

SMR 1595 - 9

**Joint DEMOCRITOS - ICTP School on
CONTINUUM QUANTUM MONTE CARLO METHODS
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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

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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 14 APRIL 1964

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 $\Psi_{\text{trial}}(\mathbf{r}_N)$. 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 $f(r) = \exp[-(2.6 \text{ \AA}/r)^6]$ the ground-state energy is found to be -0.78×10^{-38} 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.

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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.

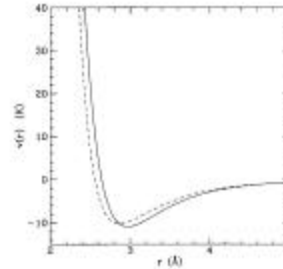


FIG. 1. The semiempirical pair potential between two helium atoms: solid line, Aziz et al. (1992); dashed line, Lennard-Jones 6-12 potential with $\epsilon = 10.22$ K and $\sigma = 2.558$ Å.

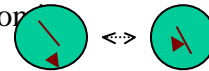
- Two isotopes:
 - ^3He (fermion: antisymmetric trial function, spin 1/2)
 - ^4He (boson: symmetric trial function, spin zero)

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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

$$c_6 r^{-6} + c_8 r^{-8} + \dots$$



- 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:

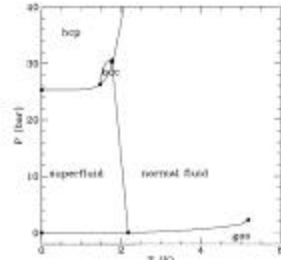


FIG. 2. The phase diagram of ⁴He.

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

$$\mathbf{I} \equiv \frac{\hbar^2}{2m_i}$$

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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:

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

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

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

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

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

Gives a cusp condition on u .

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

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

$$e r^{-n} = 2\mathbf{I} (a m r^{-m-1})^2 \text{ for } n > 2$$

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

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

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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

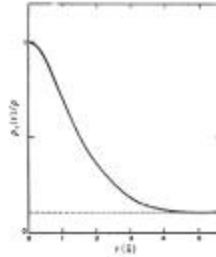
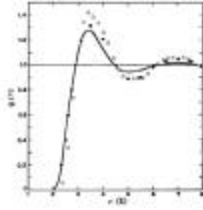


FIG. 3. The single-particle density matrix as a function of separation. The dashed curve indicates the asymptotic limit for large $r, r' \rightarrow \infty$ is ≈ 0.11 .

- 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%

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

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Derivation of momentum formula

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

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

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

- 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:

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

(states occupied with the Boltzmann distribution.)

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

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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

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

$$n(r, r') = \int dr_2 \dots dr_N \mathcal{Y}^*(r, r_2, \dots) \mathcal{Y}(r', r_2, \dots)$$

$$= \left\langle \frac{\mathcal{Y}^*(r', r_2, \dots)}{\mathcal{Y}(r, r_2, \dots)} \right\rangle$$

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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

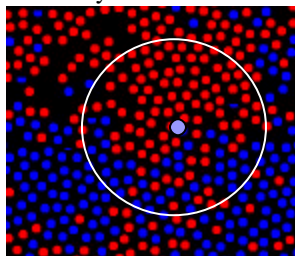
$$g(r) = \langle \sum_{i < j} \delta(r_i - r_j - r) \rangle (2 \Omega / N^2)$$

Density-density correlation function

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

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

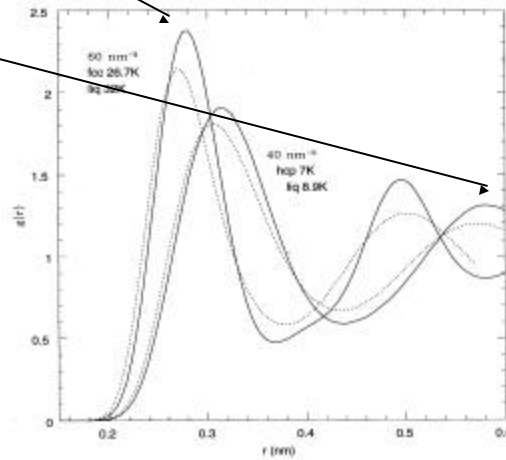
A function gives more information than a number!



