Improved Wavefunctions

Generalized Feynman-Kacs formula

- Let's calculate the average population resulting from DMC starting from a single point R_0 after a time `t'.

$$P(R_0;t) = \int dR \frac{\psi(R)}{\psi(R_0)} \left\langle R \left| e^{-t(H-E_T)} \right| R_0 \right\rangle = \left\langle \left\langle e^{-\int_0^t dt E_L(t)} \right\rangle \right\rangle_{|\psi|}$$

expand the density matrix in terms of exact eigenstates

$$P(R_0;t) = \int dR \frac{\psi(R)}{\psi(R_0)} \sum_\alpha \phi_\alpha^*(R) \phi_\alpha(R_0) e^{-t(E_\alpha - E_T)}$$

$$\lim_{t\to\infty} P(R_0;t) = \frac{\phi_0(R_0)}{\psi(R_0)} \langle \psi \phi_0 \rangle$$

$$\frac{\phi_0(R_0)}{\psi(R_0)} \sim e^{-\int_0^t dt \langle\langle E_L(t) \rangle\rangle_{|\psi|}}$$

Wavefunctions beyond Jastrow

- Use method of residuals construct a sequence of increasingly better trial wave functions. Justify from the Importance sampled DMC.
- Zeroth order is Hartree-Fock wavefunction
- First order is Slater-Jastrow pair wavefunction (RPA for electrons gives an analytic formula)
- Second order is 3-body backflow wavefunction
- Three-body form is like a squared force. It is a bosonic term that does not change the nodes.

$$\exp\{\sum_i [\sum_j \xi_{ij}(r_{ij})(\mathbf{r}_i - \mathbf{r}_j)]^2\}$$

smoothing

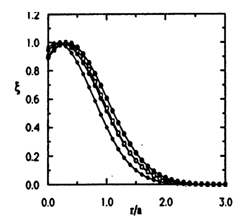
$$\phi_{n+1}(R) \approx \phi_n(R) e^{-\tau<\phi_n^{-1} H \phi_n>}$$

$$\phi_0 = e^{i\sum_j \mathbf{k}_j \bullet \mathbf{r}_j}$$

$$E_0 = V(R)$$

$$\phi_1 = \phi_0 e^{-U(R)}$$

$$E_1 = U(R) - [\nabla W(R)]^2 + i\sum_j \mathbf{k}_j \bullet (\mathbf{r}_j - \nabla_j Y(R))$$



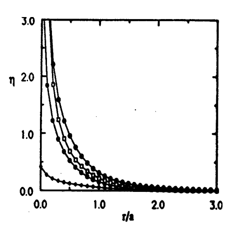
Backflow wave function

- Backflow means change the coordinates to quasi- coordinates.
- Leads to a much improved energy and to improvement in nodal surfaces. Couples nodal surfaces together.

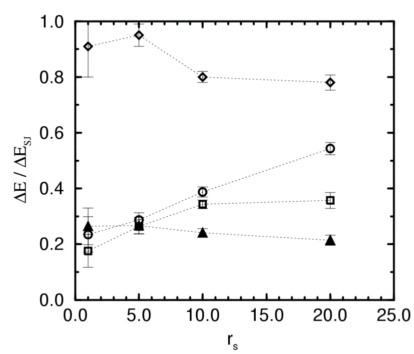
Kwon PRB 58, 6800 (1998).

$$Det\{e^{i\mathbf{k}_i\mathbf{r}_j}\} \Rightarrow Det\{e^{i\mathbf{k}_i\mathbf{x}_j}\}$$

$$\mathbf{x}_i = \mathbf{r}_i + \sum_j \eta_{ij}(r_{ij})(\mathbf{r}_i - \mathbf{r}_j)$$



3DEG

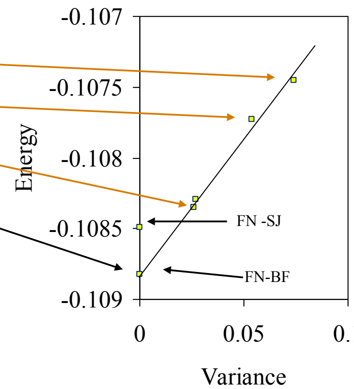


Dependence of energy on wavefunction

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.
- Using 3B-BF gains a factor of 4.
- Using DMC gains a factor of 4.



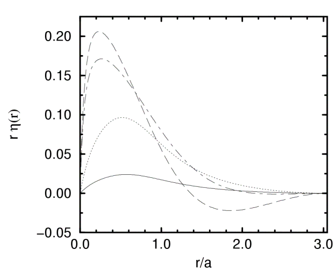
Ceperley Finite Size effects

Analytic backflow

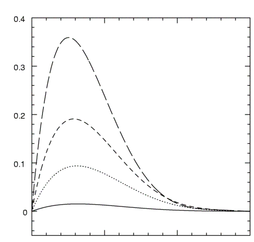
Holzmann et al, Phys. Rev. ***E 68****, 046707:1-15(2003).*

- Start with analytic Slater-Jastrow using Gaskell trial function
- Apply Bohm-Pines collective coordinate transformation and express Hamiltonian in new coordinates
- Diagonalize resulting Hamiltonian.
- Long-range part has Harmonic oscillator form.
- Expand about k=0 to get backflow and 3-body forms.
- Significant long-range component to BF

OPTIMIZED BF



ANALYTIC BF



r_s=1,5,10,20

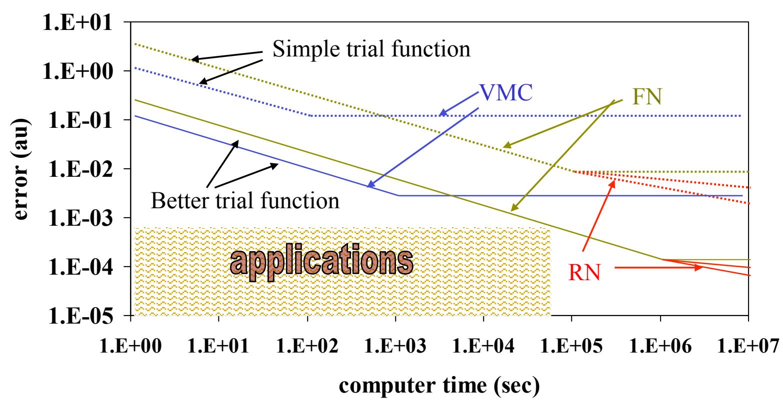
- 3-body term is non-symmetric

$$\Psi_2(R)\exp\{\sum_i \vec{\nabla}_i W_y(R)\vec{\nabla}_i W_u(R)\}$$

Ceperley Finite Size effects

Summary of T=0 methods:

Variational(VMC), Fixed-node(FN), Released-node(RN)



Problems with projector methods

- Fixed-node is a super-variational method
- DMC dynamics is determined by Hamiltonian
- Zero-variance principle allows very accurate calculation of ground state energy if trial function is good.
- Projector methods need a trial wavefunction for accuracy. They are essentially methods that perturb from the trial function to the exact function. (Note: if you don't use a trial function, you are perturbing from the ideal gas)
- Difficulty calculating properties other than energy. We must use "extrapolated estimators" or "forward walking".

$$f(R,\infty) = \phi_0(R)\psi_T(R) \text{ not } |\phi_0(R)|^2$$

- Bad for phase transitions and finite temperature