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Joint DEMOCRITOS - ICTP School on

CONTINUUM QUANTUM MONTE CARLO METHODS

12 - 23 January 2004

QMC FOR EXTENDED SYSTEMS

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These are preliminary lecture notes, intended only for distribution to participants.

QMC for extended systems

- Calculation of the Momentum distribution
- Trial Function beyond Slater-Jastrow: back flow and 3-body
- Quantum solids
- Ewald Sums for Charged systems
- Twist Averaged Boundary Conditions
- Some Results for the electron gas

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.

PHYSICAL REVIEW VOLUME 138, NUMBER 2A 19 APRIL 1965

Ground State of Liquid He⁴†

W. L. McMillan*
Department of Physics, University of Illinois, Urbana, Illinois
(Received 16 November 1964)

The properties of the ground state of liquid He⁴ 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 Michels. 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 -0.78×10^{-16} 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.

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.

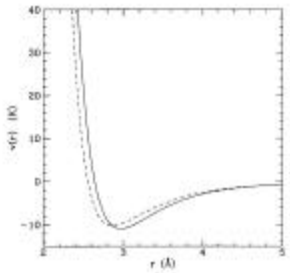

FIG. 1. The semiempirical pair potential between two helium atoms: solid line, Aziz *et al.* (1992); dashed line, Lennard-Jones 6-12 potential with $\epsilon = 10.22$ K and $\sigma = 2.556$ Å.

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

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Helium interaction

- Repulsion at short distances because of overlap of atomic cores.
- Attraction at long distance because of the dipole-induced-dipole force. Dispersion interaction $c_6 r^{-6} + c_8 r^{-8} + \ldots$.

- He-He interaction is the most accurate. Use all available low density data (virial coefficients, quantum chemistry calculations, transport coefficients, ….) Good to better than 0.1K (work of Aziz over last 20 years).
- Three body interactions are small but not zero.

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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:

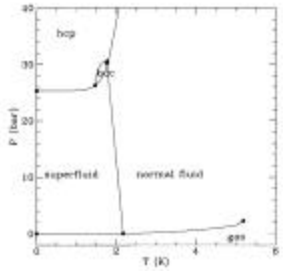

FIG. 3. The phase diagram of ^{4}He.

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

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

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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:

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

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

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

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

$U(r)=\alpha r^{-m}$

$$er^{-n} = 2l\left(a\, mr^{-m-1}\right)^2 \quad \text{for} \quad n > 2$$

$$m = \frac{n}{2} - 1$$

$$a = \frac{1}{m}\sqrt{\frac{e}{2l}}$$

Gives a cusp condition on u.

$$-e^2 r^{-1} = 2l\nabla^2 u(r) = 2l\left(u'' + \frac{D-1}{r}u'\right)$$

$$u'(0) = -\frac{e^2}{2l(D-1)}$$

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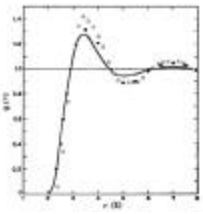
Other quantum properties

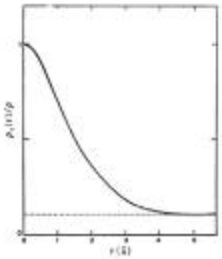
- Kinetic energy
- Potential energy
- Pair correlation function
- Structure function
- Pressure (virial relation)

Like properties from classical simulations

No upper bound property

Only first order in accuracy





- 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%

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

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

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

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

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

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

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

Where:

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

(states occupied with the Boltzmann distribution.)

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

Calculation of n(r)

Naïve procedure

- Generate sample with VMC
- Take one particle at random and displace by a distance r.
- Find ratio of trial function for old and new position.
- O(1) work/1 distance

$$n(r,r') = \int dr_2 \ldots dr_N \psi^*(r,r_2\ldots)\psi(r',r_2\ldots) = \left\langle \frac{\psi^*(r',r_2,\ldots)}{\psi(r,r_2,\ldots)} \right\rangle$$

McMillan procedure

- Generate sample with VMC
- Determine change of trial function if each particle is destroyed. a_k
- Insert a new particle at a random position in the box and determine trial function for the insertion "b"
- For each k perform the average b/a_k and add to $n(|r-r_k|)$.
- Repeat for O(N) insertions.
- O(N) work/$O(N^2)$ distances

