or "spin down." Acceptable wave functions are antisymmetric with respect to the exchange of coordinates of like-spin electrons:

$$\psi_F(R) \equiv \psi_F(r_1 \ldots r_i \ldots r_j \ldots r_N) = -\psi_F(r_1 \ldots r_j \ldots r_i \ldots r_N)$$

when i and j denote like-spin electrons. This is the "Pauli principle."

Negative walkers

That means that the solutions we seek are not everywhere positive—not a promising situation for a Monte Carlo method.

A naïve answer to this problem is to assign algebraic signs to our walkers. In fact, we will use ***ensembles of pairs of walkers carrying opposite signs.***

The "sign problem"

We use positive and negative walkers, R^+ and R^-, along with an antisymmetric trial function, $\psi_A(R)$, and a non-symmetric positive "guiding function", $\psi_G(R)$, replacing the importance function, so that the energy estimator becomes

$$E = \frac{\sum_k [H\psi_A(R_k^+)/\psi_G(R_k^+) - H\psi_A(R_k^-)/\psi_G(R_k^-)]}{\sum_k [\psi_A(R_k^+)/\psi_G(R_k^+) - \psi_A(R_k^-)/\psi_G(R_k^-)]}.$$

If the asymptotic distributions for R^+ and R^- are the same, then this estimator will give zero over zero, not an efficient Monte Carlo procedure.

We call the method "statistically stable" if the average denominator is not equal to zero.

We must break the dynamical symmetry that would otherwise give the same distribution for plus and minus walkers.

At the same time, we must limit the magnitude of the symmetric component of the walker distribution, so that it does not dominate asymptotically.

The "sign problem"—continued

Recall the eigenfunction expansion, now singling out the "bosonic" ground state and the higher "fermionic" mode:

$$\psi(R,\tau) = \sum_k a_k e^{-E_k \tau} \psi_k(R) = a_0 e^{-E_0 \tau} \psi_S(R) + ...+ a_F e^{-E_F \tau} \psi_F(R) + ...$$

Since the part of the walker distribution that contributes to an integral weighted with $\psi_F(R)$ decays exponentially; a simple Monte Carlo treatment of a fermion system will become inefficient exponentially fast because

$$E_F > E_0 .$$

One can defeat the decay by growing the population of walkers exponentially fast, demanding exponentially growing computing work.

For extensive systems, $E_F - E_0 \propto N$ so that the exponential decay is exacerbated in larger systems.

We note also that ***the Pauli principle is a non-local constraint***, at variance with the local character of diffusion equations and the random walks we use.

The "fixed-node" approximation

The standard method in the practice of Quantum Monte Carlo is totake an antisymmetric trial function, $\psi_A(R)$, and carry out the kind of random walk with drift and diffusion described above, subject to the boundary condition that the walk ***not cross the nodes*** of $\psi_A(R)$. This procedure gives an upper bound to the energy of the system.

In current practice, it has been refined in many important ways by:

- Investigating the mathematical, topological, and physical character of

  antisymmetric trial functions.

- Using expansions over large bases with many parameters.

- Using highly sophisticated optimization methods to improve $\psi_A(R)$.

As yet, it remains a method with uncontrolled approximations.

Correlation and Cancellation (1)

