Two-dimensional 3He

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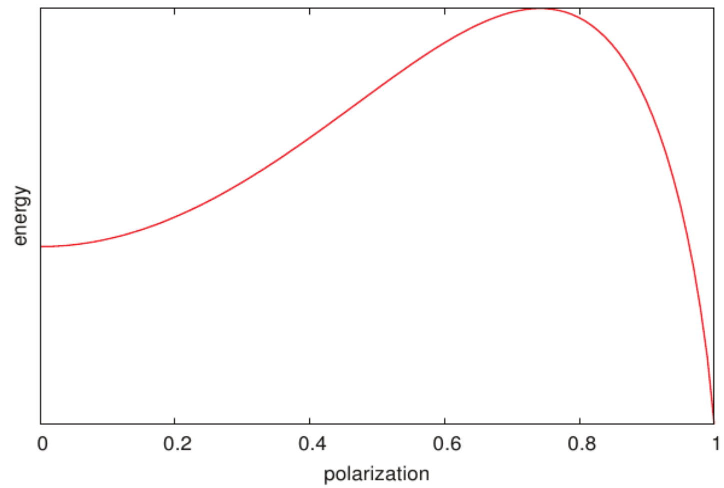
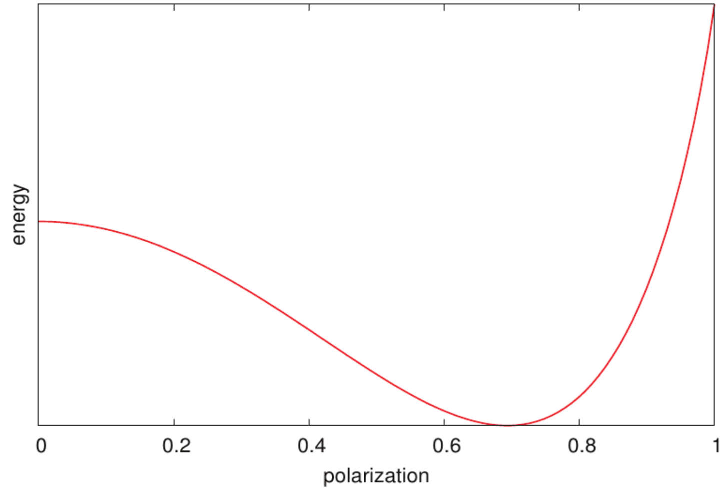
thanks to: S. Baroni, E. Vitali, M. Nava, D. Galli

- Itinerant ferromagnetism: an interaction-driven FL instability
  - some examples from QMC
  - 3He: quasi-localized model or paramagnon model?
- Two-dimensional 3He
  - experiments
  - QMC simulations
    * fixed-node results (3D)
    * unbiased fermionic ground state energy as an excitation
    * results
- Dynamic structure factor
  - neutron scattering data
  - QMC results from imaginary-time correlation functions

Bloch $E(\zeta) = \frac{A}{r_s^2}\left[(1+\zeta)^{5/3} + (1-\zeta)^{5/3}\right] - \frac{B}{r_s}\left[(1+\zeta)^{4/3} + (1-\zeta)^{4/3}\right]$