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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

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

$$S(k) = 1 + \rho \int dr \exp(ikr) (g(r) - 1) \quad (2) \text{ "FT"}$$

- 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 $g(r)$)

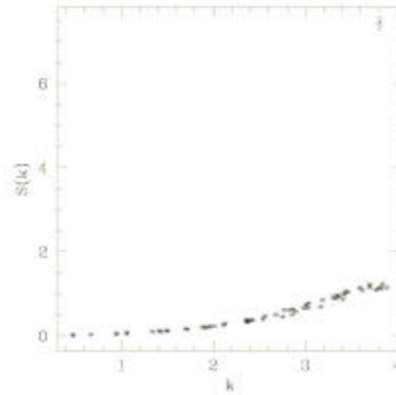
- Order parameter in solid is ρ_G where G is a particular wavevector (reciprocal lattice vector).

- 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

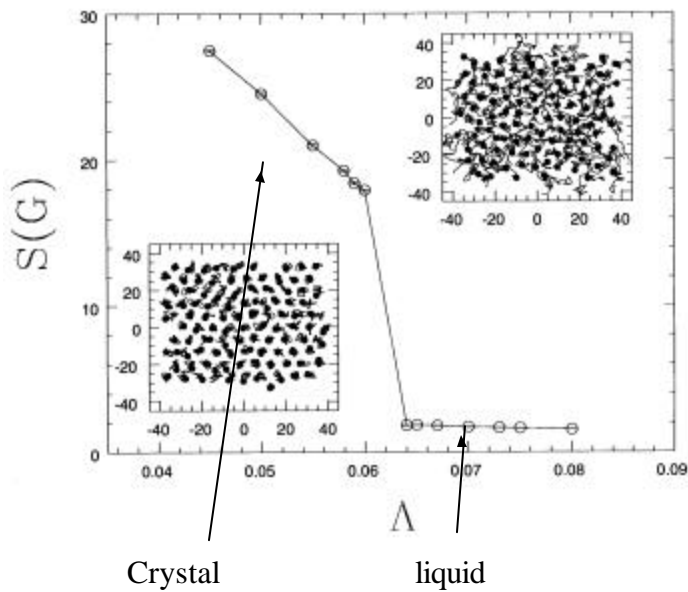
$$S(G) = 1 + (N-1)\exp(-G^2u^2/3)$$

- 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 to detect the liquid-gas transition since the compressibility should diverge as k approaches 0. (order parameter is density)

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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 determinant and sample the determinant. Use tricks from linear algebra.
- Reduces complexity to $O(N^2)$.

$$\Psi_s(R) = \text{Det} \left\{ e^{i k_j r_j} \mathbf{h}_i(\mathbf{s}_j) \right\}$$

$$\text{PBC: } k \cdot L = 2\pi n + \{\mathbf{q}\}$$

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

Slater-Jastrow trial function.

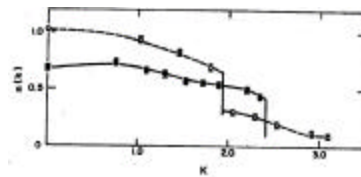
$$\det(\mathbf{f}_k(r_j^T)) = \det(\mathbf{f}_k(r_j)) \sum_k \mathbf{f}_k(r_j^T) \mathbf{M}_{k,i}^{-1}$$

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

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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.