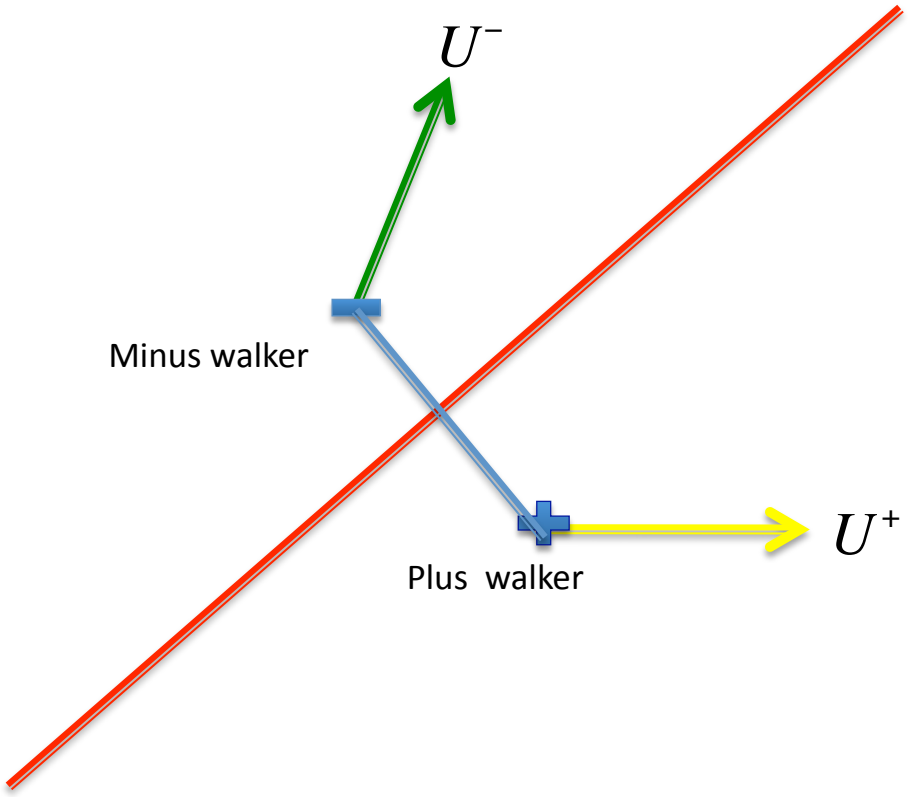
We use simple diffusion Monte Carlo for both walkers, but ***correlate the diffusion steps*** by using correlated Gaussian vectors:

If U^+ is the vector of gaussians for a plus walker, then we use U^- for its minus partner, where $U^- = U^+ - 2\frac{U^+ \cdot (R^+ - R^-)}{|R^+ - R^-|^2}(R^+ - R^-)$.

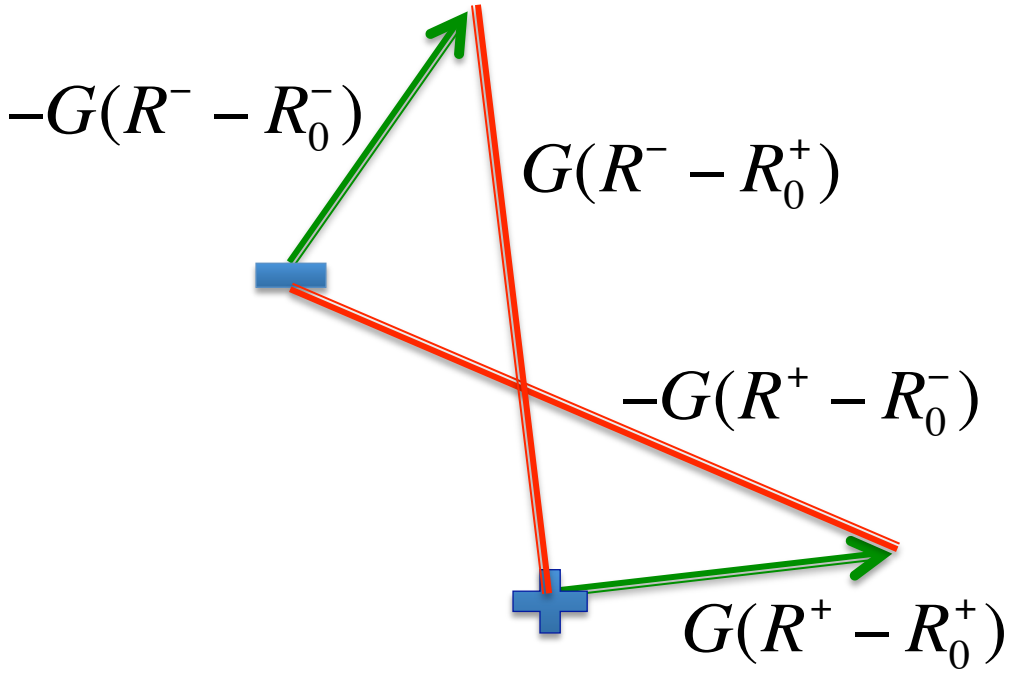
The Euclidean distance between the walkers, $|R^+ - R^-|$, undergoes a random walk in one dimension. Given periodic boundary conditions, or a finite system, this brings the pair of walkers ***arbitrarily close in linear time or better*** in any number of dimensions, which permits them to cancel each other with high probability. In simple DMC, and in the free-fermion system, a pair of walkers diffusing from (R_0^+, R_0^-) to (R^+, R^-) continues with probability