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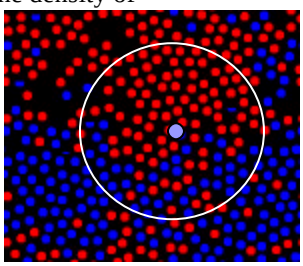
Pair Correlation Function, g(r)

Primary quantity in a liquid is the probability distribution of pairs of particles. Given a particle at the origin what is the density of surrounding particles

$g(r) = < \Sigma_{i<j} \delta (r_i - r_j - r) > (2\ \Omega/N^2)$

Density-density correlation function



From g(r) you can calculate all pair quantities (potential, pressure, …)

$$V = \sum_{i<j} v(r_{ij}) = \frac{N r}{2} \int d^3 r v(r) g(r)$$

A function gives more information than a number!

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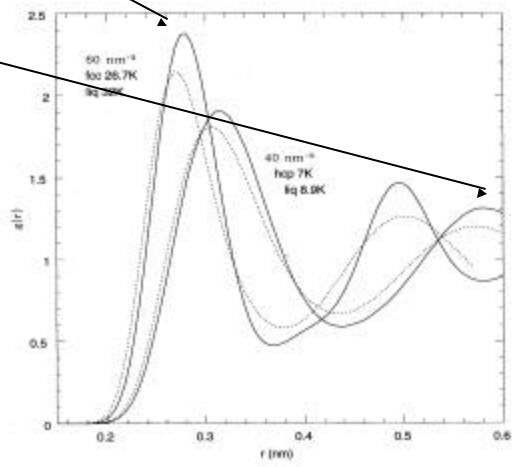
g(r) in liquid and solid helium

- First peak is at inter-particle spacing. (shell around the particle)
- goes out to r<L/2 in periodic boundary conditions.



(The static) structure factor S(k)

- The Fourier transform of the pair correlation function is the structure factor

$$S(k) = \langle|\rho_k|^2\rangle/N \qquad (1)\ \text{“direct”}$$

$$S(k) = 1 + \rho \int dr\, \exp(ikr)\,(g(r)-1) \qquad (2)\ \text{“FT”}$$

- problem with (2) is to extend g(r) to infinity
- S(K) is measured in neutron and X-Ray scattering experiments.
- Can provide a direct test of the assumed potential.
- Used to see the state of a system:

  liquid, solid, glass, gas? (much better than g(r))

- Order parameter in solid is ρ_G where G is a particular wavevector (reciprocal lattice vector).

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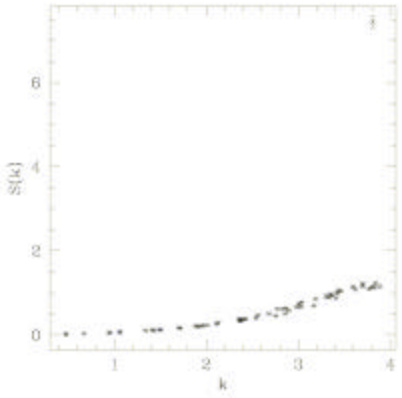
- In a perfect lattice S(k) will be non-zero only on the reciprocal lattice vectors G: S(G) = N
- At non-zero temperature (or for a quantum system) this structure factor is reduced by the Debye-Waller factor

$$S(G) = 1 + (N-1)\exp(-G^2u^2/3)$$

- To tell a liquid from a crystal we see how S(G) scales as the system is enlarged. In a solid, S(k) will have peaks that scale with the number of atoms.