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

$$= \left\langle \frac{\mathbf{y}^*(r, r_2 \dots)}{\mathbf{y}(r', r_2 \dots)} \right\rangle$$

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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:

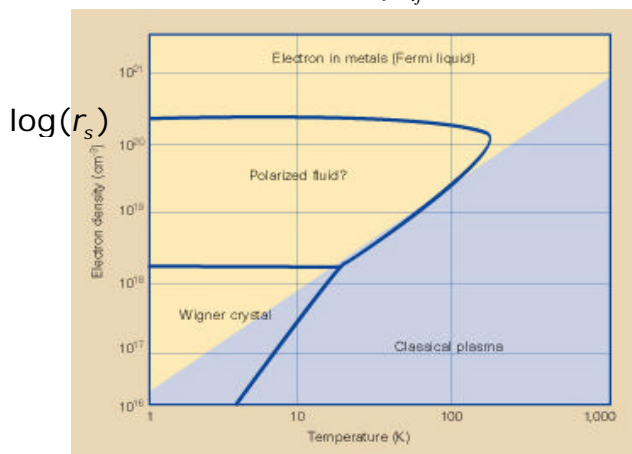
- Density
- Temperature

$$r_s = a/a_0$$

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

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

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



$\Gamma < r_s$ classical OCP

$\Gamma = 175$ classical melting

$\log(\Gamma)$

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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.

$$2ru_k = \sqrt{\frac{V_k}{Ik^2}} \propto \frac{1}{k^2}$$

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

$$2ru_k = -\frac{1}{S_k} + \sqrt{\frac{1}{S_k^2} + \frac{V_k}{Ik^2}} \quad S_k = \text{ideal structure factor}$$

- 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.

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

Long range properties important

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

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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

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

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:

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

- 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.

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

$$V = \sum_k f_k (|\mathbf{r}_k|^2 - N) \quad \text{where } \mathbf{r}_k = \sum_i e^{i\mathbf{k} \cdot \mathbf{r}_i}$$

$$\text{and } \mathbf{j}_k = \frac{1}{\Omega} \int d\mathbf{r} e^{i\mathbf{k} \cdot \mathbf{r}} \mathbf{f}(r)$$

$$\text{For } f(r) = e^2/r \Rightarrow \mathbf{j}_k = \frac{4\mathbf{p}e^2}{k^2}$$

- 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

$$f(r) = \frac{\text{erfc}(\mathbf{k}r)}{r} \quad \text{decays fast at large } r$$

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

\mathbf{k} = convergence parameter

- If we make it large enough we can use the minimum image potential in r-space.

- Extra term for insulators:
$$V_{dipole} = \frac{2\mathbf{p}}{(2\mathbf{e} + 1)\Omega} \left| \sum_i \mathbf{m}_i \right|^2$$

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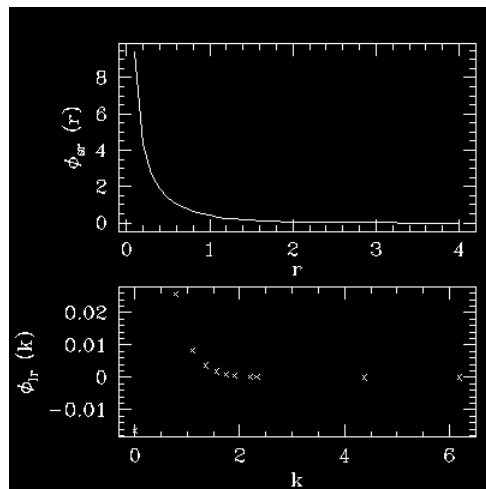
How to do it

- r-space part same as short-ranged potential O(N^{3/2})
- k-space part:
 1. Compute $\exp(ik_0 x_i) = (\cos(ik_0 x_i), \sin(ik_0 x_i))$, $k_0 = 2\pi/L$ O(N)
 $\forall i$.
 2. Compute powers $\exp(i2k_0 x_i) = \exp(ik_0 x_i) * \exp(ik_0 x_i)$ O(N^{3/2})
etc. This way we get all values of $\exp(ik \cdot r_i)$ with just multiplications.
 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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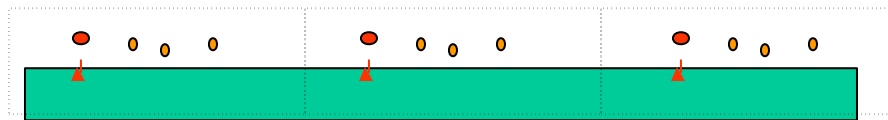
Optimized Ewald

- 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!

