# The Variational Monte Carlo Method

The theorem + restrictions

Upper and lower bounds: variance

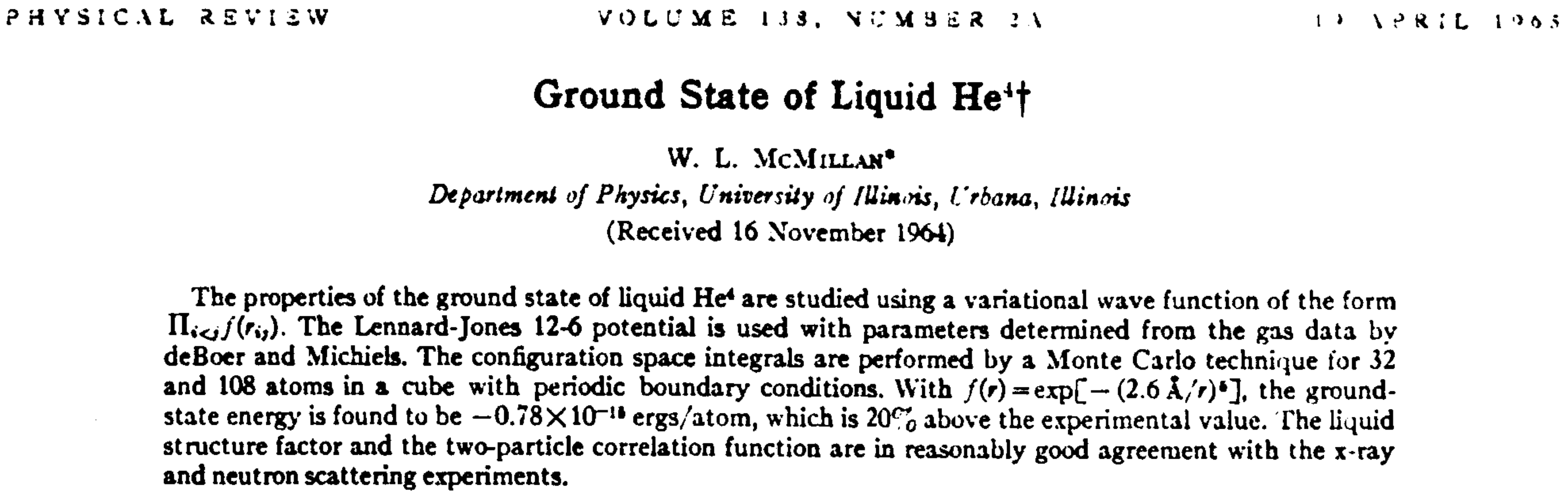
How to do the variation.

McMillan's calculation on liquid $^4$He

Fermion VMC

# First Major QMC Calculation

- PhD thesis of W. McMillan (1964) University of Illinois.
- VMC calculation of ground state of liquid helium 4.
- Applied MC techniques from classical liquid theory.
- Ceperley, Chester and Kalos (1976) generalized to fermions.



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## Ground State of Liquid He$^4$†

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(Received 16 November 1964)

The properties of the ground state of liquid He$^4$ are studied using a variational wave function of the form $\Pi_{i<j} f(r_{ij})$. The Lennard-Jones 12-6 potential is used with parameters determined from the gas data by deBoer and Michiels. The configuration space integrals are performed by a Monte Carlo technique for 32 and 108 atoms in a cube with periodic boundary conditions. With $f(r) = \exp[-(2.6\ \text{Å}/r)^5]$, the ground-state energy is found to be $-0.78\times10^{-15}$ ergs/atom, which is 20% above the experimental value. The liquid structure factor and the two-particle correlation function are in reasonably good agreement with the x-ray and neutron scattering experiments.

- Zero temperature (single state) method
- Can be generalized to finite temperature by using “trial” density matrix instead of “trial” wavefunction.

# The “Variational Theorem”

Assume $\psi(R;a)$ is a trial function where R are the quantum degrees of freedom (positions, spin) “a” are “variational “parameters.

$$E_V(a) = \frac{\langle \psi(a) H \psi(a) \rangle}{\langle \psi(a) \psi(a) \rangle} \geq E_0 = \text{exact ground state energy}$$

$$\langle \psi(a) H \psi(a) \rangle \equiv \int dR \psi^*(R;a) H \psi(R;a)$$

$$E_V(a) = E_0 \Leftrightarrow \psi(R;a) = \phi_0(R)$$

$$E_L(R;a) \equiv \frac{1}{\psi(R;a)} H \psi(R;a) = \text{"local energy" of trial function}$$

$$E_V(a) = \langle\langle E_L(R;a) \rangle\rangle_{\psi^2} \quad \text{where} \quad \langle\langle O \rangle\rangle_{\psi^2} \equiv \frac{\langle \psi(a) O \psi(a) \rangle}{\langle \psi(a) \psi(a) \rangle}$$

$$\sigma^2(a) \equiv \frac{\langle \psi(a) \left(H - E_V(a)\right)^2 \psi(a) \rangle}{\langle \psi(a) \psi(a) \rangle} = \left\langle\left\langle \left(E_L(R;a) - E_V(a)\right)^2 \right\rangle\right\rangle_{\psi^2} = \text{variance of the trial function}$$

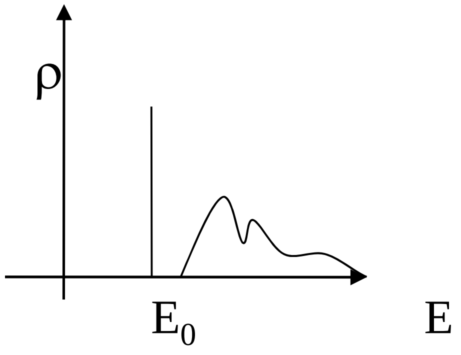
$$\frac{dE_V(a)}{da} = 2 \left\langle\left\langle \frac{d \ln \psi(R;a)}{da} \left(E_L(R;a) - E_V(a)\right) \right\rangle\right\rangle = 0$$

Conditions: matrix elements exist, symmetries and boundary conditions are correct.

Expand trial function in terms of the exact eigenfunctions:

$$\psi(R;a) = \sum_{\alpha} \phi_{\alpha}(R) \langle \alpha | \psi(a) \rangle$$

$$E_V(a)) = \frac{\sum_{\alpha} E_{\alpha} \left| \langle \alpha | \psi(a) \rangle \right|^2}{\sum_{\alpha} \left| \langle \alpha | \psi(a) \rangle \right|^2} = \int dE \rho_a(E) E$$



$$\rho_a(E) = \sum_{\alpha} \delta(E - E_{\alpha}) \frac{\left| \langle \alpha | \psi(a) \rangle \right|^2}{\left\langle \left| \psi(a) \right|^2 \right\rangle} \geq 0 \qquad \int_{-\infty}^{\infty} dE \rho(E) = 1$$

$$\sigma^2(a) = \int dE \rho_a(E) \left( E - E_V(a) \right)^2$$

$$O(a) \equiv \rho_a(E_0) = 1 - \int_{E_0+}^{\infty} dE \rho_a(E) = \frac{\left| \langle 0 | \psi(a) \rangle \right|^2}{\left\langle \left| \psi(a) \right|^2 \right\rangle} = \text{overlap with ground state}$$

Energy and variance are second order in (1-overlap).

Other properties are first order.

Temple lower bound:

$$\boxed{E_v - \frac{\sigma^2}{E_1 - E_0} \leq E_0 \leq E_v}$$

# Linear Basis approach

- Assume trial function is a linear combination of known functions: a basis $f_n(R)$.

$$\psi(R;\mathbf{a}) = \sum_{n=1}^{m} a_n f_n(R)$$

$$E_V(\mathbf{a}) = \frac{\sum_{n,m} \mathbf{a}_n^* \mathbf{a}_m H_{nm}}{\sum_{n,m} \mathbf{a}_n^* \mathbf{a}_m S_{nm}}$$

$$S_{nm} = \langle f_n f_m \rangle = \text{overlap matrix}$$

$$H_{nm} = \langle f_n H f_m \rangle = \text{Hamiltonian matrix } H$$

$$S_{nm} = \delta_{nm} \text{ in an orthonormal basis} \qquad S$$

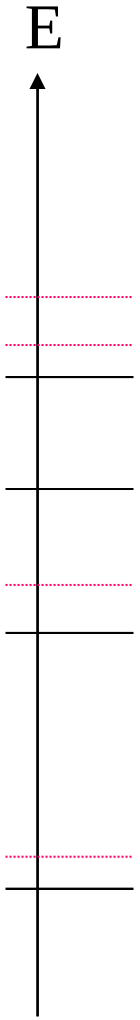
$$\frac{dE}{da} = 2\left[Ha - E_v S a\right]$$

$$Ha_\lambda = E_\lambda S_\lambda \quad \text{generalized eigenvalue problem}$$

Problem that MC solves:

Unless we use 1-particle basis, integrals are too slow to perform.

# Properties of solution to GEP



- For a basis of size m, there exist “m” eigenvalues and orthonormal eigenfunctions:

$$\psi_n(R) = \sum_{k=1}^{m} a_{k,n} f_k(R)$$

$$\langle \psi_n \psi_m \rangle = a_n^* S_{nm} a_m = \delta_{nm}$$

- McDonald’s theorem: the n$^{th}$ eigenvalue in a basis is an upper bound to the n$^{th}$ “exact eigenvalue.