- The compressibility is given by:
- We can use this is detect the liquid-gas transition since the compressibility should diverge as k approaches 0. (order parameter is density)

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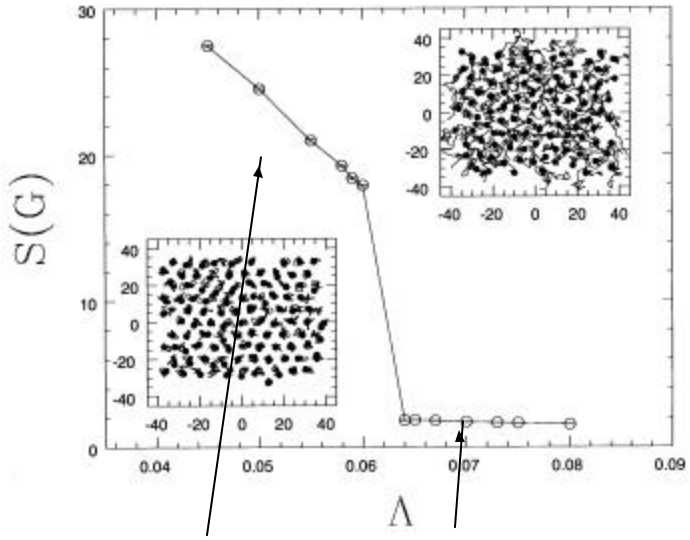

Crystal liquid

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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 $O(N^2)$.

$$\Psi_s(R) = Det\left\{e^{i k_i r_j} h_i(s_j)\right\}$$

$$\text{PBC:} \quad k \cdot L = 2p\,n + \{q\}$$

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

Slater-Jastrow trial function.

$$\det\left(f_k\left(r_j^T\right)\right) = \det\left(f_k\left(r_j\right)\right) \sum_k f_k\left(r_j^T\right) M^{-1}_{k,i}$$

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

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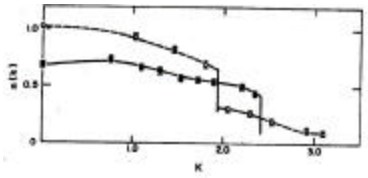
Momentum Distribution

- 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.



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

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

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The electron gas

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

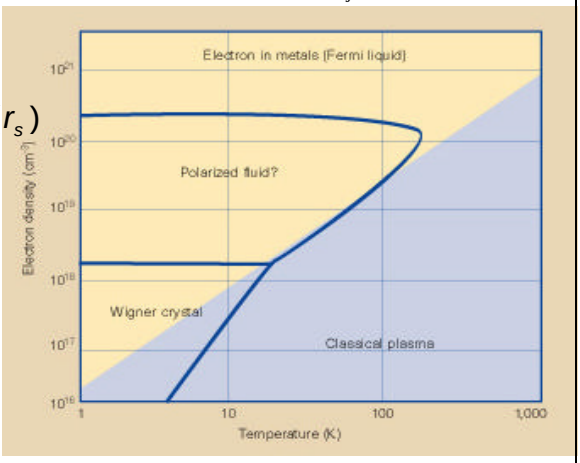
- Standard model for electrons in metals
- Basis of DFT.
- Characterized by 2 dimensionless parameters:
  - Density
  - Temperature

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

$$r_s = a/a_0$$

$$\Gamma = e^2/Ta$$

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



$\log(r_s)$

$\Gamma < r_s$ classical OCP

$\Gamma = 175$ classical melting

$\log(\Gamma)$

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.

$$2\,r\,u_k = \sqrt{\frac{V_k}{l\,k^2}} \propto \frac{1}{k^2}$$

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

$$2\,r\,u_k = -\frac{1}{S_k} + \sqrt{\frac{1}{S_k^2} + \frac{V_k}{l\,k^2}} \qquad S_k = \text{ideal structure factor}$$

- 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.

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

Long range properties important

- Give rise to dielectric properties
- Energy is insensitive to u_k at small k
- Those modes converge $t \sim 1/k^2$

Periodic distances

- Minimum Image Convention:take the closest distance

$$|r|_M = \min (r+nL)$$

Potential is cutoff so that V(r)=0 for r>L/2 .

- Image potential

$$V_I = \Sigma\, v(r_i-r_j+nL)$$

For long range potential this leads to the Ewald image potential. You need a back ground and convergence method.

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Charged systems

How can we handle charged systems?