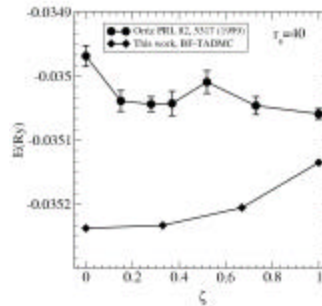
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Comparison of Trial functions

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

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

- 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 .

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

expand the density matrix in terms of exact eigenstates

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

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

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

Wavefunctions beyond Jastrow

- Use method of residuals construct a sequence of increasingly better trial wave functions. Justify from the Importance sampled DMC.

$$\mathbf{f}_{n+1}(R) \approx \mathbf{f}_n(R) e^{-t \langle \mathbf{f}_n^{-1} H \mathbf{f}_n \rangle} \quad \downarrow \text{smoothing}$$

$$\mathbf{f}_0 = e^{i \sum_j \mathbf{k}_j \cdot \mathbf{r}_j}$$

- Zeroth order is Hartree-Fock wavefunction

$$E_0 = V(R)$$

- First order is Slater-Jastrow pair wavefunction (RPA for electrons gives an analytic formula)

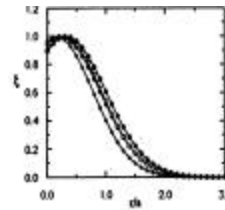
$$\mathbf{f}_1 = \mathbf{f}_0 e^{-U(R)}$$

- Second order is 3-body backflow wavefunction

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

- Three-body form is like a squared force. It is a bosonic term that does not change the nodes.

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



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Backflow- 3B Wave functions

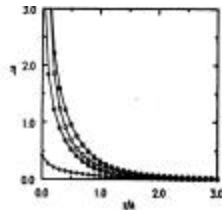
- Backflow means change the coordinates to quasi-coordinates.

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

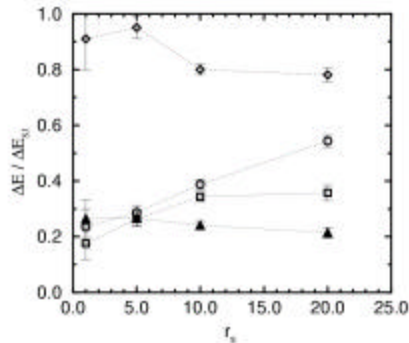
$$\mathbf{x}_i = \mathbf{r}_i + \sum_j \mathbf{h}_{ij}(r_{ij})(\mathbf{r}_i - \mathbf{r}_j)$$

- Leads to a much improved energy and to improvement in nodal surfaces. Couples nodal surfaces together.

Kwon PRB 58, 6800 (1998).



3DEG



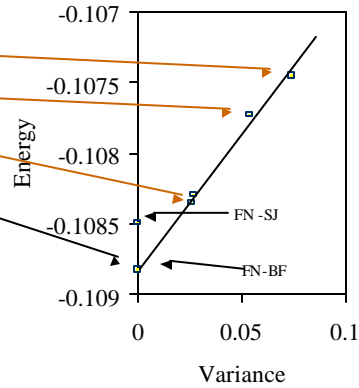
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Dependence of energy on wavefunction

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.