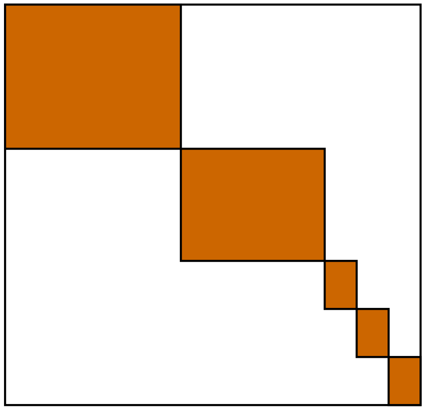
$$E_0 \le E_1 \le E_2 \le \ldots \le E_m$$

$$E_n^{ex} \le E_n$$

- We can always lower all the energies by augumenting the basis
- When basis is complete, we get exact answers!

# Symmetry reduces complexity

- If an operator P commutes with H: $[P,H]=0$ we can reduce complexity by working in a basis with that symmetry.
  - rotational symmetry use $Y_{lm.}$
  - Translation symmetry: use plane waves.
  - Inversion symmetry: even/odd functions
- Matrix elements are non-zero only for states within the same "sector".
- By reordering we can block diagonalize
- Reduces complexity from $M^3$ to $k(M/k)^3=M^3/k^2$.
- McDonald's theorem applies to each sector individually.



# The Variational Method

- Approximate the solution to an eigenvalue problem with a trial function
- Upper bound guaranteed.
- In a linear basis, problem reduces to the generalized eigenvalue problem for a finite-sized matrix.
- Problems:
  - What goes in, comes out.
  - How do access convergence?
  - Have to do the matrix elements
  - What is the complexity?
    - Eigenvalue problem is $M^3$
    - Basis needs to scale exponentially with number of particles.

# Notation

- Individual coordinate of a particle $r_i$
- All 3N coordinates $R = (r_1, r_2, \ldots. r_N)$
- R can depend on "imaginary time", "time slice" or "Trotter index" "t" or on iteration number.

- Total potential energy = V(R)
- Kinetic energy = $-\lambda \sum_{i=1}^{N} \nabla_i^2$ where $\lambda \equiv \frac{\hbar^2}{2m}$
- Hamiltonian = $\hat{H} = \hat{T} + \hat{V}$

# Variational Monte Carlo (VMC)

- Variational Principle. Given an appropriate trial function:
  - Continuous
  - Proper symmetry
  - Normalizable
  - Finite variance
- Quantum chemistry uses a product of single particle functions
- With MC we can use any "computable" function.

$$E_V = \frac{\int dR \langle \psi | H | \psi \rangle}{\int dR \langle \psi \psi \rangle} \geq E_0$$

$$\sigma^2 = \frac{\int dR \langle \psi | H^2 | \psi \rangle}{\int dR \langle \psi \psi \rangle} - E_V^2$$

- Sample R from $|\psi|^2$ using MCMC.
- Take average of local energy:
- Optimize $\psi$ to get the best upper bound

$$E_L(R) = \Re\left[\psi^{-1}(R) H \psi(R)\right]$$

$$E_V = \langle E_L(R) \rangle_{\psi^2} \geq E_0$$

- Better wavefunction, lower variance! "Zero variance" principle. (non-classical)

# Liquid helium
# the prototypic quantum fluid

- Interatomic potential is known more accurately than any other atom because electronic excitations are so high.
- A helium atom is an elementary particle. A weakly interacting hard sphere.

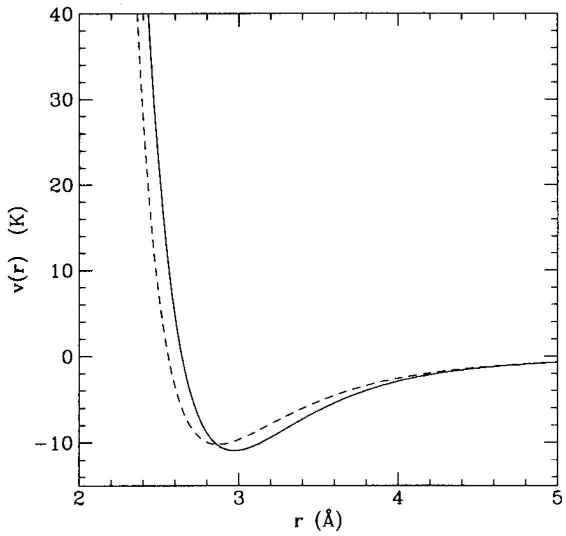


**FIG. 1.** The semiempirical pair potential between two helium atoms: solid line, Aziz *et al.* (1992); dashed line, Lennard-Jones 6-12 potential with $\epsilon = 10.22$ K and $\sigma = 2.556$ Å.

- Two isotopes:
  - $^3$He (fermion: antisymmetric trial function, spin 1/2)
  - $^4$He(boson: symmetric trial function, spin zero)

# Helium phase diagram

- Because interaction is so weak helium does not crystallize at low temperatures. Quantum exchange effects are important
- Both isotopes are quantum fluids and become superfluids below a critical temperature.
- One of the goals of computer simulation is to understand these states, and see how they differ from classical liquids starting from non-relativistic Hamiltonian:

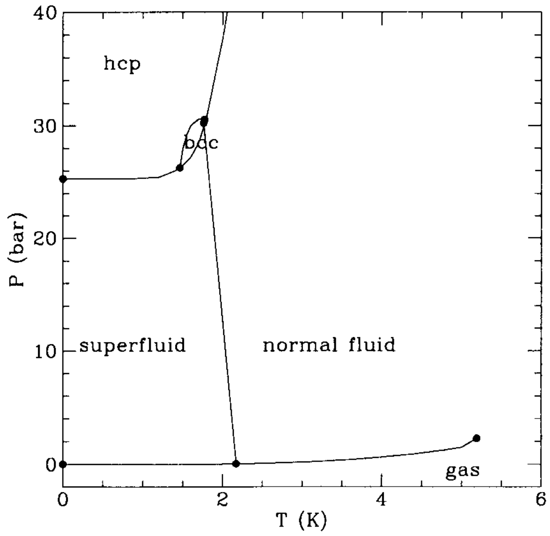


FIG. 2. The phase diagram of $^4$He.

$$\widehat{H} = -\sum_i \frac{\hbar^2}{2m_i}\nabla_i^2 + V(R)$$

$$\lambda \equiv \frac{\hbar^2}{2m_i}$$

# Trial function for helium

- We want finite variance of the local energy.
- Whenever 2 atoms get close together wavefunction should vanish.
- The pseudopotential u(r) is similar to classical potential
- Local energy has the form:

  G is the pseudoforce:

$$\psi(R) = \prod_{i<j} e^{-u(r_{ij})}$$

$$E_\psi(R) = \sum_{i<j} v(r_{ij}) - 2\lambda\nabla^2 u(r_{ij}) - \lambda\sum_i G_i^2$$

$$G_i = \sum \nabla_i u(r_{ij})$$

If v(r) diverges as $\varepsilon r^{-n}$ how should u(r) diverge? Assume:

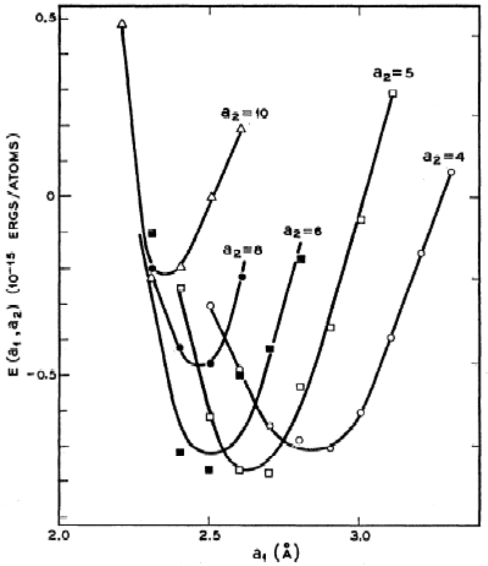
$U(r)=\alpha r^{-m}$ →

$$\boxed{\begin{aligned} &\varepsilon r^{-n} = 2\lambda\left(\alpha m r^{-m-1}\right)^2 \quad \text{for } n > 2 \\ &m = \frac{n}{2} - 1 \\ &\alpha = \frac{1}{m}\sqrt{\frac{\varepsilon}{2\lambda}} \end{aligned}}$$

Gives a cusp condition on u.

$$\boxed{\begin{aligned} &-e^2 r^{-1} = 2\lambda\nabla^2 \mathrm{u(r)} = 2\lambda\left(u'' + \frac{D-1}{r}u'\right) \\ &u'(0) = -\frac{e^2}{2\lambda(D-1)} \end{aligned}}$$

# Optimization of trial function



- Try to optimize u(r) using reweighting (correlated sampling)
  - Sample R using P(R)= $\psi^2(R,a_0)$
  - Now find minima of the analytic function $E_v(a)$
  - Or minimize the variance (more stable but wavefunctions less accurate).
- Statistical accuracy declines away from $a_0$.

