Fermions?

- How can we do fermion simulations? The initial condition can be made real but not positive (for more than 1 electron in the same spin state)
- In *transient estimate* or *released-node* methods one carries along the sign as a weight and samples the modulus.

$$\phi(t) = e^{-(\hat{H}-E_T)t}\,\mathrm{sign}(\phi(R,0))\,|\phi(R,0)|$$

- Do not forbid crossing of the nodes, but carry along sign when walks cross.
- What's wrong with node release:
  - Because walks don't die at the nodes, the computational effort increases (bosonic noise)
  - The signal is in the cancellation which dominates

Monte Carlo can add but not subtract

Transient Estimate Approach

$$\Psi(\beta) = e^{-\frac{\beta}{2}H}\Psi$$

$$Z(\beta) = \langle \Psi(\beta)\Psi(\beta)\rangle = \langle \Psi e^{-\beta H}\Psi\rangle = \int dR_0 \ldots dR_p \Psi(R_0)\langle R_0 e^{-\tau H} R_1\rangle \ldots \langle R_{p-1} e^{-\tau H} R_p\rangle \Psi(R_p)$$

$$E(\beta) = \frac{\langle \Psi(\beta) H \Psi(\beta)\rangle}{\langle \Psi(\beta)\Psi(\beta)\rangle} = \langle E_L(R_0)\rangle_\beta \qquad \tau = \frac{\beta}{p}$$

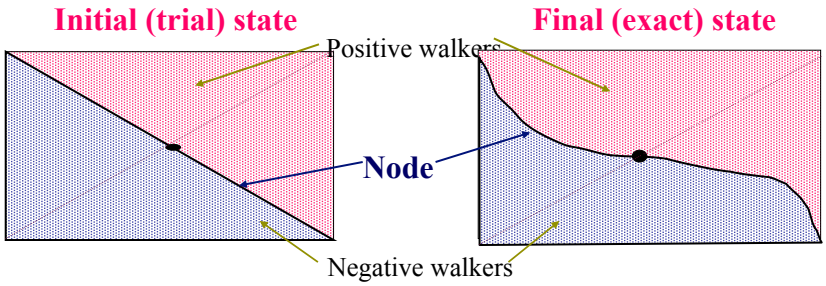
- Ψ(β) converges to the exact ground state
- E is an upper bound converging to the exact answer monotonically

$$Z(\beta) = \int dR_0 \ldots dR_p \left|\Psi(R_0)\right| \left|\langle R_0 e^{-\tau H} R_1\rangle \ldots \langle R_{p-1} e^{-\tau H} R_p\rangle\right| \left|\Psi(R_p)\right| \sigma(R_0)\sigma(R_P)$$

$$\frac{Z_{\mathrm{fermi}}}{Z_{\mathrm{bose}}} = \langle \sigma(R_0)\sigma(R_P)\rangle$$

Model fermion problem: Particle in a box

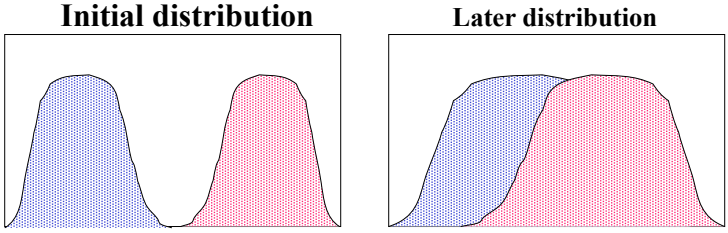
Symmetric potential: V(**r**) =V(-**r**)
Antisymmetric state: f(**r**)=-f(-**r**)



Sign of walkers fixed by initial position. They are allowed to diffuse freely. f(r)= number of positive-negative walkers. Node is dynamically established by diffusion process. (cancellation of positive and negative walkers.)

$$\langle E(t)\rangle = \frac{\sum \sigma(0)\sigma(t)E(t)}{\sum \sigma(0)\sigma(t)}$$