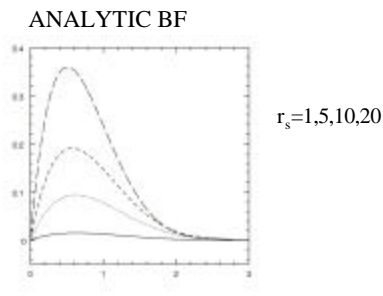
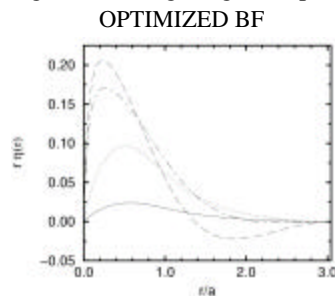


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Analytic backflow

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



- 3-body term is non-symmetric

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

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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

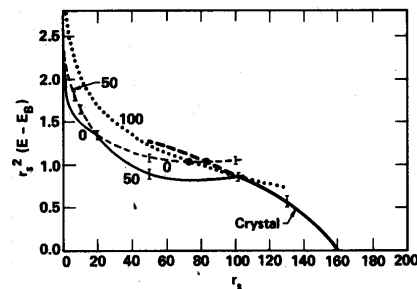
- Jastrow trial function does not “freeze” at appropriate density.
- Solution is to break spatial symmetry “by hand.”
- Introduce a bcc lattice $\{Z_i\}$
- bcc has the lowest Madelung energy, but others may have lower zero point energy.
- Introduce localized one-body terms (Wannier functions).
- Make 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.

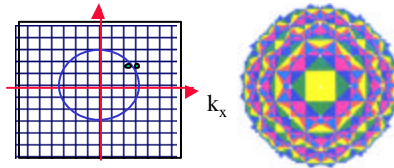


Twist averaged boundary conditions

- In periodic boundary conditions (Γ point), the wavefunction is periodic \Rightarrow **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 $r \rightarrow r+L$
- If one integrates over all phases the momentum distribution changes from a lattice of k-vectors to a fermi sea.
- Smaller finite size effects

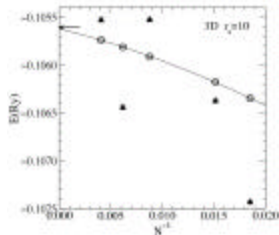
$$\mathbf{j} = e^{i\mathbf{k}r}$$

$$kL = 2\pi n + \mathbf{q}$$

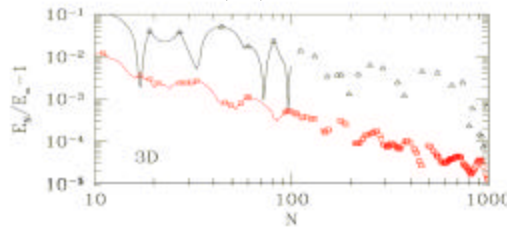


$$\Psi(x+L) = e^{i\theta} \Psi(x)$$

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



PBC
TABC



Twist averaged MC

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

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

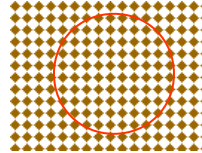
- Within GCE, change the number of electrons
- Within TA-VMC
 - Initialize twist vector.
 - Run usual VMC (with warmup)
 - Resample twist angle within cube
 - (iterate)
- Or do in parallel.

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 \mathbf{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.

$$\vec{k}_n = \frac{2\mathbf{p}}{L}\vec{n} + \frac{\mathbf{q}}{L}$$

$$k_n \leq k_F$$



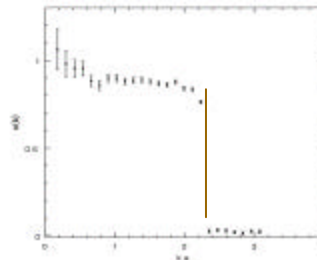
- After we average over θ (TA) we get a sphere of filled states.
- **Is there a problem with Ewald sums as the number of electrons varies?**
No! average density is exactly that of the background. We only work with averaged quantities.

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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?