$$E_V(a) = \frac{\int \psi(a) H \psi(a)}{\int |\psi(a)|^2}$$

$$= \frac{\sum_k w(R_i,a) E(R_i,a)}{\sum_k w(R_i,a)}$$

$$w(R_i,a) = \frac{|\psi(R,a)|^2}{P(R)}$$

$$E(R,a) = \psi^{-1}(R,a) H \psi(R,a)$$

$$N_{eff} = \frac{\left[\sum_i w_i\right]^2}{\sum_i w_i^2}$$

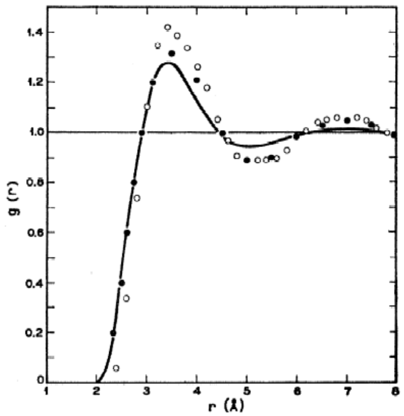
# Other quantum properties

- Kinetic energy
- Potential energy
- Pair correlation function
- Structure function
- Pressure (virial relation)

Like properties from classical simulations

No upper bound property

Only first order in accuracy



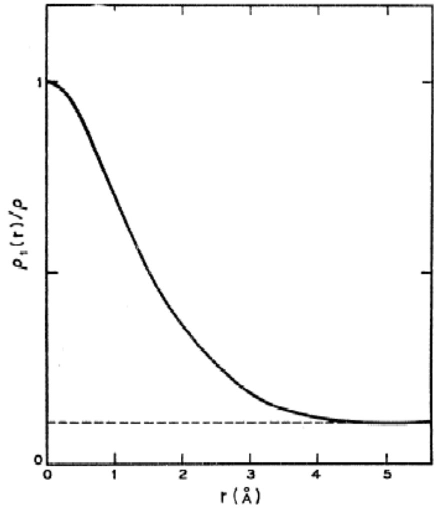


FIG. 7. The single-particle density matrix as a function of separation. The dashed curve indicates the asymptotic limit for large $r$, $\rho_1(r) \sim \rho_0 = 0.11\rho$.

- Momentum distribution
  - Non-classical showing effects of bose or fermi statistics
  - Fourier transform is the single particle off-diagonal density matrix
- Compute with McMillan Method.
- Condensate fraction ~10%

$$n(r,r') = \int dr_2 ... dr_N \psi^*(r,r_2...)\psi(r',r_2...)$$

$$= \left\langle \frac{\psi^*(r',r_2,...)}{\psi(r,r_2,...)} \right\rangle$$

# Derivation of momentum formula

- Suppose we want the probability $n_k$ that a given atom has momentum hk.
- Find wavefunction in momentum space by FT wrt all the coordinates and integrating out all but one electron

$$\Pr(k_1,..k_N) = \left| \int dR\ e^{-i(k_1 r_1 + ... + k_N r_N)} \Psi(R) \right|^2$$

$$n_k = \int dk_2....dk_N \Pr(k, k_2, ...k_N)$$

- Expanding out the square and performing the integrals we get.

$$n_k = \int \frac{d^3 r d^3 s}{(2\pi)^3 V} \exp(-ik(r-s)) n(r,s) = \int \frac{d^3 r}{(2\pi)^3} e^{-ikr} n(r)$$

Where:

$$n(r,s) = \frac{V}{Q} \int dr_2 ... dr_N \psi^*(r, r_2 ... r_N) \psi(s, r_2 ... r_N)$$

(states occupied with the Boltzmann distribution.)

*For a homogeneous system,* $n(r,s)=n(|r-s|)$

# Fermions: antisymmetric trial function

- At mean field level the wavefunction is a Slater determinant. Orbitals for homogenous systems are a filled set of plane waves.
- We can compute this energy analytically (HF).
- To include correlation we multiply by a pseudopotential. We need MC to evaluate properties.
- New feature: how to compute the derivatives of a deteminant and sample the determinant. Use tricks from linear algebra.
- Reduces complexity to O(N$^2$).

$$\Psi_s(R) = Det\left\{e^{ik_i r_j}\eta_i\left(\sigma_j\right)\right\}$$

$$PBC: \quad k \cdot L = 2\pi n + \{\theta\}$$

$$\Psi_{SJ}(R) = Det\{e^{ik_i r_j}\}e^{-\sum_{i<j} u(r_{ij})}$$

*Slater-Jastrow trial function.*

$$\det\left(\phi_k\left(r_j^T\right)\right) = \det\left(\phi_k\left(r_j\right)\right)\sum_k \phi_k\left(r_j^T\right)M_{k,i}^{-1}$$

$$\frac{1}{\det(M)}\frac{\partial \det\left(M\right)}{\partial a} = Tr\left\{M^{-1}\frac{\partial M}{\partial a}\right\}$$

# The electron gas

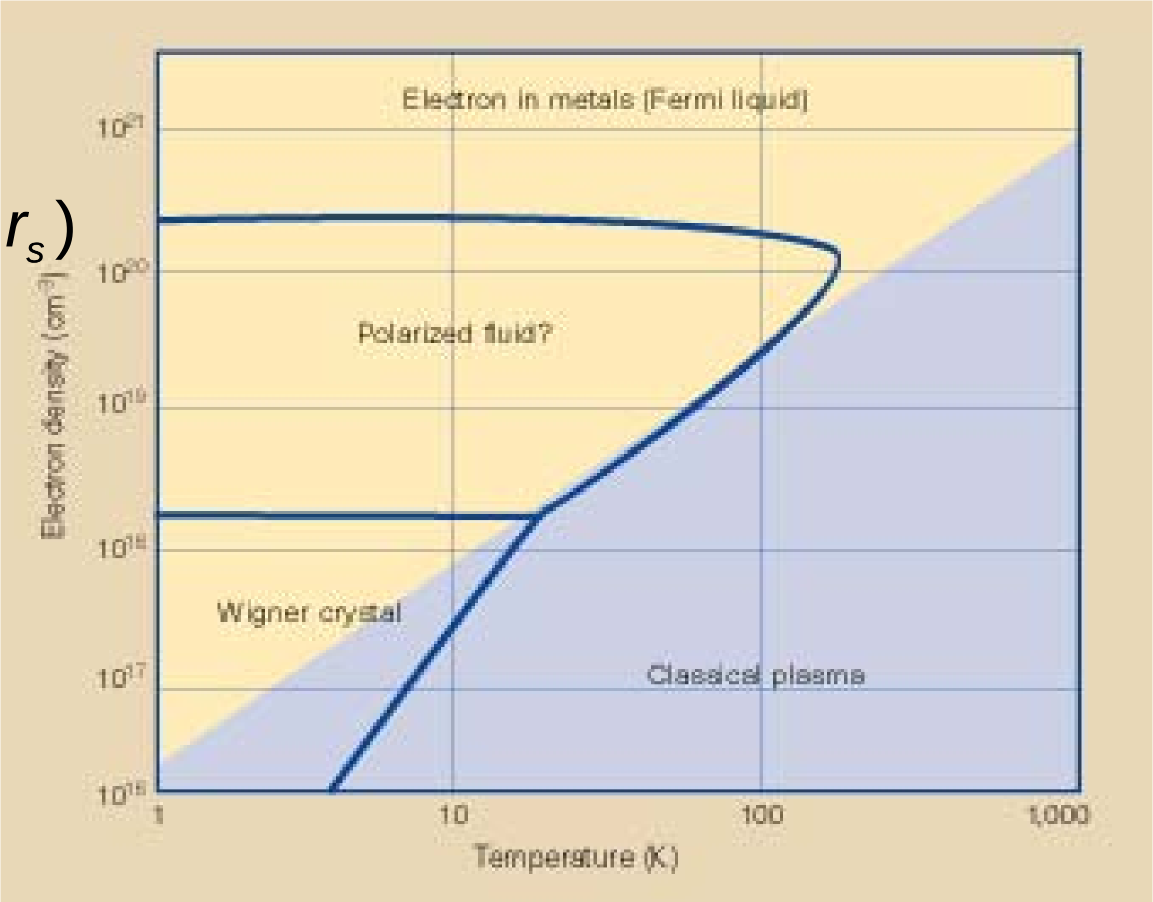
*D. M. Ceperley, Phys. Rev. B 18, 3126 (1978)*

$$H = -\frac{\hbar^2}{2m}\sum_i \nabla_i^2 + \sum_{i<j}\frac{1}{r_{ij}}$$

- Standard model for electrons in metals
- Basis of DFT.
- Characterized by 2 dimensionless parameters:
  - Density
  - Temperature

$$\boxed{\begin{aligned} r_s &= a/a_0 \\ \Gamma &= e^2/Ta \end{aligned}}$$

- What is energy?
- When does it freeze?
- What is spin polarization?
- What are properties?



