Brief introduction to sign problems for many-electron systems in the continuum

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- Quantum Monte Carlo
  - Zero temperature methods
  - Path Integral methods
- The "sign problem"

Variational Monte Carlo (VMC)

(McMillan 1965)

- Put correlation directly into the wavefunction.
- Integrals are hard to do: need MC.
- VMC has no sign problem, and classical complexity
- Take sequence of increasingly better wavefunctions. Stochastic optimization is important!
- Progress in optimization, multiple determinants, tensor networks,….
- **Can we make arbitrarily accurate functions?** Method of residuals says how to do this.

- Posit a wavefunction $\Psi(\mathbf{R},\mathbf{a})$
- sample $|\Psi(\mathbf{R},\mathbf{a})|^2$ with random walk.
- minimize energy or variance of $\Psi(\mathbf{R},\mathbf{a})$ with respect to $\mathbf{a}$
- Zero variance principle

$$e(R) \equiv \Psi(R)^{-1} H \Psi(R) = residual$$

$$E_V = \left\langle e(R) \right\rangle_{|\Psi^2|} \quad \sigma^2 = \left\langle \delta e(R)^2 \right\rangle_{|\Psi^2|}$$

$$\Psi_2(R) = Det\{\phi_i(\mathbf{r}_j)\} e^{-\sum_{i<j} u_{ij}(r_{ij})}$$

$$\Psi_{n+1}(R) \approx \Psi_n(R) e^{-\underbrace{<e(R)>}}$$