$$\max\{0, 1 - \exp[\frac{(R^- - R_0^+)^2 - (R^- - R_0^-)^2}{2\delta\tau}]\}.$$

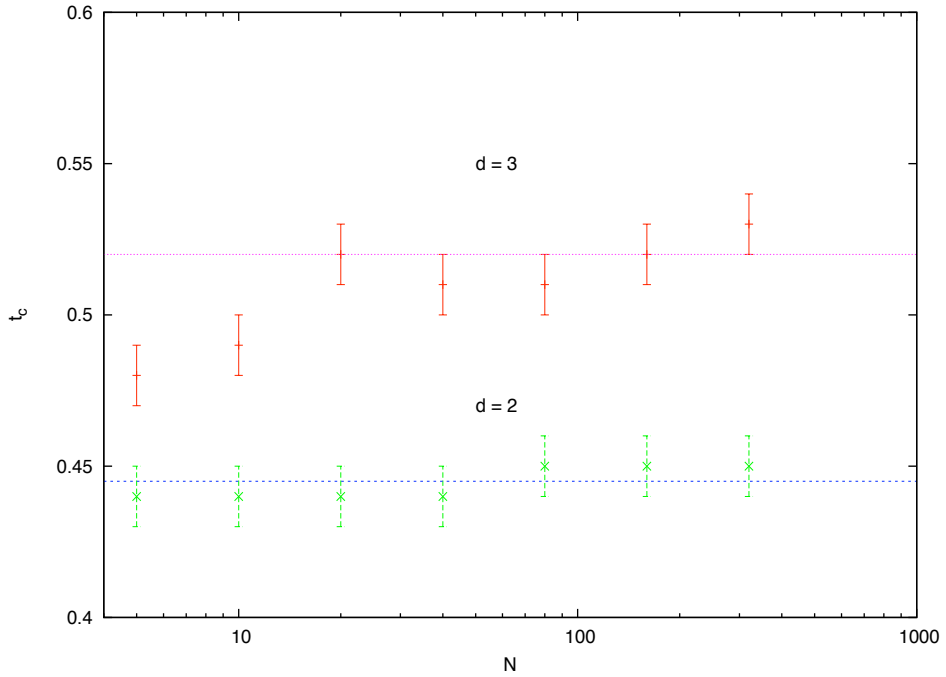
Correlated diffusion of plus and minus walkers