$\log(r_s)$

$\log(\Gamma)$

$\Gamma < r_s$ classical OCP

$\Gamma = 175$ classical melting

# Jastrow factor for the e-gas

- Look at local energy either in r space or k-space:
- r-space as 2 electrons get close gives cusp condition
- K-space, charge-sloshing or plasmon modes.

$$2\rho u_k = \sqrt{\frac{V_k}{\lambda k^2}} \propto \frac{1}{k^2}$$

- Can combine 2 exact properties in the Gaskell form. Write $E_V$ in terms structure factor making “random phase approximation.” (RPA).

$$2\rho u_k = -\frac{1}{S_k} + \sqrt{\frac{1}{S_k^2} + \frac{V_k}{\lambda k^2}}$$

- Optimization can hardly improve this form for the e-gas in either 2 or 3 dimensions. RPA works better for trial function than for the energy.
- NEED EWALD SUMS because potential trial function is long range, it also decays as 1/r, but it is not a simple power.

$$\lim_{r\to\infty} u(r) = \begin{cases} r^{-1} & \text{3D} \\ r^{-1/2} & \text{2D} \\ \log(r) & \text{1D} \end{cases}$$

Long range properties important

- Gives rise to dielectric properties
- Energy is insensitive to $u_k$

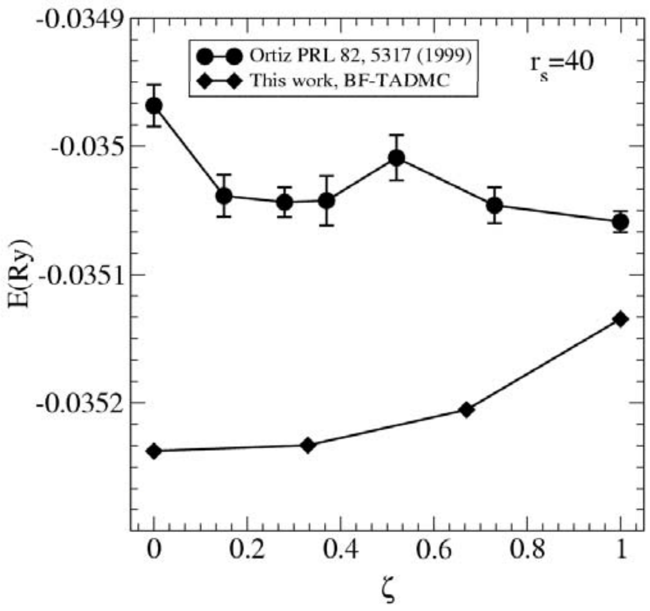
# Comparison of Trial functions

- What do we choose for the trial function in VMC and DMC?
- Slater-Jastrow (SJ) with plane wave orbitals :

$$\Psi_2(R) = Det\{\phi_k(r_j)\}e^{-\sum_{i<j} u_{ij}(r_{ij})}$$

- For higher accuracy we need to go beyond this form.
- Include backflow-three body.

Example of incorrect physics within SJ

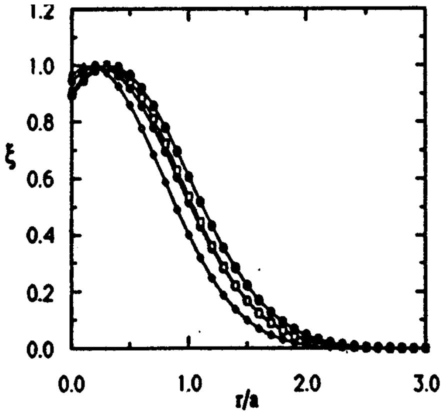


# Wavefunctions beyond Jastrow

$$\phi_{n+1}(R) \approx \phi_n(R)\, e^{-\tau \langle \phi_n^{-1} H \phi_n \rangle}$$

smoothing

- Use method of residuals construct a sequence of increasingly better trial wave functions.
- 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.



$$\Psi_2(R)\exp\{\sum_i [\sum_j \xi_{ij}(r_{ij})(\mathbf{r}_i - \mathbf{r}_j)]^2\}$$

# Backflow- 3B Wave functions

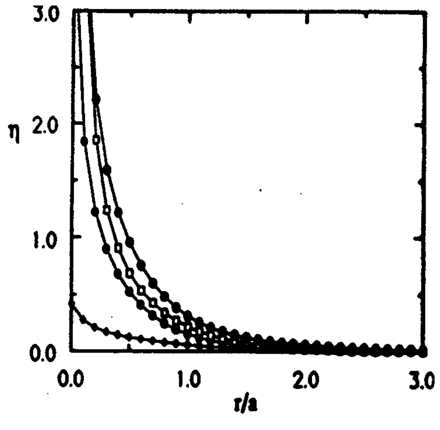
- Backflow means change the coordinates to quasi- coordinates.

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

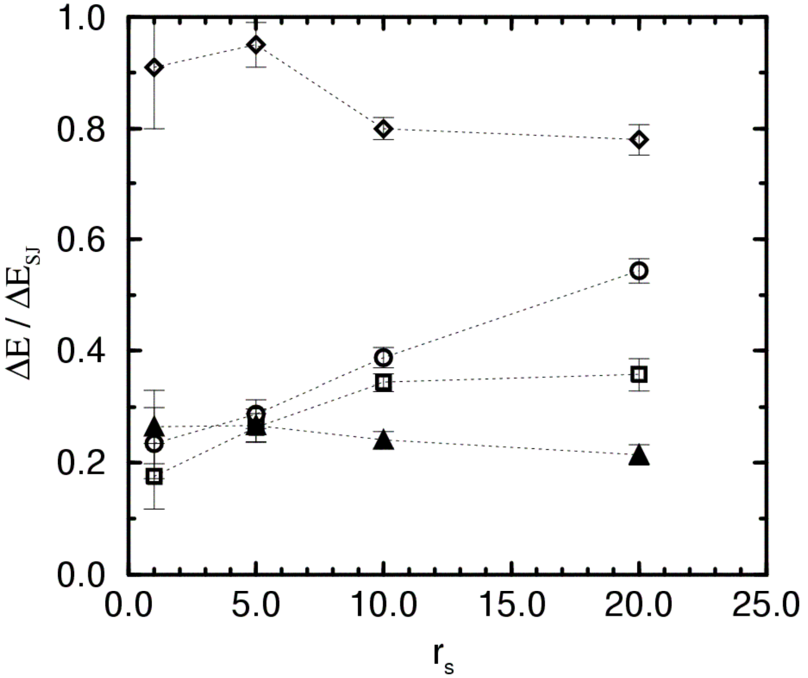
$$\mathbf{x}_i = \mathbf{r}_i + \sum_j \eta_{ij}(r_{ij})(\mathbf{r}_i - \mathbf{r}_j)$$

- Leads to a much improved energy

*Kwon PRB 58, 6800 (1998).*



3DEG

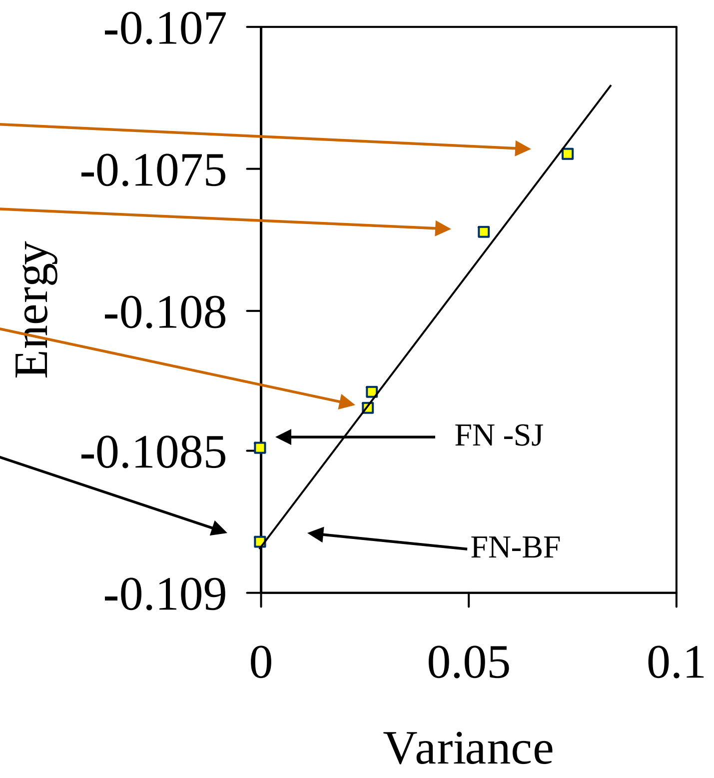


# Dependence of energy on wavefunction

3d Electron fluid at a density $r_s=10$

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

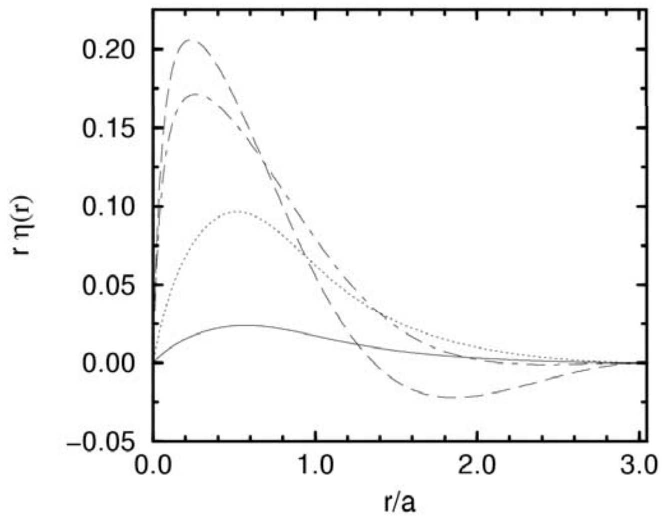
- Wavefunctions
  - Slater-Jastrow (SJ)
  - three-body (3)
  - backflow (BF)
  - fixed-node (FN)
- Energy $<\phi |H| \phi>$ converges to ground state
- Variance $<\phi [H-E]^2 \phi>$ to zero.
- Using 3B-BF gains a factor of 4.
- Using DMC gains a factor of 4.