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

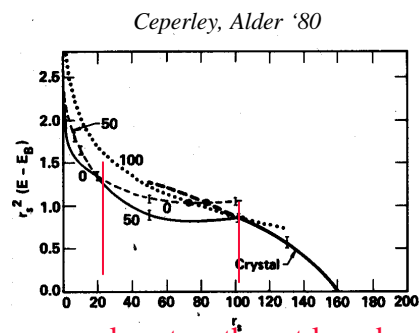
- Bloch 1929 got polarization from exchange interaction:
 - $r_s > 5.4$ 3D
 - $r_s > 2.0$ 2D
- Stoner 1939: include electron screening: contact interaction
- Herring 1960
- Ceperley-Alder 1980 $r_s > 20$ is partially polarized
- **Young-Fisk experiment on doped CaB_6 1999 $r_s \sim 25$.**
- Ortiz-Balone 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

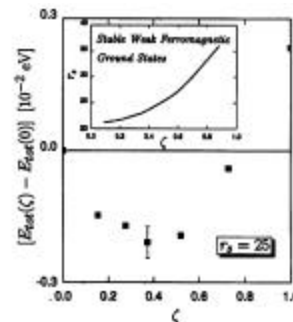
3d electron gas

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



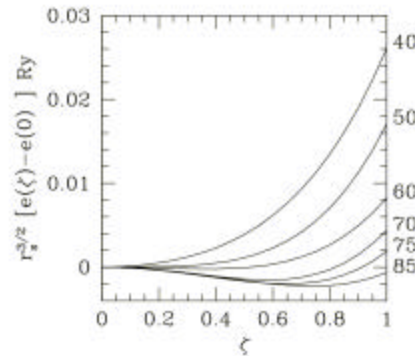
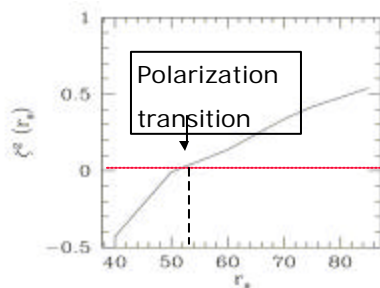
Energies are very close together at low density!

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



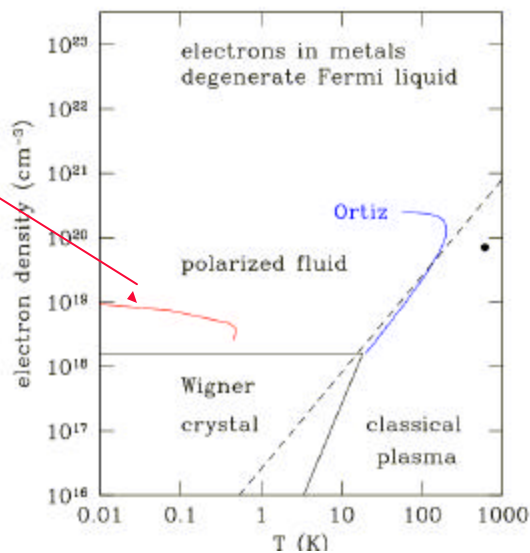
Polarization of 3DEG

- 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.

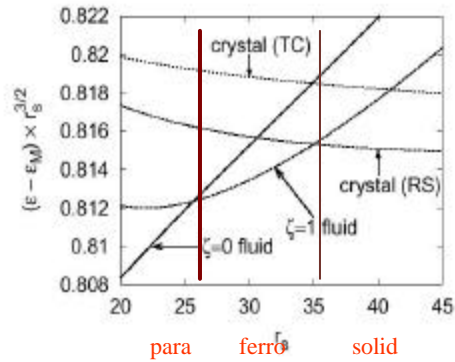
Energies of various phases are nearly identical

Attaccalite et al:

PRL 88, 256601 (2002)

2d electron gas

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



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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.

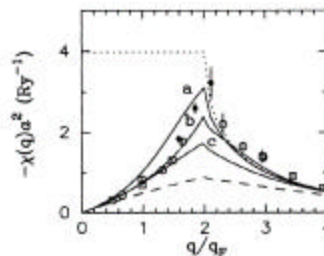


FIG. 4. Linear static response function $\chi(q)$ of the 2D electron fluid at $r_s = 5$. The squares, empty circles, and full

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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.