Scaling in Released-Node

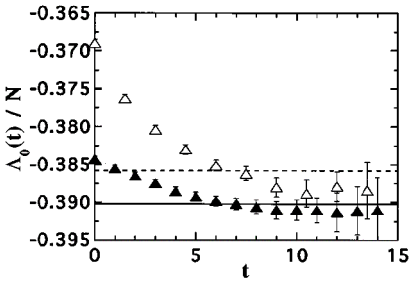


- At any point, positive and negative walkers will tend to cancel so the signal is drown out by the fluctuations.
- Signal/noise ratio is : $e^{-t[E_F - E_B]}$ **t**=projection time
  E_F and E_B are Fermion, Bose energy (proportional to **N**)
- Converges but at a slower rate. Higher accuracy, larger **t**.
- For general excited states:
  Exponential complexity! $\text{CPUtime} \propto \varepsilon^{-2(1+\frac{E_F}{E_g})} \approx \varepsilon^{-2N\frac{e_F}{E_g}}$
- Not a fermion problem but an excited state problem.
- Cancellation is difficult in high dimensions.

Exact fermion calculations

- Possible for the electron gas for up to 60 electrons.
- 2DEG at rs=1 N=26
- Transient estimate calculation with SJ and BF-3B trial functions.

$$\left\langle \Psi_T \left| e^{-tH} \right| \Psi_T \right\rangle$$



General statement of the "fermion problem"

- Given a system with **N** fermions and a known Hamiltonian and a property **O.** (usually the energy).
- How much time **T** will it take to estimate **O** to an accuracy **ε**? How does **T** scale with **N** and **ε**?
- If you can map the quantum system onto an equivalent problem in classical statistical mechanics then:

$$T \propto N^{\alpha} \varepsilon^{-2} \qquad \text{With } 0 < \alpha < 4$$

This would be a "solved" quantum problem!

- All approximations must be controlled!
- Algebraic scaling in N!

e.g. properties of Boltzmann or Bose systems in equilibrium.

"Solved Problems"

- 1-D problem. (simply forbid exchanges)
- Bosons and Boltzmanons at any temperature
- Some lattice models: Heisenberg model, 1/2 filled Hubbard model on bipartite lattice (Hirsch)
- Spin symmetric systems with purely attractive interactions: u<0 Hubbard model, nuclear Gaussian model.
- Harmonic oscillators or systems with many symmetries.
- Any problem with $\langle i|H|j\rangle \leq 0$
- Fermions in special boxes
- Other lattice models

- Kalos and coworkers have invented a pairing method but it is not clear whether it is approximation free and stable.

The sign problem

- The fermion problem is intellectually and technologically very important.
- Progress is possible but ***danger***-the problem maybe more subtle than you first might think. New ideas are needed.
- No fermion methods are perfect but QMC is competitive with other methods and more general.
- The fermion problem is one of a group of related problems in quantum mechanics (**e.g** dynamics).
- Feynman argues that general many-body quantum simulation is exponentially slow on a classical computer.
- Maybe we have to "solve" quantum problems using "analog" quantum computers: programmable quantum computers that can emulate any quantum system.

Fixed-node method

- Initial distribution is a pdf.
  It comes from a VMC simulation. $f(R,0) = |\psi_T(R)|^2$
- Drift term pushes walks away from the nodes.
- Impose the condition: $\phi(R) = 0$ when $\psi_T(R) = 0.$
- This is the fixed-node BC
- Will give an upper bound to the exact energy, the best upper bound consistent with the FNBC.

$$E_{FN} \geq E_0$$
$$E_{FN} = E_0 \text{ if } \phi_0(R)\psi(R) \geq 0 \text{ all } R$$

- f(R,t) has a discontinuous gradient at the nodal location.
- Accurate method because Bose correlations are done exactly.
- Scales well, like the VMC method, as N^3. Classical complexity.
- Can be generalized from the continuum to lattice finite temperature, magnetic fields, …
- One needs trial functions with accurate nodes.

Proof of fixed-node theorem

Suppose we solve S.E. in a subvolume V determined by the nodes of an antisymetric trial function.

$\hat{H}\phi_{FN} = E_{FN}\phi_{FN}$ inside V

Extend the solution to all space with the permutation operator.

$$\hat{\phi}_{FN}(R) \equiv \frac{1}{N!}\sum_P (-1)^P \phi_{FN}(PR)$$

Inside a given sub-volume only permutations of a given sign (±) contribute.

Hence the extend solution is non-zero.