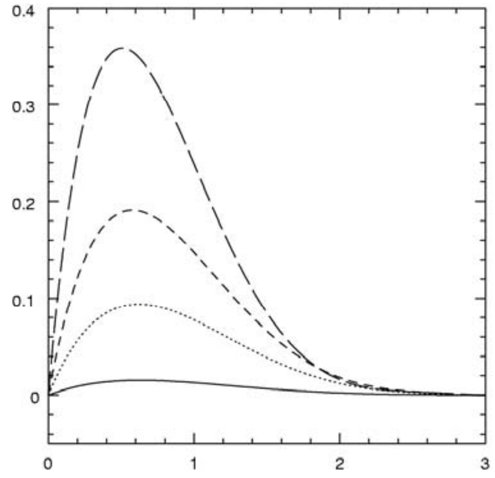
# Analytic backflow

- 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 3body forms.
- Significant long-range component to BF

OPTIMIZED BF



ANALYTIC BF

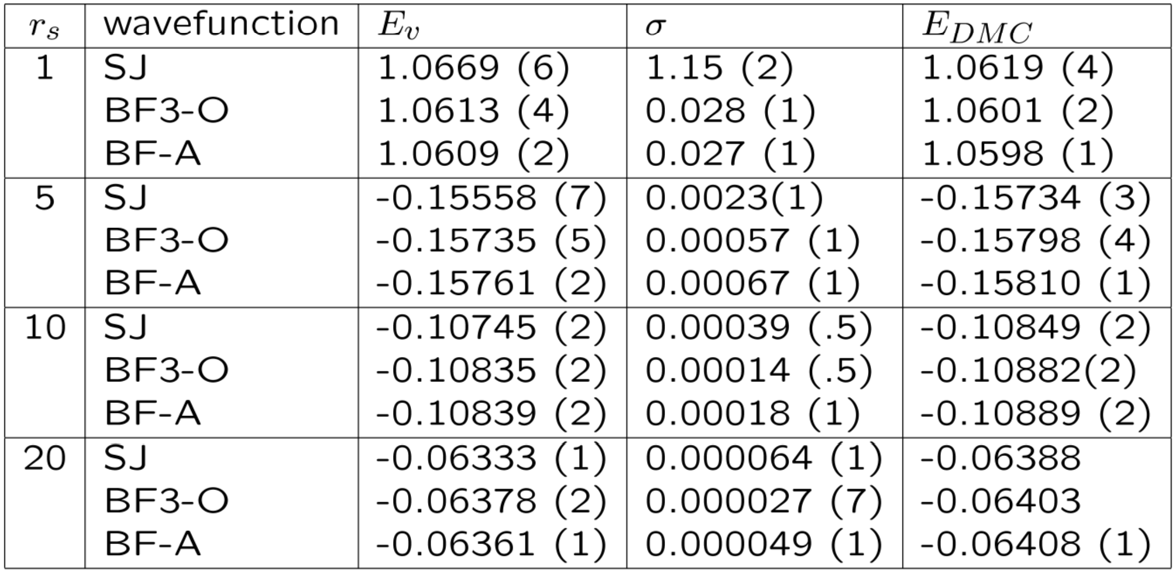


$r_s$=1,5,10,20

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

- 3-body term is non-symmetric!

# Results of Analytic tf



| $r_s$ | wavefunction | $E_v$ | $\sigma$ | $E_{DMC}$ |
|---|---|---|---|---|
| 1 | SJ | 1.0669 (6) | 1.15 (2) | 1.0619 (4) |
| | BF3-O | 1.0613 (4) | 0.028 (1) | 1.0601 (2) |
| | BF-A | 1.0609 (2) | 0.027 (1) | 1.0598 (1) |
| 5 | SJ | -0.15558 (7) | 0.0023(1) | -0.15734 (3) |
| | BF3-O | -0.15735 (5) | 0.00057 (1) | -0.15798 (4) |
| | BF-A | -0.15761 (2) | 0.00067 (1) | -0.15810 (1) |
| 10 | SJ | -0.10745 (2) | 0.00039 (.5) | -0.10849 (2) |
| | BF3-O | -0.10835 (2) | 0.00014 (.5) | -0.10882(2) |
| | BF-A | -0.10839 (2) | 0.00018 (1) | -0.10889 (2) |
| 20 | SJ | -0.06333 (1) | 0.000064 (1) | -0.06388 |
| | BF3-O | -0.06378 (2) | 0.000027 (7) | -0.06403 |
| | BF-A | -0.06361 (1) | 0.000049 (1) | -0.06408 (1) |

- Analytic form $E_{VMC}$ better for $r_s<20$ but not for $r_s \geq 20$.
- Optimized variance is smaller than analytic/
- Analytic nodes always better! (as measured by $E_{DMC}$)
- Form ideal for use at smaller $r_s$ since it will minimize optimization noise and lead to more systematic results vs N, $r_s$ and polarization.
- Saves human & machine optimization time.
- Also valuable for multi-component system of metallic hydrogen.

# Wigner Crystal Trial Function

- Jastrow trial function does not "freeze" at appropriate density.
- Solution is to break spatial symmetry "by hand."
- Introduce a bcc lattice

  $\{Z_i\}$
- bcc has the lowest Madelung energy, but others may have lower zero point energy.
- Introduce localized one-body terms (Wannier functions).
- Non-symmetric but provides a very good description of a quantum crystal.
- More complicated trial functions and methods are also possible.

$$\psi(R) = \prod_{i<j} e^{-u(r_{ij})}$$

$$\psi(R) = \prod_{i} \phi\left(r_i - Z_i\right) \prod_{i<j} e^{-u(r_{ij})}$$

$$\phi(r) = e^{-Cr^2}$$

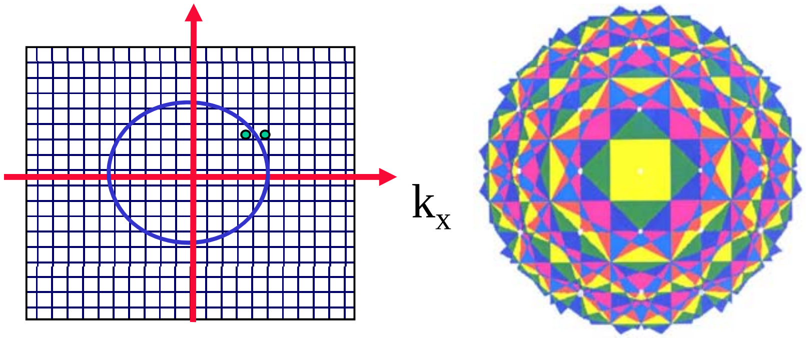
"C" is a variational parameter to be optimized.

# Twist averaged boundary conditions

- In periodic boundary conditions (Γ point), the wavefunction is periodic⇒**Large finite size effects for metals because of shell effects.**
- Fermi liquid theory can be used to correct the properties.
- In twist averaged BC we use an arbitrary phase θ as r →r+L
- If one integrates over all phases the momentum distribution changes from a lattice of k-vectors to a fermi sea.
- Smaller finite size effects

$$\varphi = e^{ikr}$$

$$kL = 2\pi n + \theta$$

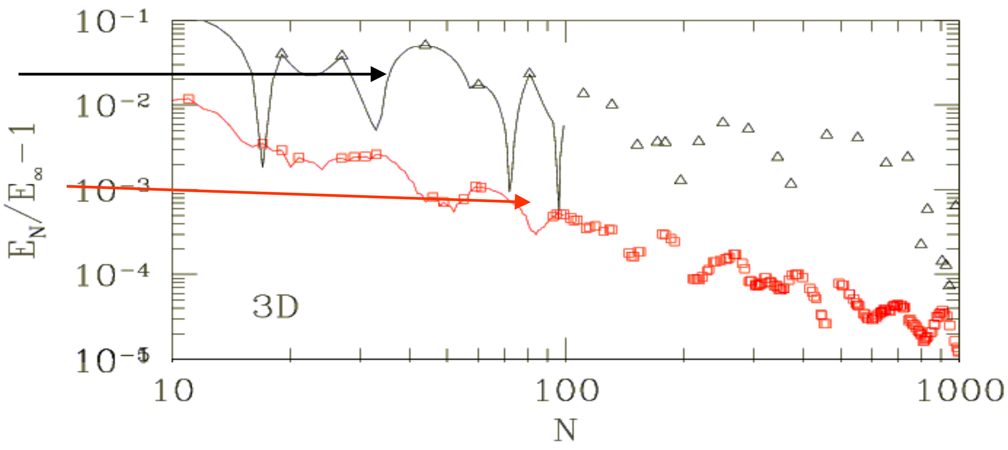


$$\Psi(x+L) = e^{i\theta}\Psi(x)$$

$$\bar{A} = \frac{1}{(2\pi)^3}\int_{-\pi}^{\pi} d^3\theta \left\langle \Psi_\theta A \Psi_\theta \right\rangle$$

Error with PBC

Error with TABC



Cepe

# Twist averaged MC

- Make twist vector dynamical by changing during the random walk.

$$\boxed{-\pi < \theta_i \leq \pi \qquad \mathrm{i} = (1,2,3)}$$

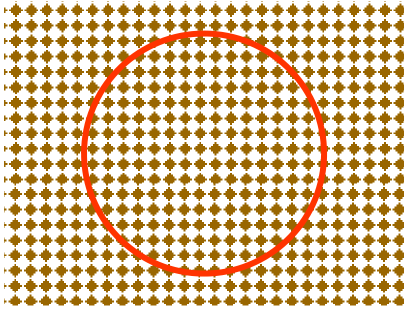
- Within GCE, change the number of electrons
- Within TA-VMC
  - Initialize twist vector.
  - Run usual VMC (with warmup)
  - Resample twist angle within cube
  - (iterate)
- Or do in parallel.