Cancelation of plus and minus walkers

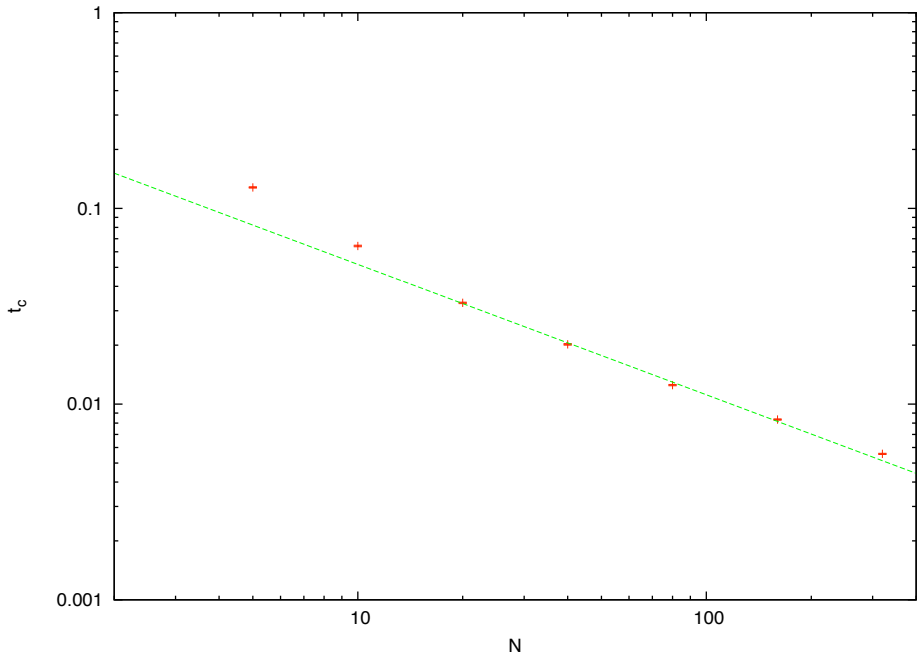


Imaginary time to cancellation for free fermions



Average imaginary time to cancelation for N free particles in d dimensions

Imaginary time to cancel—Pöschl-Teller potential



Average imaginary time to cancel for N particles interacting via $1/\cosh^2$ potential

$$t_c(N) = 0.24 N^{-2/3}$$

Correlation and Cancellation (2)

We use simple diffusion Monte Carlo for both walkers, but

each walker separately executes correct drift and diffusion steps.

This has the effect of reducing the overlap with symmetric test functions, while not affecting the overlap with antisymmetric test functions.

But by itself, this procedure does not break the symmetry.

The "plus-minus symmetry"

We have introduced rules that define stochastic dynamics for a pair of random walkers, (R^+,R^-), each of which lives in a 3N-dimensional Euclidean space.

Let $\rho(R^+,R^-,\tau)$ be the joint density of walkers (R^+,R^-) at imaginary time τ.

The stochastic dynamics define an operator, $K(R^+,R^- \mid R'^+,R'^- \mid \delta\tau)$, that

advances the density in imaginary time:

$$\rho(R^+,R^-,\tau+\delta\tau) = e^{E_S\delta\tau}\iint K(R^+,R^- \mid R'^+,R'^- \mid \delta\tau)\rho(R'^+,R'^-,\tau)dR'^+\,dR'^-$$

If $K(R^+,R^- \mid R'^+,R'^- \mid \delta\tau)$ is invariant under exchange of the labels, +,–,

$$K(R^-,R^+ \mid R'^-,R'^+ \mid \delta\tau) = K(R^+,R^- \mid R'^+,R'^- \mid \delta\tau)$$

then, asymptotically,

$$\rho_\infty(R^+,R^-) = \lim_{\tau\to\infty}\rho(R^+,R^-,\tau) = \rho_\infty(R^-,R^+)$$

so that the sum over pairs of walkers needed in the energy quotient

$\sum_k [\psi_A(R_k^+)/\psi_G(R_k^+) - \psi_A(R_k^-)/\psi_G(R_k^-)]$ is asymptotically zero: Not stable!

Breaking the plus/minus symmetry (1)

Quite generally, if the evolution depends in any way on the +/− labels of the pair, the symmetry is broken, a necessary condition for stability.

For example:

If $\psi_A(R^+) - \psi_A(R^-) < 0$ use the antithetic correlated dynamics described above.

Else: if $\psi_A(R^+) - \psi_A(R^-) > 0$ move R^+ and R^- in parallel, *i,e.,* set

$$U^- = U^+ .$$

with no cancellation.

We call this "parallel dynamics."

Repairing

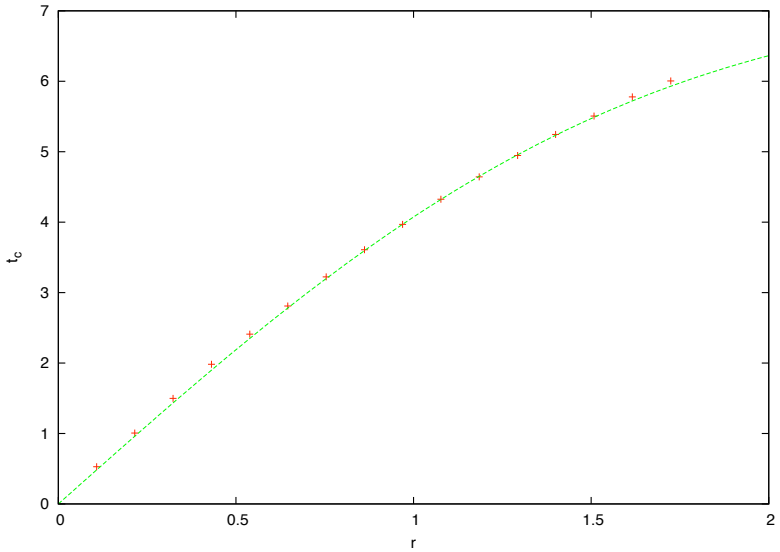
If P is an odd permutation then, on the average, the descendants of a walker at R^+ have exactly the negative of the expectations (weighted with an antisymmetric function) of the descendants of PR^+.