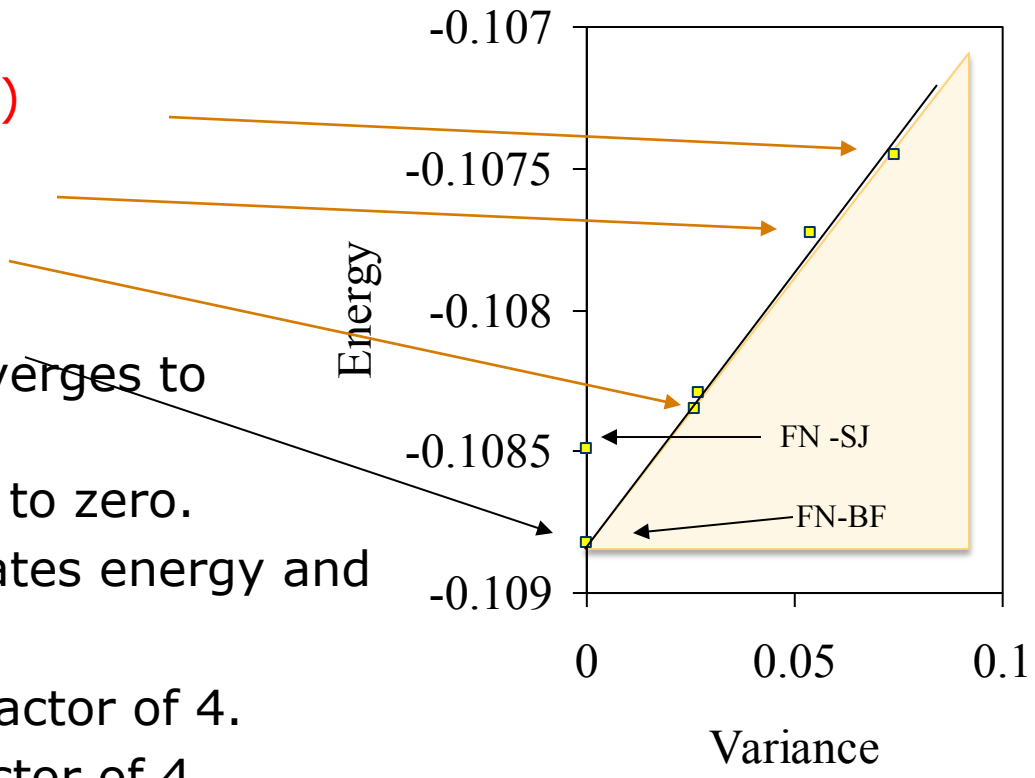
smoothing

Dependence of energy on wavefunction

3d Electron fluid at a density r_s=10

Kwon, Ceperley, Martin, Phys. Rev. ***B58****,6800, 1998*

- Wavefunctions
  - Slater-Jastrow (SJ)
  - three-body (3)
  - backflow (BF)
  - fixed-node (FN)
- Energy <f |H| f> converges to ground state
- Variance <f $[H-E]^2$ f> to zero.
- Temple inequality relates energy and variance
- Using 3B-BF gains a factor of 4.
- Using DMC gains a factor of 4.



Bayesian methods can provide tight upper and lower bounds

Projector Monte Carlo

e.g. Diffusion Monte Carlo (DMC)

- Automatic way to get better wavefunctions.
- Project single state using the Hamiltonian

$$\Psi(R,t) = e^{-(\mathrm{H}-\mathrm{E})\mathrm{t}}\Psi(R,0)$$

- This is a diffusion + branching operator.
- **But is this a probability?**
- **Yes!** for bosons since ground state can be made real and non-negative. **But** all excited states must have sign changes.
- In exact methods one carries along the sign as a weight and samples the modulus. This leads to the famous sign problem

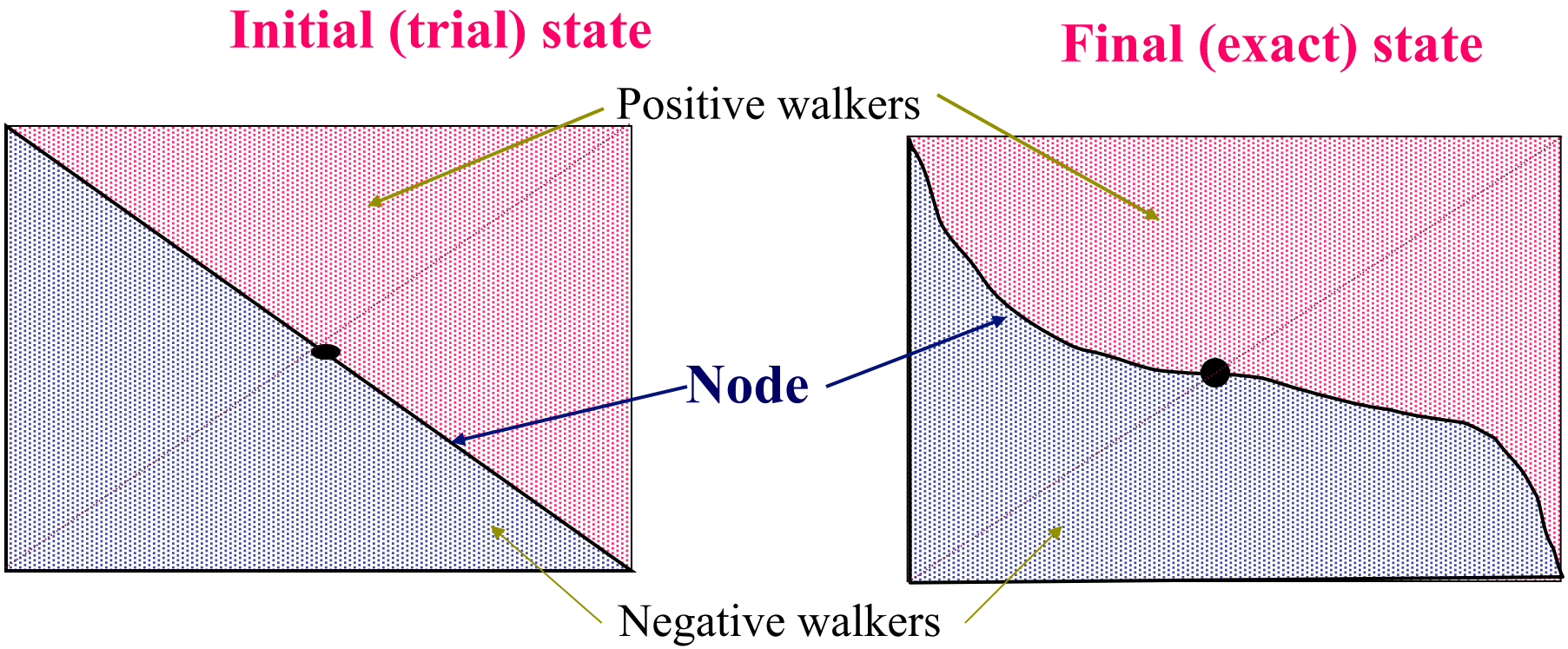
$$\phi(t) = e^{-(\mathrm{H}-\mathrm{E})\mathrm{t}}\ \mathrm{sign}(\phi(R,0))\,|\,\phi(R,0)\,|$$