# Grand Canonical Ensemble QMC

- GCE at T=0K: choose N such that E(N)-μN is minimized.
- According to Fermi liquid theory, interacting states are related to non-interacting states and described by **k**.
- Instead of N, we input the fermi wavevector(s) $\mathbf{k_F}$. Choose all states with $k < k_F$ (assuming spherical symmetry)
- N will depend on the twist angle θ. = number of points inside a randomly placed sphere.

$$\vec{k}_n = \frac{2\pi}{L}\vec{n} + \frac{\vec{\theta}}{L}$$

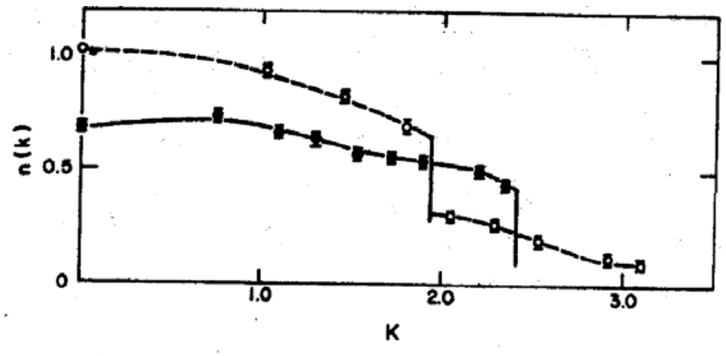
$$k_n \le k_F$$



- After we average over θ (TA) we get a sphere of filled states.
- Is there a problem with Ewald sums as the number of electrons varies? No! average density is exactly that of the background. We only work with averaged quantities.

# Momentum Distribution

- Momentum distribution
  - Non-classical showing effects of bose or fermi statistics
  - Fourier transform is the single particle off-diagonal density matrix
- Compute with McMillan Method.



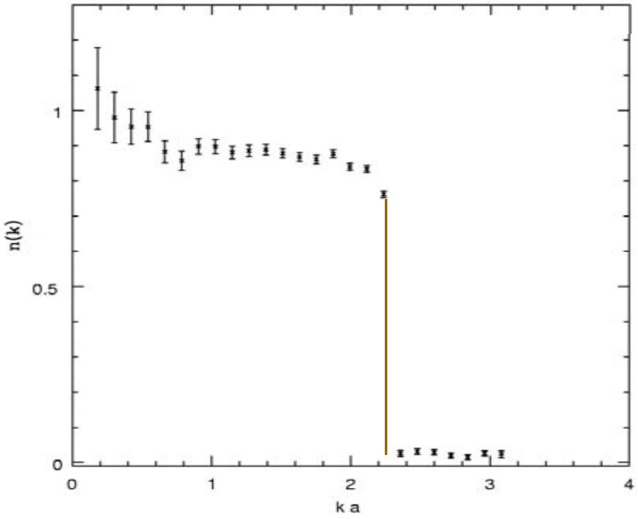
$$n(r,r') = \frac{1}{Z}\int dr_2 ... dr_N \psi^*(r,r_2...)\psi(r',r_2...)$$

$$= \left\langle \frac{\psi^*(r,r_2...)}{\psi(r',r_2...)} \right\rangle$$

# Single particle size effects

- Exact single particle properties with TA within HF
- Implies momentum distribution is a continuous curve with a sharp feature at $k_F$.
- With PBC only 5 points on curve

$r_s=4$  N=33 polarized



- No size effect within single particle theory!
- Kinetic energy will have much smaller size effects.

$$T = \int d^3k \frac{\hbar^2}{2m} k^2 n(k)$$

# Potential energy

- Write potential as integral over structure function:

$$V = \int d^3k \frac{4\pi}{k^2} S(k) \qquad S(k) = \left\langle \rho_{-k} \rho_k \right\rangle = 1 + (N-1) \left\langle e^{i(r_1 - r_2)k} \right\rangle$$

- Error comes from 2 effects.
  - Approximating integral by sum
  - Finite size effects in S(k) at a given k.

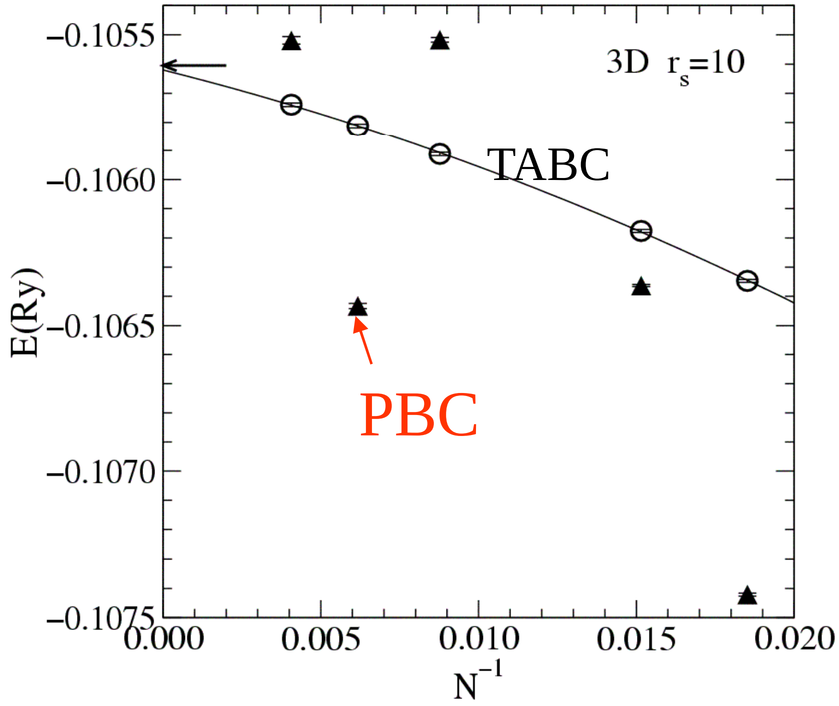
$$S_{HF}(k) = 1 - \frac{2}{N} \sum_{q,q'} \delta_{q-q'+k}$$

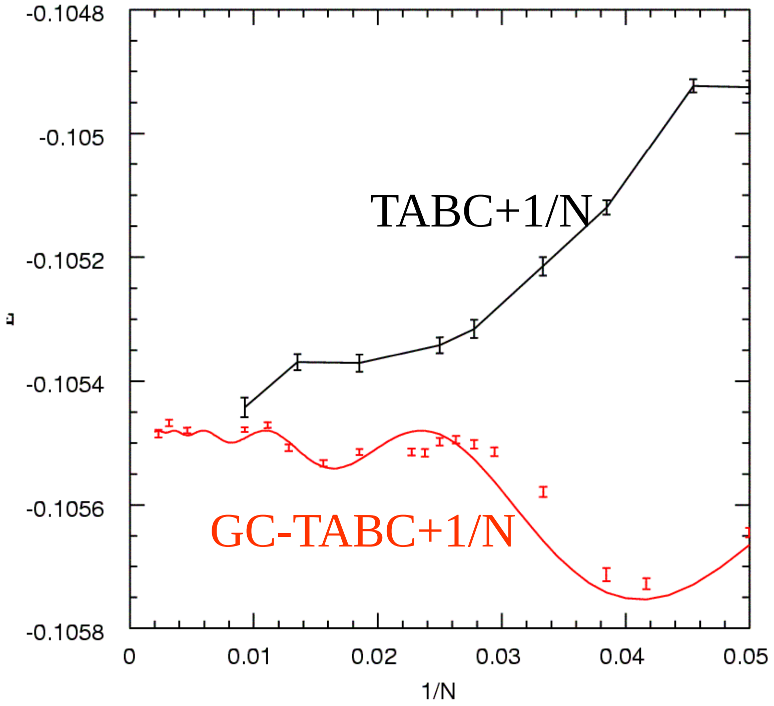
- Within HF we get exact S(k) with TABC.
- Discretization errors come only from non-analytic points of S(k).
  - the absence of the k=0 term in sum. We can put it in by hand since we know the limit S(k) at small k (plasmon regime)

  - Remaining size effects are smaller, coming from the non-analytic behavior of S(k) at $2k_F$.

$$S(k) = \frac{k^2}{2m\omega_p} \Rightarrow \Delta E = \frac{\omega_p}{N}$$

# 3DEG at $r_s$=10





We can do simulations with N=42!

Size effects now go like: $$\Delta E = aN^{-5/3}cos^2(k_F L + \pi/16)$$

We can cancel this term at special values of N!