No bias is introduced if a walker at R^+ is replaced, with probability ½ , by the pair of walkers (R^+, PR^+) for ***any*** odd permutation P.

This is analogous to applying an antisymmetrizing operator.

The figure shows the cancellation time for 80 free fermions as a function of the initial Euclidean separation of the pair.

We can adjust the average cancellation time by choosing different permutations.



$$t_c(r) = 0.82r(6-r)$$

Breaking the plus/minus symmetry (2)

That means that the plus/minus symmetry can be broken by explicit separation and "repairing" one or another of a pair (R^+, R^-).

Choose one of the pair at random; suppose it to be R^+. Next choose an odd permutation, P, to produce pair (R^+, PR^+). We let the choice of P depend on R^+ in the following way:

If $\psi_A(R^+) > 0$, choose P so that $|R^+ - PR^+|$ is large ;

If $\psi_A(R^+) < 0$, choose P so that $|R^+ - PR^+|$ is small.

If the walker to be repaired is R^-, then the sense of the inequalities is reversed.

Now the evolution depends explicitly on the +/− labels of the pair.

The symmetry is broken.

Importance Sampling (2)

In the experiments we have recently carried out, we use two distinct stages of importance functions. In the first stage, which uses simple DMC, we set the importance function for both walkers to be a ***symmetric*** function, $\psi_S(R)$, an approximation to the ground state of the Hamiltonian.

Symmetry breaking using different permutations guarantees stability, but not necessarily a practical level of computational efficiency. It can be improved with the introduction of a ***second-stage importance function***, $\Psi_2(R^+,R^-)$, using ratios of this function before and after a move of $\delta\tau$ to determine the outcome of a branching process.

To specify the form of this new function, write the denominator of the energy quotient as

$$D(R^+,R^-) = \frac{\psi_A(R^+)}{\psi_S(R^+)} - \frac{\psi_A(R^-)}{\psi_S(R^-)}$$

Two-dimensional Free Fermions

For the two-dimensional free fermion system, we use a constant symmetric function, and a Slater determinant with distorted plane waves as orbitals.

$$\psi_A = \left\| e^{-i\vec{k}_\alpha \cdot \vec{r}_\beta} + \zeta e^{-3i\vec{k}_\alpha \cdot \vec{r}_\beta} \right\|$$
$$\psi_S = 1$$

ζ is an adjustable constant designed to create controllably bad nodal surfaces.

It is easy to get a fixed-node energy 10% too high.