Evaluate the variational energy of the extended trial function.

$$E_0 \leq \frac{\sum_{PP'} (-1)^{P+P'} \int dR \phi^*_{FN}(PR)\hat{H}\phi_{FN}(P'R)}{\sum_{PP'} (-1)^{P+P'} \int dR \phi^*_{FN}(PR)\phi_{FN}(P'R)} = E_{FN} \leq E_{VMC}$$

Surfaces do not contribute to the integral since the solution vanishes there.

Nodal Properties

If we know the sign of the exact wavefunction (the nodes), we can solve the fermion problem with the fixed-node method.

- If f(R) is real, nodes are f(R)=0 where R is the 3N dimensional vector.
- Nodes are a 3N-1 dimensional surface. (Do not confuse with single particle orbital nodes!)
- Coincidence points $\mathbf{r}_i = \mathbf{r}_j$ are 3N-3 dimensional hyper-planes
- In 1 spatial dimension these "points" exhaust the nodes: *fermion problem is easy to solve in 1D* with the "no crossing rule."
- Coincidence points (and other symmetries) only constrain nodes in higher dimensions, they do not determine them.
- The nodal surfaces define nodal volumes. How many nodal volumes are there? **Conjecture**: there are typically *only* 2 different volumes (+ and -) except in 1D. (but only demonstrated for free particles.)

Nodal Picture: 2d slice thru 322d space

- Free electron
- Other electrons

- Nodes pass thru their positions
- Divides space into 2 regions
- Wavelength given by interparticle spacing

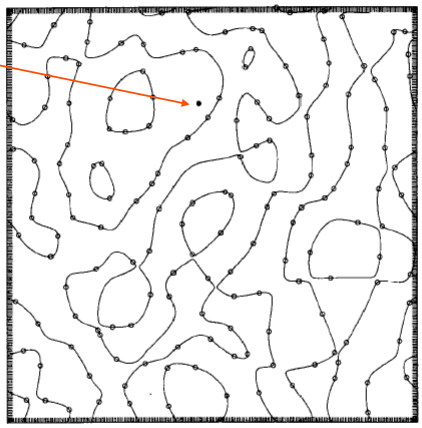


Fig. 3. A 2D cross section of the ground-state wave function of 161 free (polarized) fermions in a periodic square. All 161 particle positions were sampled using variational Monte Carlo from $\phi(R)^2$. The filled circle indicates the original position of the first particle. The other 160 particles are fixed at positions indicated by the open circles, and nodes of the wave function as a function of the position of the first particle are plotted. The resolution of the contouring program is approximately half of the fine scale shown around the border of the plot.

SPIN?

- How do we treat spin in QMC?
- For extended systems we use the S_z representation.
- We have a fixed number of up and down electrons and we antisymmetrize among electrons with the same spin.
- This leads to 2 Slater determinants.
- For a given trial function, its real part is also a trial function (but it may have different symmetries), for example momentum

$$\left(e^{ikr}, e^{-ikr}\right) \quad \text{or} \quad \left(\cos(kr), \sin(kr)\right)$$

- For the ground state, without magnetic fields, spin-orbit interaction we can always work with real functions.
- However, in some cases it may be better to work with complex functions.

Fixed-Phase method

Ortiz, Martin, DMC 1993

- Generalize the FN method to complex trial functions: $\Psi(R) = e^{-U(R)}$
- Since the Hamiltonian is Hermitian, the variational energy is real:

$$E_V = \frac{\int dR\, e^{-2\Re U(R)} \left[V(R) + \lambda \nabla^2 U(R) - \lambda \left[\Re \nabla U(R)\right]^2 + \lambda \left[\Im \nabla U(R)\right]^2 \right]}{\int dR\, e^{-2\Re U(R)}}$$

- We see only one place where the energy depends on the phase of the wavefunction.
- We fix the phase, then we add this term to the potential energy. In a magnetic field we get also the vector potential.

$$\text{effective potential} = V(R) + \sum_i \lambda_i \left[A(r_i) + \Im \nabla_i U(R) \right]^2$$

- We can now do VMC or DMC and get upper bounds as before.
- The imaginary part of the local energy will not be zero unless the right phase is used.
- Used for twisted boundary conditions, magnetic fields, vortices, phonons, spin states, …