- Just treat like short-ranged potential: cutoff potential at r>L/2. Problems:
  - Effect of discontinuity never disappears ((1/r) (r^2) gets bigger.
  - Will not have correct dispersion because Poisson equation is not satisfied
  - Even a problem with dipolar forces.
- Image potential solves this:

$$V_I = \Sigma\, v(r_i-r_j+n\,L)$$

  - But summation diverges. We need to resum. This gives the ewald image potential.
  - For one component system we have to add a background to make it neutral.
  - Even the trial function is long ranged and needs to be resummed.

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Ewald summation method

- Key idea is to split potential into k-space part and real-space part. We can do since FT is linear.

  V = $\sum_{i<j,L} f(r_i - r_j + nL)$

  V = $\sum_k f_k \left(|r_k|^2 - N \right)$ where $r_k = \sum_i e^{ik \cdot r_i}$

  and $j_k = \frac{1}{\Omega} \int dr e^{i k \cdot r} f(r)$

  For $f(r) = e^2/r \Rightarrow j_k = \frac{4\pi e^2}{k^2}$

- Hence converges slowly at large r (in r-space)
- And at large k (in k-space)

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Classic Ewald

- Split up using Gaussian charge distribution

  $f(r) = \frac{erfc(kr)}{r}$ decays fast at large r

  $f_k = \frac{4\pi e^{-(k/2k)^2}}{k^2}$ decays fast at large k

  k = convergence parameter

- If we make it large enough we can use the minimum image potential in r-space.
- Extra term for insulators: $V_{dipole} = \frac{2\pi}{(2\varepsilon + 1)\Omega} \left| \sum_i m_i \right|^2$

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How to do it

- r-space part same as short-ranged potential — $O(N^{3/2})$
- k-space part:
  1. Compute $\exp(ik_0 x_i)=(\cos(ik_0 x_i), \sin(ik_0 x_i))$, $k_0=2\pi/L$ $\forall$ i. — $O(N)$
  2. Compute powers $\exp(i2k_0 x_i)= \exp(ik_0 x_i)*\exp(ik_0 x_i)$ etc. This way we get all values of $\exp(ik \cdot r_i)$ with just multiplications. — $O(N^{3/2})$
  3. Sum over particles to get ρ_k all k. — $O(N^{3/2})$
  4. Sum over k to get the potentials. — $O(N^{1/2})$
  5. Forces can also be done by taking gradients. — $O(N^{3/2})$
- Constant terms to be added. — $O(1)$
- Checks: perfect lattice: V=-1.4186487/a (cubic lattice).

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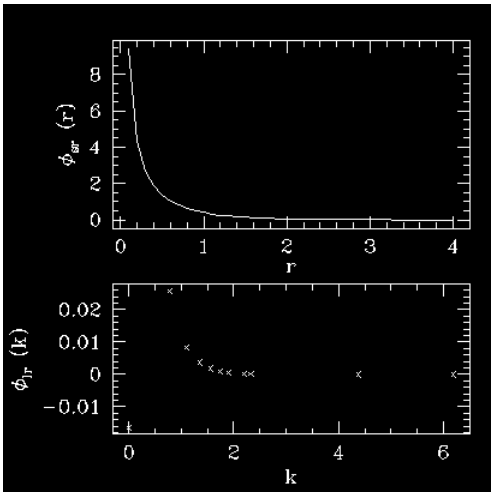
Short and long range potentials

- Potential in r-space
- Potential in k-space



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Optimzed Ewald

- Division into Long-range and short-ranged function is convenient but is it optimal? No
- Trial functions are also long-ranged but not simply 1/r. We need a general procedure.
- Natoli-Ceperley procedure. What division leads to the highest accuracy for a given radius in r and k?
- Leads to a least squares problem.
- FITPN code does this division.
  - Input is fourier transform of desired function on grid appropriate to the supercell
  - Output is a spline of short ranged function and table of long ranged function.

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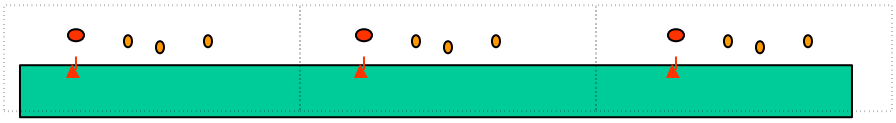
Problems with Image potential

- Introduces a lattice structure which may not be appropriate.
- Example: a charge layer.