N= 15, 42, 92, 168, 279,…

# Brief History of Ferromagnetism in electron gas

What is polarization state of fermi liquid at low density?

$$\zeta = \frac{N_{\uparrow} - N_{\downarrow}}{N_{\uparrow} + N_{\downarrow}}$$

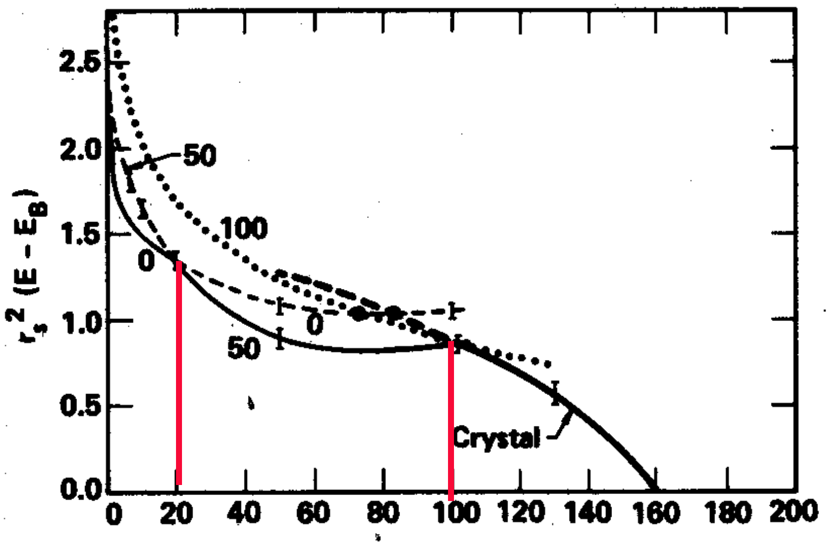
- Bloch 1929 got polarization from exchange interaction:
  - $r_s > 5.4$ 3D
  - $r_s > 2.0$ 2D
- Stoner 1939: include electron screening: contact interaction
- Herring 1960
- Ceperley-Alder 1980 $r_s > 20$ is partially polarized
- Young-Fisk experiment on doped $CaB_6$ 1999 $r_s \sim 25$.
- Ortiz-Balone 1999 : ferromagnetism of e gas at $r_s > 20$.
- Zong et al Redo QMC with backflow nodes and TABC.

# T=0 calculations with FN-DMC

3d electron gas

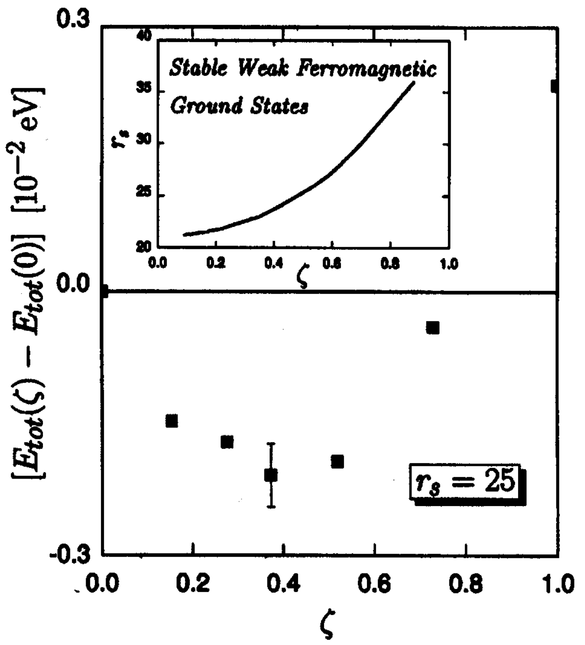
- $r_s<20$ unpolarized
- $20<r_s<100$ partial
- $100<r_s$ Wigner crystal

Ceperley, Alder ‘80



Energies are very close together at low density!

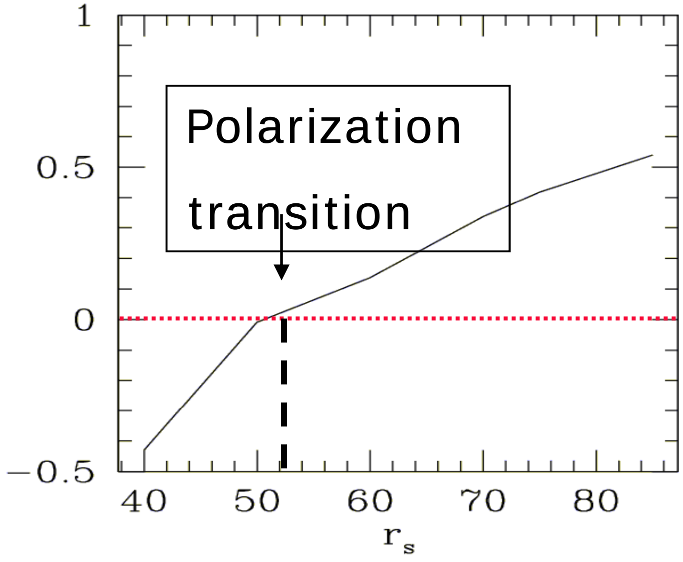
More recent calculations of *Ortiz, Harris and Balone PRL 82, 5317 (99)* confirm this result but get transition to crystal at $r_s=65$.



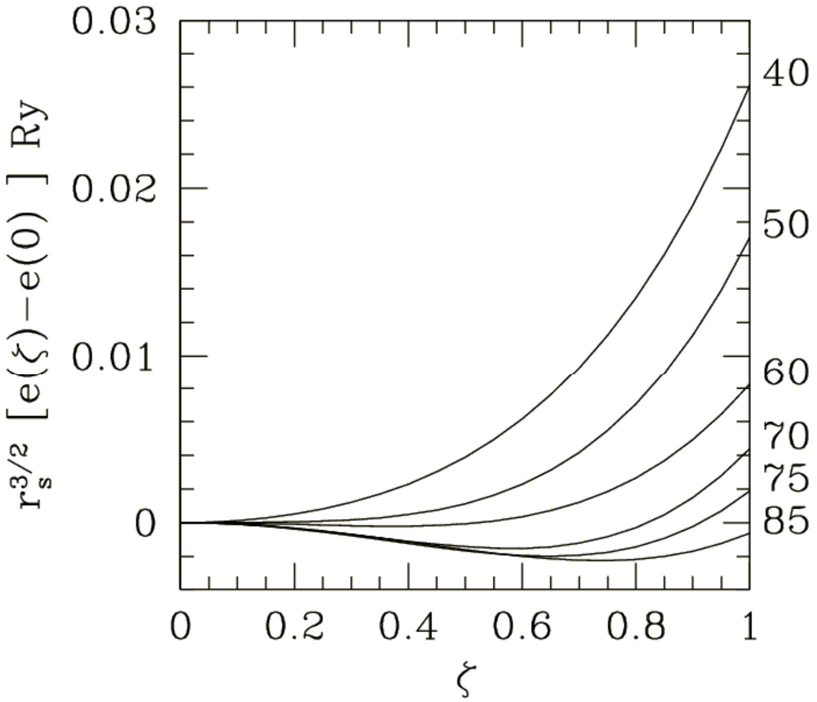
# Polarization of 3DEG

- We see second order partially polarized transition at $r_s$=52
- Is the Stoner model (replace interaction with a contact potential) appropriate? Screening kills long range interaction.
- Wigner Crystal at $r_s$=105

- Twist averaging makes calculation possible--much smaller size effects.
- Jastrow wavefunctions favor the ferromagnetic phase.
- Backflow 3-body wavefunctions more paramagnetic

