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

- VMC calculation of ground state of liquid helium 4.
- Applied MC techniques from classical liquid theory.
- Ceperley, Chester and Kalos (1976) generalized to fermions.

**Ground State of Liquid He**

W. L. McMillan

Department of Physics, University of Illinois, Urbana, Illinois

(Received 16 November 1964)

The properties of the ground state of liquid He are studied using a variational wave function of the form $\Pi_{\alpha} \phi(r_\alpha)$. 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 $\phi(r) = \exp[-(2.6 \AA/r)^6]$, the ground-state energy is found to be $-0.78 \times 10^{-14}$ 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.

\[
E_v(a) = \frac{\langle \psi(a)|H|\psi(a) \rangle}{\langle \psi(a)\psi(a) \rangle} \geq E_0 = \text{exact ground state energy}
\]

\[
\langle \psi(a)H\psi(a) \rangle = \int dR \psi^*(R; a)H\psi(R; a)
\]

\[
E_v(a) = E_0 \iff \psi(R; a) = \phi_0(R)
\]

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

\[
E_v(a) = \langle \langle E_L(R; a) \rangle \rangle_{\psi^2} \quad \text{where} \quad \langle \langle O \rangle \rangle_{\psi^2} = \frac{\langle \psi(a)O\psi(a) \rangle}{\langle \psi(a)\psi(a) \rangle}
\]

\[
\sigma^2(a) = \frac{\langle \psi(a)(H-E_v(a))^2\psi(a) \rangle}{\langle \psi(a)\psi(a) \rangle} = \langle \langle (E_L(R; a) - E_v(a))^2 \rangle \rangle_{\psi^2} = \text{variance of the trial function}
\]

\[
\frac{dE_v(a)}{da} = 2\langle \langle \frac{d \ln \psi(R; a)}{da} (E_L(R; a) - E_v(a)) \rangle \rangle = 0
\]

Conditions: \textbf{matrix elements exist, symmetries and boundary conditions are correct.}
Expand trial function in terms of the exact eigenfunctions:

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

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

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

$$\sigma^2(a) = \int dE \rho_{a}(E) (E - E_v(a))^2$$

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

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

**Temple lower bound:**

$$E_v - \frac{\sigma^2}{E_1 - E_0} \leq E_0 \leq E_v$$
Linear Basis approach

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

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

$$E_V(a) = \sum_{n,m} a^*_n a_m H_{nm}$$

Problem that MC solves:

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

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

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

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

$$\frac{dE}{da} = 2[H a - E_V S a]$$

$$H a_\lambda = E_\lambda S a_\lambda \text{ generalized eigenvalue problem}$$
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.
  \[ E_0 \leq E_1 \leq E_2 \leq \ldots \leq E_m \]
  \[ E_n^{ex} \leq E_n \]

- We can always lower all the energies by augmenting 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

\[ E_L (R) = \Re \left[ \psi^{-1} (R) H \psi (R) \right] \]
\[ E_V = \langle E_L (R) \rangle_{\psi} \geq E_0 \]

- 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.

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

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

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

\[
\lambda \equiv \frac{\hbar^2}{2m_i}
\]

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

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

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

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

$U(r) = \alpha r^m$

Gives a cusp condition on $u$.

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

\[u'(0) = -\frac{e^2}{2\lambda(D-1)}\]

$$\varepsilon r^{-n} = 2\lambda \left(\alpha m r^{-m-1}\right)^2 \text{ for } n > 2$$

\[m = \frac{n}{2} - 1\]

$$\alpha = \frac{1}{m} \sqrt{\frac{\varepsilon}{2\lambda}}$$
Optimization of trial function

\[ E_V(a) = \frac{\int \psi(a) H \psi(a)}{\int \left| \psi(a) \right|^2} \]

\[ \sum_k w(R_i, a) E(R_i, a) \]

\[ \sum_k w(R_i, a) \]

\[ w(R_i, a) = \frac{\left| \psi(R, a) \right|^2}{P(R)} \]