  - We assume charge structure continues at large r.
  - Actually nearby fluid will be anticorrelated.
  - This means such structures will be penalized.
- One should always consider the effects of boundary conditions, particularly when electrostatic forces are around!

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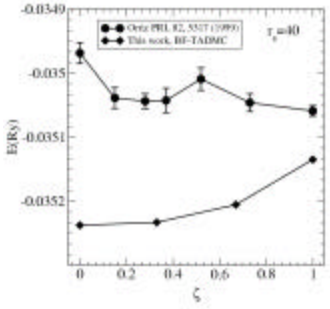
Comparison of Trial functions

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

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

- For higher accuracy we need to go beyond this form.
- Need correlation effects in the nodes.
- Include backflow-three body.

Example of incorrect physics within SJ



Generalized Feynman-Kacs formula

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

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

expand the density matrix in terms of exact eigenstates

$$P(R_0;t) = \int dR \frac{y(R)}{y(R_0)} \sum_a f_a^*(R) f_a(R_0) e^{-t(E_a - E_T)}$$

$$\lim_{t\to\infty} P(R_0;t) = \frac{f_0(R_0)}{y(R_0)} \langle y f_0 \rangle$$

$$\frac{f_0(R_0)}{y(R_0)} \sim e^{-\int_0^t dt \langle\!\langle E_L(t) \rangle\!\rangle_{|y|}}$$

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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.

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

smoothing

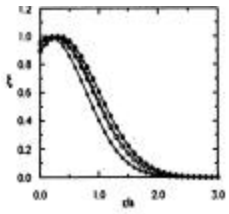
$$f_{n+1}(R) \approx f_n(R) e^{-t\langle f_n^{-1} H f_n\rangle}$$

$$f_0 = e^{i\sum_j \mathbf{k}_j \bullet \mathbf{r}_j}$$

$$E_0 = V(R)$$

$$f_1 = f_0 e^{-U(R)}$$

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



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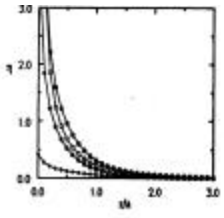
Backflow- 3B Wave functions

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

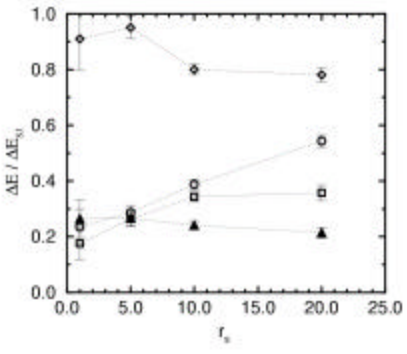
Kwon PRB 58, 6800 (1998).

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

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



3DEG

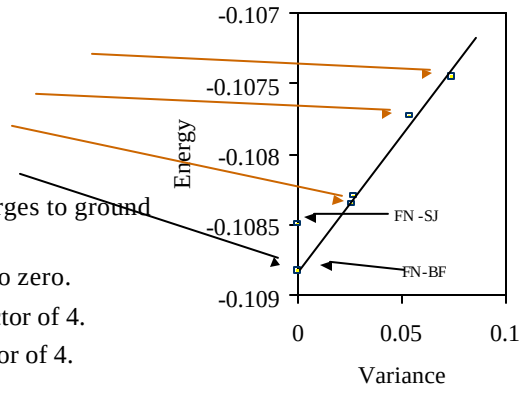


Dependence of energy on wavefunction

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 $\langle\phi |H| \phi\rangle$ converges to ground state
- Variance $\langle\phi [H-E]^2 \phi\rangle$ to zero.
- Using 3B-BF gains a factor of 4.
- Using DMC gains a factor of 4.



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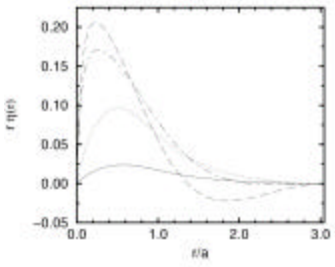
Analytic backflow

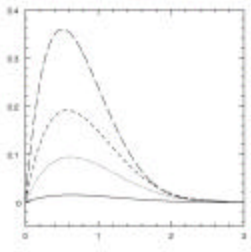
Holzmann et al, Phys. Rev. ***E 68****, 046707:1-15(2003).*

- 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

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

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Results of Analytic tf

r_s	wavefunction	E_v	σ	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.