- Zero variance principle still applies: fluctuations only due to trial function error.

Model fermion problem: Particle in a box

Symmetric potential: $V(\mathbf{r}) = V(-\mathbf{r})$

Antisymmetric state: $\Psi(\mathbf{r}) = -\Psi(-\mathbf{r})$

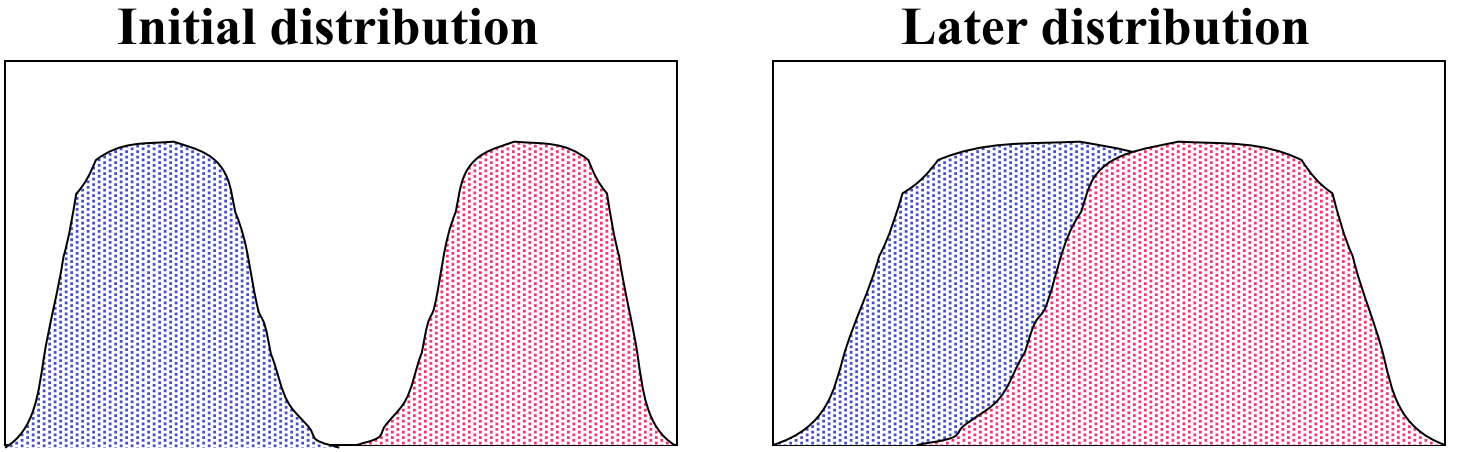


Sign of walkers fixed by initial position. They are allowed to diffuse freely.

$\Psi(r)$= number of positive-negative walkers.

Node is dynamically established by cancellation of positive and negative walkers.