Second-stage Importance Function & Stability

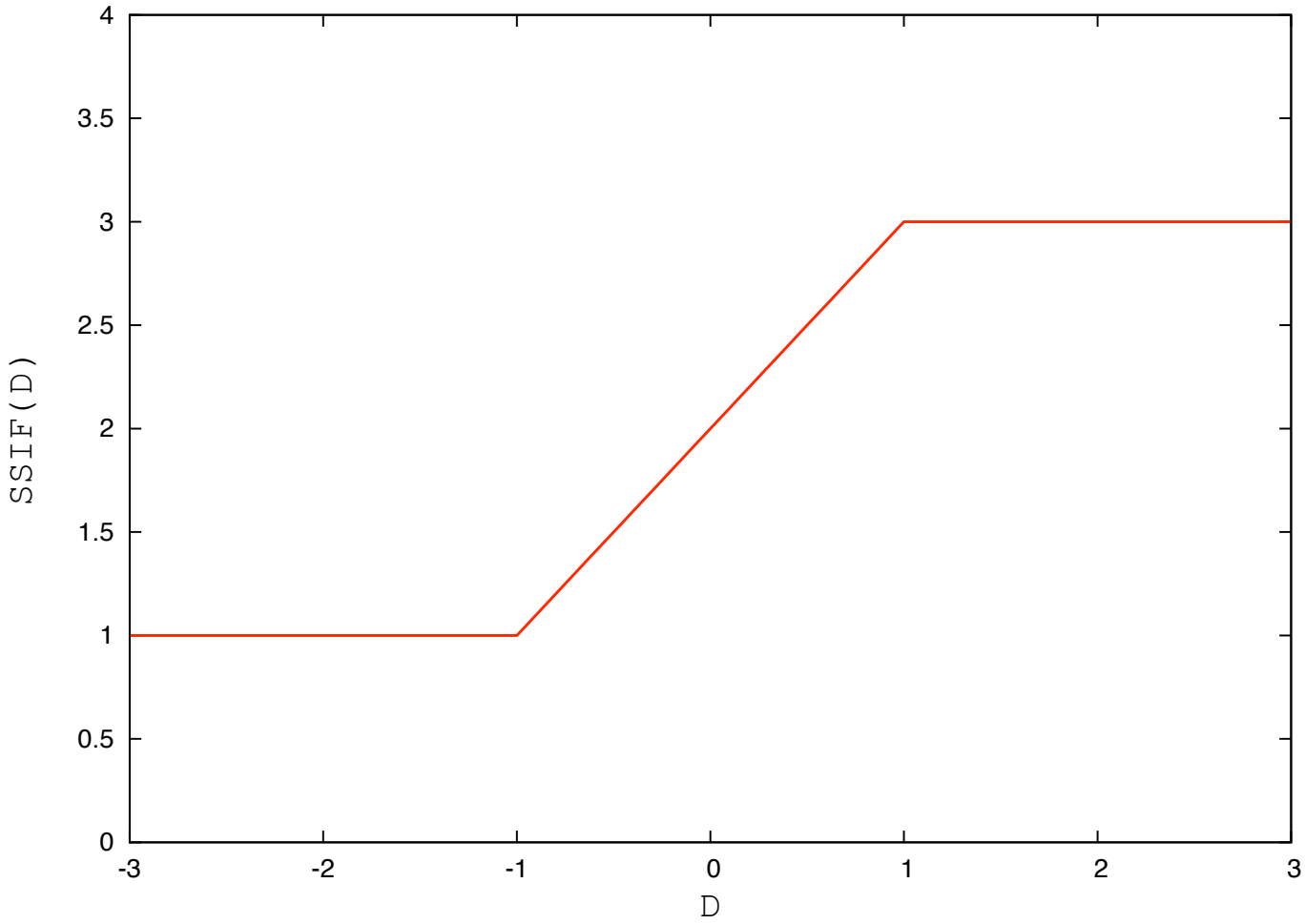
Then

$$\Psi_2(R^+, R^-) = SSIF(D)$$

with parameters to be determined to optimize efficiency.

The stochastic operator that advances the walkers is not invariant under interchange of the signs of the walkers, so that the equilibrium distribution will in general have a non-zero overlap with the antisymmetric function ψ_A.

Second-stage Importance Function-- SSIF(D)



Dynamics of stability

- ***First-stage importance*** ψ_S drives walkers to its maxima.
- ***Correlation of gaussians*** brings plus and minus walkers together.
- ***Cancellation of walkers reduces symmetric component of distribution.***
- ***Repairing with permutations that depend on the sign of the walker*** breaks the +/- symmetry. For example, a walker on the correct side of the nodal surface can live longer before cancellation than a walker on the wrong side.
- *D* is the energy denominator: $\psi_A(R^+) / \psi_S(R^+) - \psi_A(R^-) / \psi_S(R^-)$
- ***Second stage importance*** causes pairs with positive *D* to drift apart and tend to avoid cancellation.
- Pairs with negative *D* do not drift apart and cancellation is more likely for them.
- ***The total effect is to produce a population of walkers having a stable overlap with an antisymmetric function, which within a linear time-step error correctly gives fermionic estimators.***
- ***For free Fermions, it is exact, except for population bias***

Conclusions

- All computational steps introduce no bias for free fermions.
- The method is manifestly stable.
- ***The sign problem is not intractable!***
- What's next?
  - —Understanding the structure of the Importance Function
  - — More efficient sampling
  - —Quantum expectations
  - —2D e-gas.
  - —Polarized ^{3}He.
  - —"Ultracold Fermions"
  - —Quantum Chemistry (finite systems)
  - —Hubbard models
  - —. . .