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

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

- 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 \( a_0 \).
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 \( \sim 10\% \)

\[
n(r, r') = \int dr_2...dr_N \psi^*(r, r_2...)(r', r_2...)
\]
\[
= \frac{\langle \psi^*(r', r_2,...) \rangle}{\psi(r, r_2,...)}
\]

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

$$\Pr(k_1,..k_N) = \left| \int dR \ e^{-i(k_1r_1+...+k_Nr_N)}\Psi(R) \right|^2$$

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

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

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

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

\[
\Psi_s(R) = Det \left\{ e^{ik_ir_j} \eta_i(\sigma_j) \right\}
\]

PBC: \[ k \cdot L = 2 \pi n + \{\theta\} \]

\[
\Psi_{SJ}(R) = Det \left\{ e^{ik_ir_j} \right\} e^{-\sum_{i<j} u(r_{ij})}
\]

Slater-Jastrow trial function.

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

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

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

\[ \Gamma < r_s \quad \text{classical OCP} \]
\[ \Gamma = 175 \quad \text{classical melting} \]
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.

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

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

Ceperley Variational Method
Wavefunctions beyond Jastrow

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

- 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.

\[ \Psi_2(R) \exp\{\sum_i [\sum_j \xi_{ij}(r_{ij})(r_i - r_j)]^2\} \]

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Backflow- 3B Wave functions

- Backflow means change the coordinates to quasi-coordinates.

\[
\begin{align*}
\text{Det}\{e^{ik_ir_j}\} & \Rightarrow \text{Det}\{e^{ik_ir_j}\} \\
\mathbf{x}_i & = \mathbf{r}_i + \sum_j \eta_{ij}(r_{ij})(\mathbf{r}_i - \mathbf{r}_j)
\end{align*}
\]

- Leads to a much improved energy

*Kwon PRB 58, 6800 (1998).*

3DEG
Dependence of energy on wavefunction

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


- 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.
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

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

Ceperley Variational Methods

- 3-body term is non-symmetric!
## Results of Analytic tf

<table>
<thead>
<tr>
<th>$r_s$</th>
<th>wavefunction</th>
<th>$E_v$</th>
<th>$\sigma$</th>
<th>$E_{DMC}$</th>
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<td>1</td>
<td>SJ</td>
<td>1.0669 (6)</td>
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</table>

- 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.

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

\[
\psi(R) = \prod_i \phi(r_i - Z_i) \prod_{i<j} e^{-u(r_{ij})}
\]

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

“\(C\)” is a variational parameter to be optimized.
Twist averaged boundary conditions

- In periodic boundary conditions ($\Gamma$ 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 $\theta$ as $r \to r+L$
- If one integrates over all phases the momentum distribution changes from a lattice of $k$-vectors to a fermi sea.
- Smaller finite size effects

$$\varphi = e^{ikr}$$
$$kL = 2\pi n + \theta$$

$$\Psi(x + L) = e^{i\theta} \Psi(x)$$
$$\bar{A} = \frac{1}{(2\pi)^3} \int_{-\pi}^{\pi} d^3\theta \langle \Psi_\theta A \Psi_\theta \rangle$$

Error with PBC
Error with TABC
Twist averaged MC

- Make twist vector dynamical by changing during the random walk.
  \[ -\pi < \theta_i \leq \pi \quad i=(1,2,3) \]

- 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.

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Grand Canonical Ensemble QMC

• GCE at T=0K: choose N such that $E(N) - \mu N$ 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) $k_F$. Choose all states with $k < k_F$ (assuming spherical symmetry)
• $N$ will depend on the twist angle $\theta$. = number of points inside a randomly placed sphere.

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

$$k_n \leq k_F$$

• After we average over $\theta$ (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

- 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

$$r_s=4 \ N=33 \text{ polarized}$$

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

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

• 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:

$$\Delta E = aN^{-5/3}\cos^2(k_FL + \pi/16)$$

We can cancel this term at special values of $N$!

$N=15, 42, 92, 168, 279, \ldots$
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 \( r_s \sim 20 \).
- 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

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
• 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

\[ r_s = 10 \quad r_s = 20 \quad r_s = 3 \]
Recent calculations in 2D

**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*

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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)

![Graph showing error against computer time for different methods](image)