Scaling in Released-Node



- At any point, positive and negative walkers will tend to cancel so the signal is overwhelmed by the fluctuations.
- Signal/noise ratio is : $\mathbf{e}^{-\mathbf{t}[\mathbf{E_F}-\mathbf{E_B}]}$ **t**=projection time

E_F and **E_B** are Fermion, Bose energy (proportional to **N**)

$$CPUtime \propto \varepsilon^{-2(1+\frac{E_F}{E_g})} \approx \varepsilon^{-2N\frac{e_F}{E_g}}$$

Cancellation Methods

- Keep exactness and try to improve the scaling by coupling positive and negative walkers.
- Let plus and minus walkers annihilate when they are "close." (Arnow, 1980)
- "Closeness" defined in **3N** dimensions:

$$|\mathbf{R}-\mathbf{R}'|^2=\sum_{i=1}^{N}(\mathbf{r}_i-\mathbf{r}_i')^2 \propto N$$

- The density is too low in many dimensions

  growth rate >> death rate.
- The number of walkers needed to achieve dynamical stability grows exponentially in **N**.
- You do not both ***solve*** the sign problem ***and*** have a ***scalable*** algorithm.
- Alavi (2009) FCI-QMC: Work in a finite second quantized basis..
- Can we guide oppositely signed walkers together to annihilate?

Fixed-node method

- Impose the fixed-node BC condition:

$$\phi(R) = 0 \quad \text{when } \psi_T(R) = 0.$$

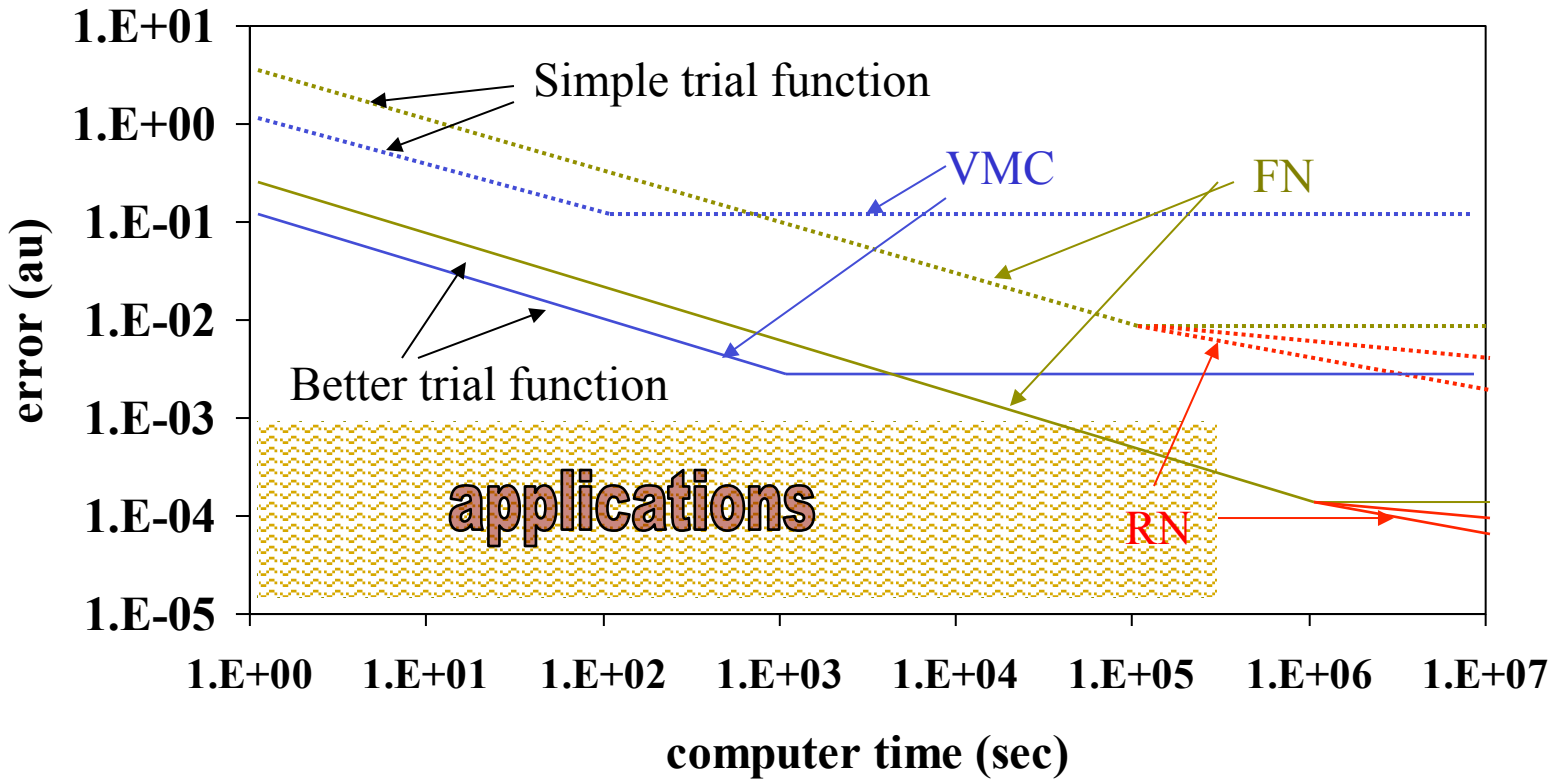
- Will give an upper bound to the exact energy, the best upper bound consistent with the FNBC.