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Wigner Crystal Trial Function

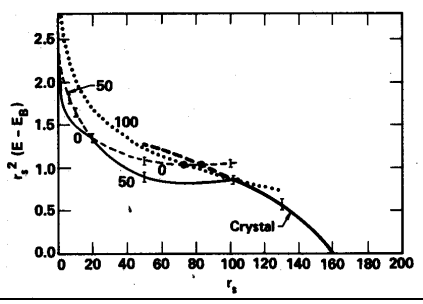
- Jastrow trial function does not "freeze" at appropriate density.
- Solution is to break spatial symmetry "by hand."
- Introduce a bcc lattice $\{Z_i\}$
- bcc has the lowest Madelung energy, but others may have lower zero point energy.
- Introduce localized one-body terms (Wannier functions).
- Make a Slater determinant possibly with spin ordering.
- More complicated trial functions and methods are also possible.

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

$$y(R)=\prod_{i} f(r_i-Z_i)\prod_{i<j} e^{-u(r_{ij})}$$

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

"C" is a variational parameter to be optimized.

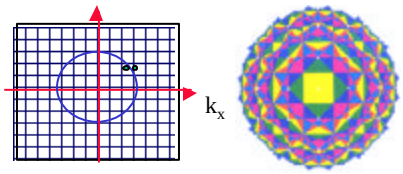


Twist averaged boundary conditions

- 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

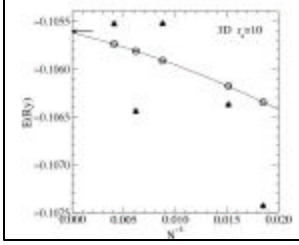
$$j = e^{ikr}$$

$$kL = 2p\,n + q$$

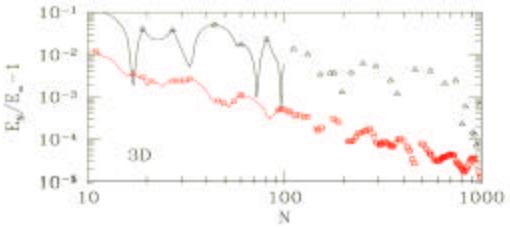


$$\Psi(x + L) = e^{iq}\Psi(x)$$

$$\bar{A} = \frac{1}{(2p)^3}\int_{-p}^{p} d^3q \,\langle \Psi_q A \Psi_q \rangle$$



PBC
TABC



Twist averaged MC

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

$$-p < q_i \le p \qquad i=(1,2,3)$$

- 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.

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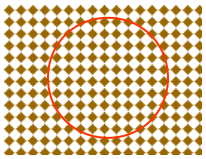
Grand Canonical Ensemble QMC

- 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.

$$\vec{k}_n = \frac{2p}{L}\vec{n} + \frac{\vec{q}}{L}$$
$$k_n \le k_F$$



- 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.

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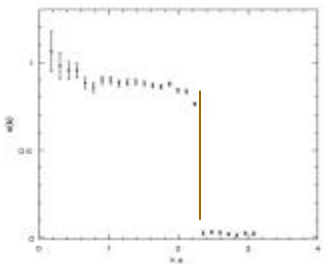
Single particle size effects

- 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.

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

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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.

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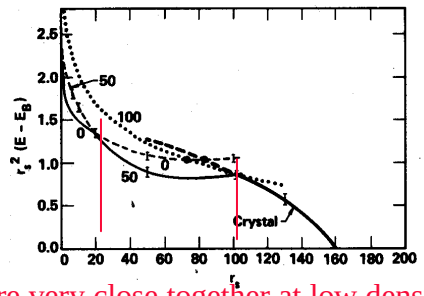
T=0 calculations with FN-DMC

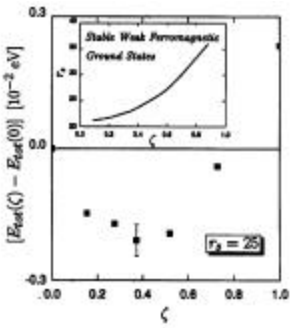
3d electron gas
- $r_s < 20$ unpolarized
- $20 < r_s < 100$ partial
- $100 < r_s$ Wigner crystal

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 $r_s = 65$.