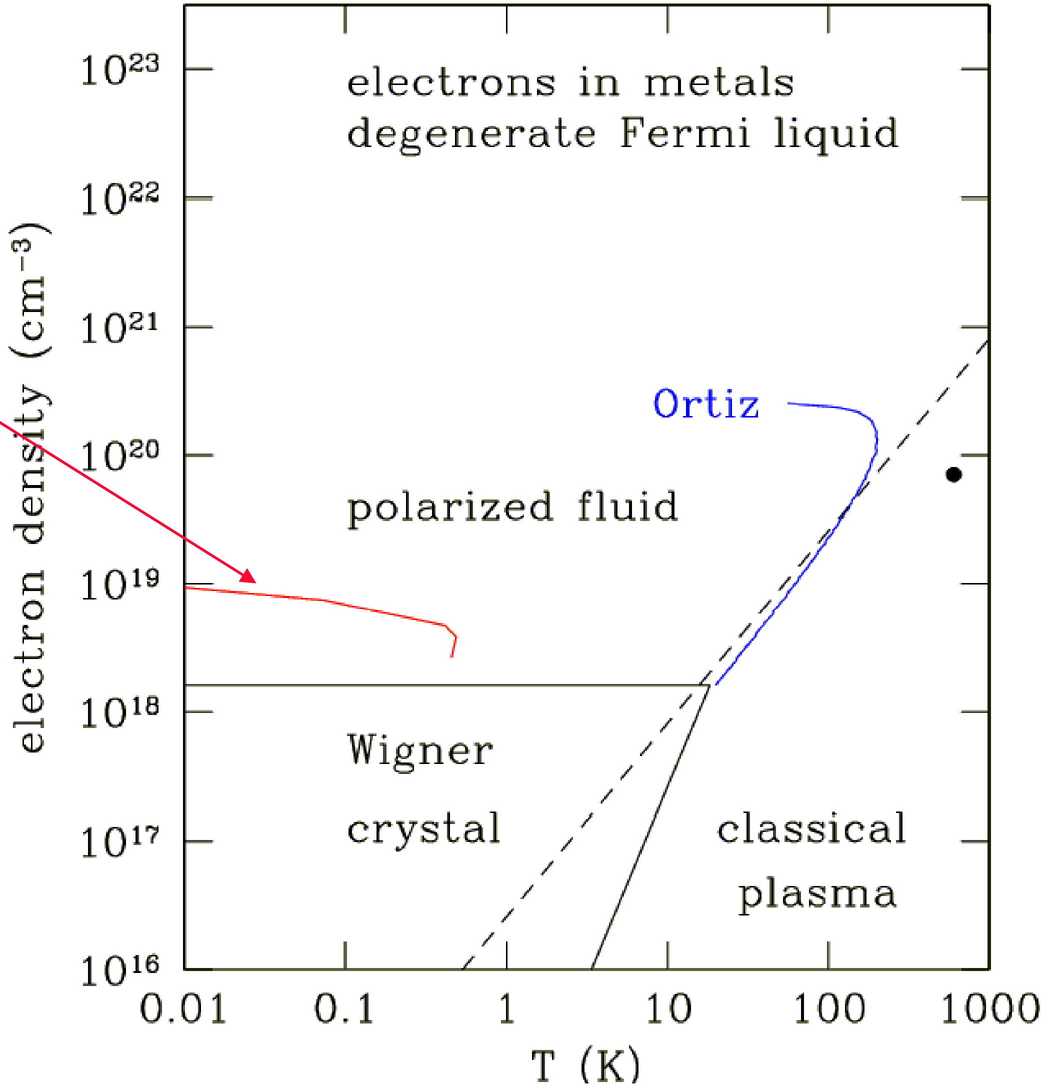

Polarization transition

ariational



# Phase Diagram

- Partially polarized phase at low density.
- But at lower energy and density than before.
- As accuracy gets higher, polarized phase shrinks
- Real systems have different units.

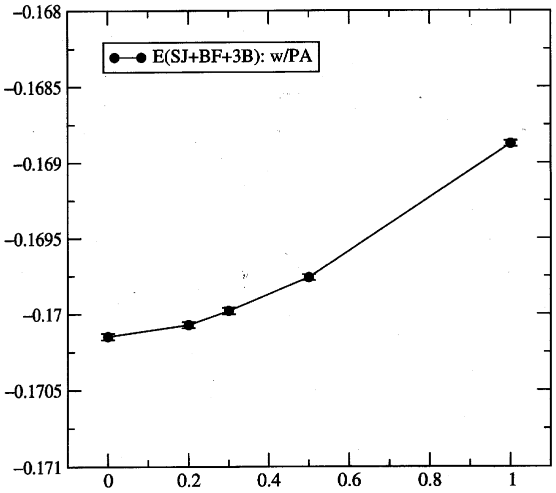


# Polarization of 2D electron gas

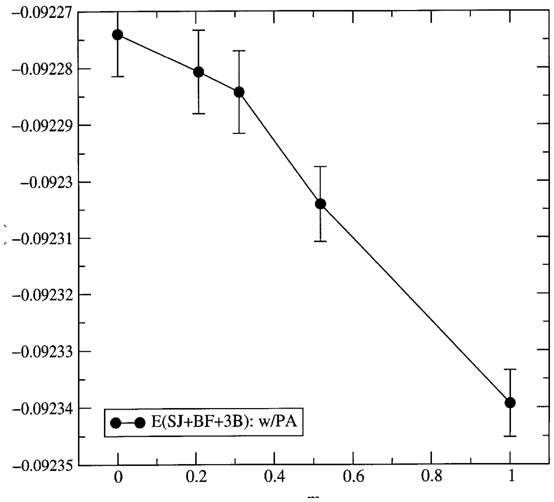
- Same general trend in 2D
- Partial polarization before freezing

Results using phase averaging and BF-3B wavefunctions

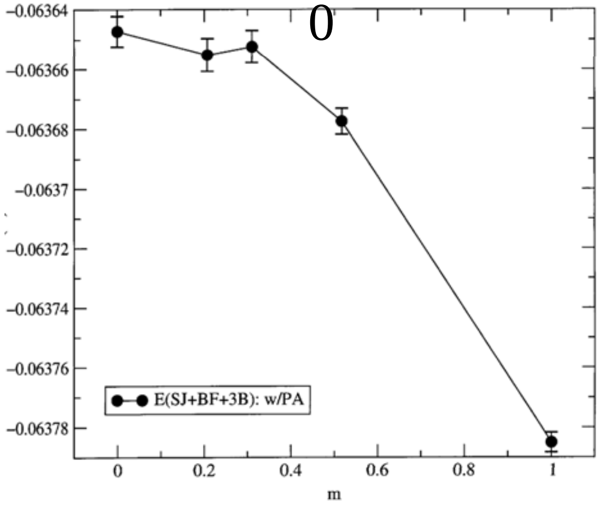
$r_s$=10



$r_s$=20



$r_s$=30



# Recent calculations in 2D

*Tanatar,Ceperley ‘89*
*Rapisarda, Senatore ‘95*
*Kwon et al ‘97*

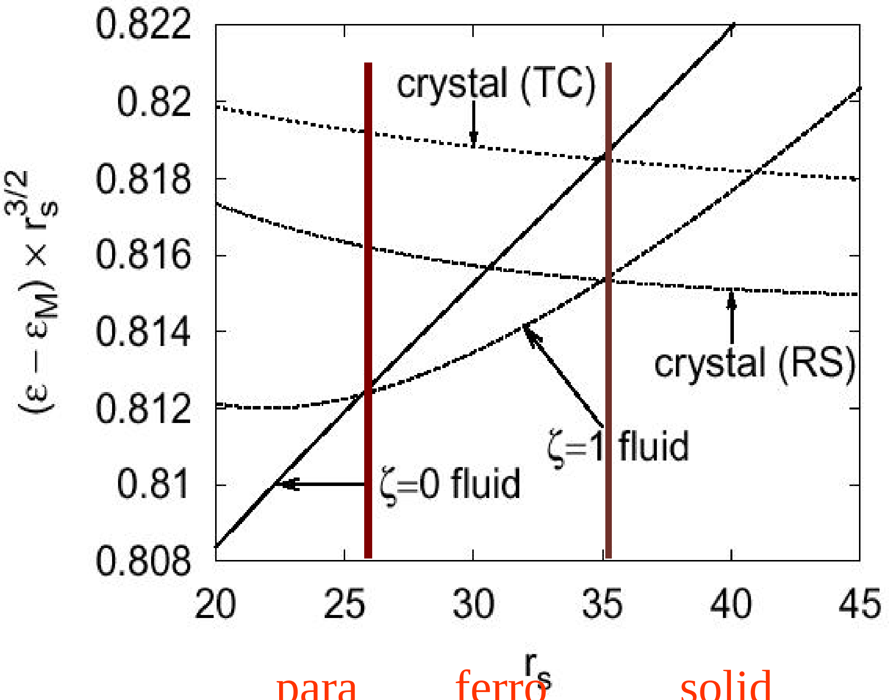
**T=0 fixed-node calculation:**

Also used high quality backflow wavefunctions to compute energy vs spin polarization.

Energies of various phases are nearly identical

*Attaccalite et al:*

*cond-mat/0109492*



para ferro solid

2d electron gas

- $r_s < 25$ unpolarized
- $25 < r_s < 35$ polarized
- $r_s > 35$ Wigner crystal

# Linear response for the egas

- Add a small periodic potential.
- Change trial function by replacing plane waves with solutions to the Schrodinger Eq. in an effective potential.
- Since we don’t care about the strength of potential use trial function to find the potential for which the trial function is optimal.
- Observe change in energy since density has mixed estimator problems.

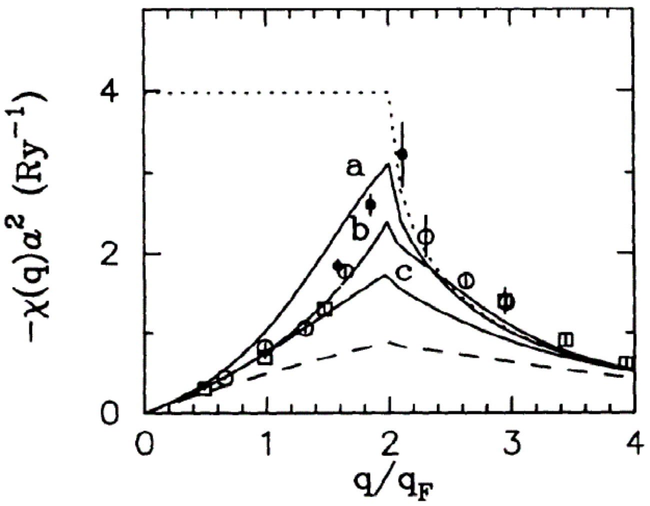


FIG. 4. Linear static response function $\chi(q)$ of the 2D electron fluid at $r_s = 5$. The squares, empty circles, and full

# Fermi Liquid parameters

- Do by correlated sampling: Do one long MC random walk with a guiding function (something overlapping with all states in question).
- Generate energies of each individual excited state by using a weight function

$$w_\alpha(R) = \frac{\phi_\alpha(R)}{\psi_G(R)}$$

$$\psi_G^{\ 2} = \sum_\alpha |\phi_\alpha(R)|^2$$

- "Optimal Guiding function" is
- Determine particle hole excitation energies by replacing columns:fewer finite size effects this way. Replace columns in slater matrix
- Case where states are orthogonal by symmetry is easier, but non-orthogonal case can also be treated.
- Back flow needed for some excited state since Slater Jastrow has no coupling between unlike spins.

# Summary of T=0 methods:

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