$$E_V \geq E_{FN} \geq E_0$$

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

- Φ(R,t) has a discontinuous gradient at the nodal location.
- Accurate method because Bose correlations are done exactly.
- Scales like the VMC method, as N^3 or better.
- But we need to know the nodes!

Summary of T=0 methods:
Variational(VMC),
Fixed-node(FN),
Released-node(RN)



"Direct" Fermion Path Integrals

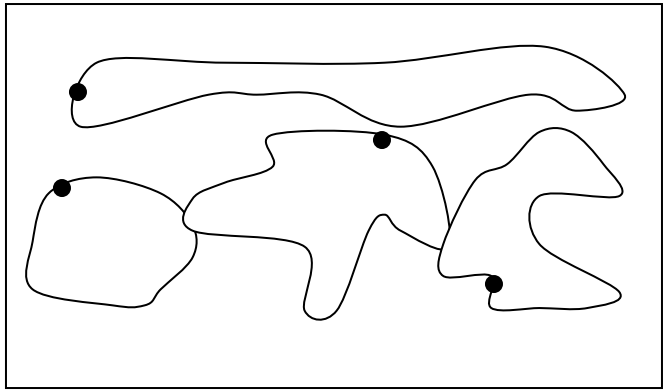
- Path integrals map quantum mechanics into a system of cross-linking closed "polymers."

$$Z = \sum_{p=1}^{N!} \frac{(-1)^P}{N!} \int dR_1 \ldots dR_M e^{-\sum_{i=1}^{M} S(R_i, R_{i+1})}$$

$R_0 = P R_M$, **P** permutation,

$S(R_i, R_{i+1})$ is "boltzmannon action"

4 quantum paths



- Bosons are easy: simply sample **P**.
- Fermions: sample the "action" and carry **$(-1)^P$** as a weight.
- Observable is **even P - odd P.** scales exponentially in N and T^{-1}!

$$\text{CPUtime} \propto \varepsilon^{-2} e^{2N[\mu_F - \mu_B]/k_B T}$$

Generalizations of Fixed-Node method

- Positive temperature: restricted fermion path integrals. Similar to zero temperature method: Exact nodes imply exact answer.
- Lattices with auxiliary fields (Fahy, Zhang …). Requires projection on a Slater determinant to be always positive.

Some methods require magnitude of trial function to be correct, not just the nodes:

- Magnetic fields or complex wavefunctions: fixed-phase method. (Ortiz et al., Carlson) Input phase and solve for modulus.
- Lattice fixed-node: (Bemmel et al). Requires trial function "near" the sign changes.

Can we do quantum dynamics with fixed-node?

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:

$$T \propto N^{\alpha} \varepsilon^{-2} \qquad \text{With } 0 < \alpha < 3$$

This would be a "solved" quantum problem!

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

Materials problem: "Solve" electronic structure problems with "chemical accuracy" (<<300K /atom) on systems containing thousands of electrons with available computer power.