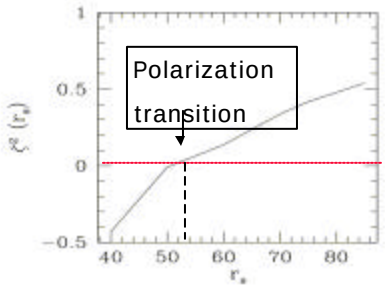
Polarization of 3DEG

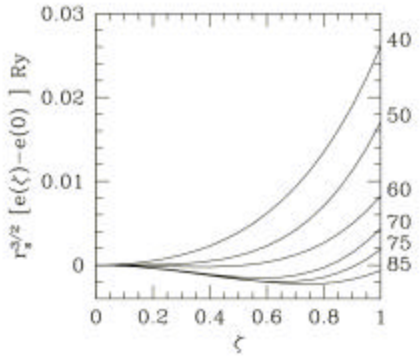
- We see second order partially polarized transition at r_s=52
- Is the Stoner model (replace interaction with a contact potential) appropriate? Screening kills long range interaction.
- Wigner Crystal at r_s=105

•Twist averaging makes calculation possible--much smaller size effects.

•Jastrow wavefunctions favor the ferromagnetic phase.

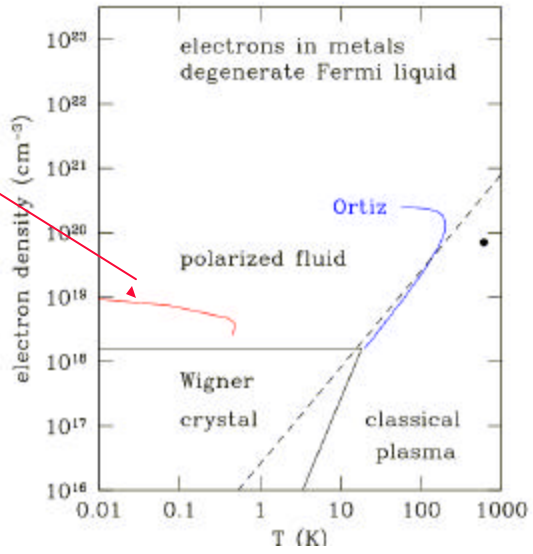
•Backflow 3-body wavefunctions more paramagnetic





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.



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Recent calculations in 2D

Tanatar,Ceperley '89
Rapisarda, Senatore '95
Kwon et al '97

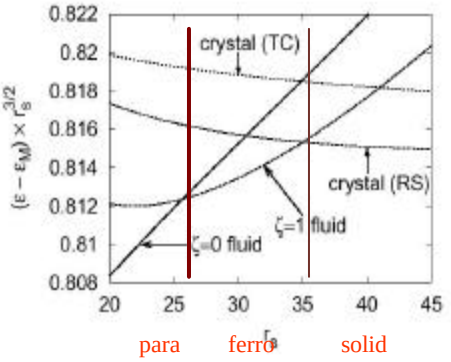
T=0 fixed-node calculation:

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

Energies of various phases are nearly identical

Attaccalite et al:

PRL 88, 256601 (2002)



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.

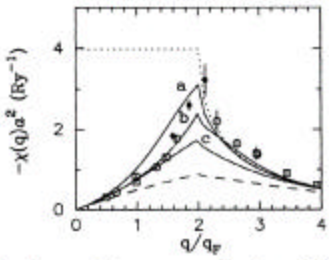


FIG. 4. Linear static response function $\chi(q)$ of the 2D electron fluid at $r_s = 5$. The squares, empty circles, and full

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

$$w_a(R) = \frac{f_a(R)}{y_G(R)}$$

- "Optimal Guiding function" is

$$y_G^2 = \sum_a |f_a(R)|^2$$

- 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 states since Slater Jastrow has no coupling between unlike spins.

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