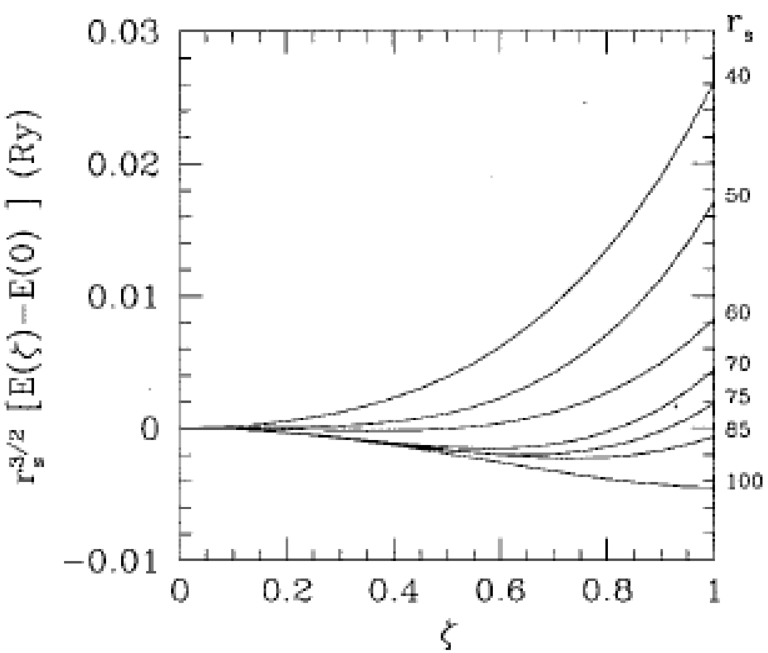


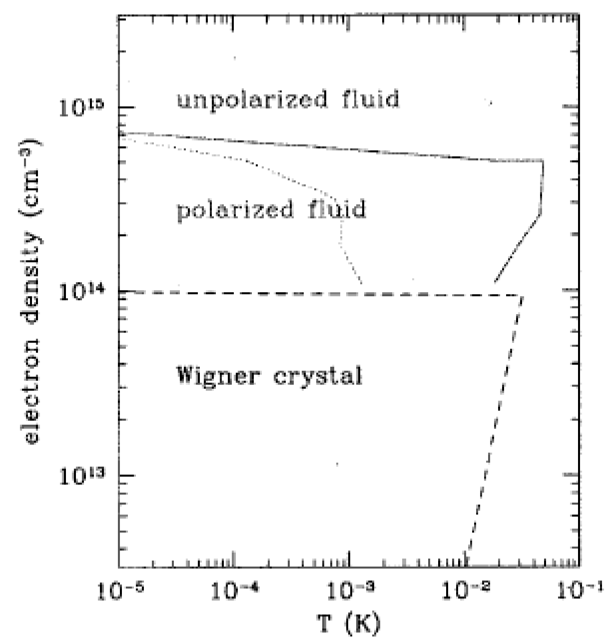
Stoner $E \propto (1+\zeta)^{5/3} + (1-\zeta)^{5/3} + 0.054 g\, r_s^2 (1-\zeta^2)$

Itinerant ferromagnetism

- 3D electron gas

Energy vs spin polarization



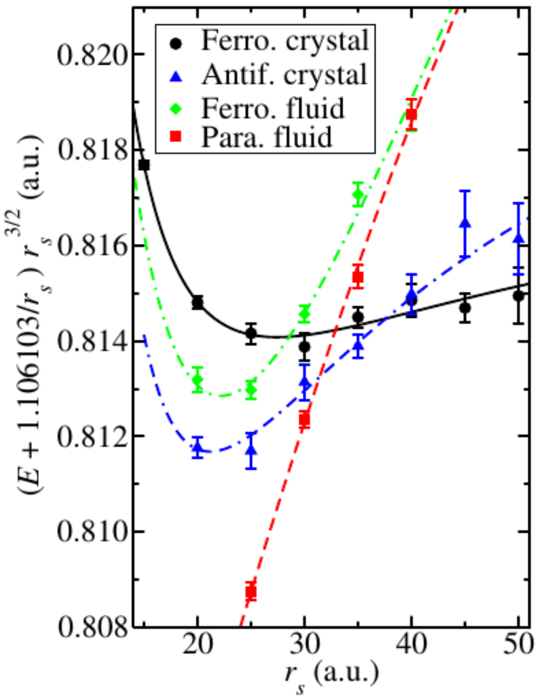


Phase diagram
(via an effective Stoner model)

F. Zong, C. Lin and D. Ceperley (2002)

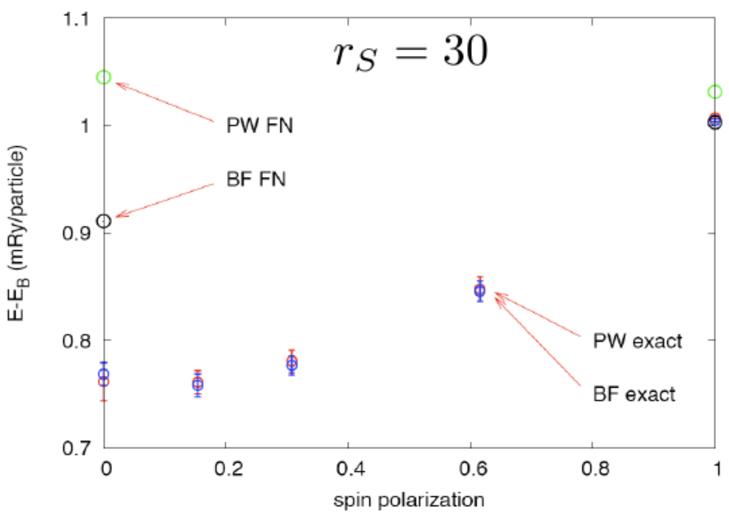
Itinerant ferromagnetism

- 2D electron gas



Phase diagram, fixed node,
N. Drummond and R. Needs, PRL (2009)

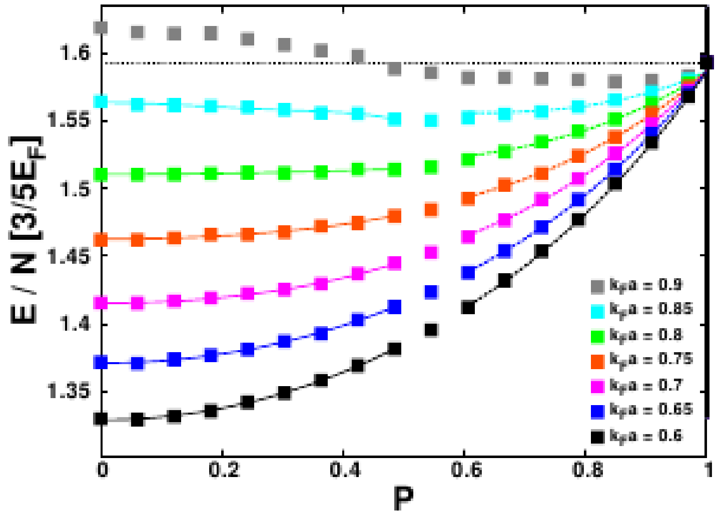
Energy vs polarization, TE,
E. Vitali, SM, S. Baroni



Itinerant ferromagnetism

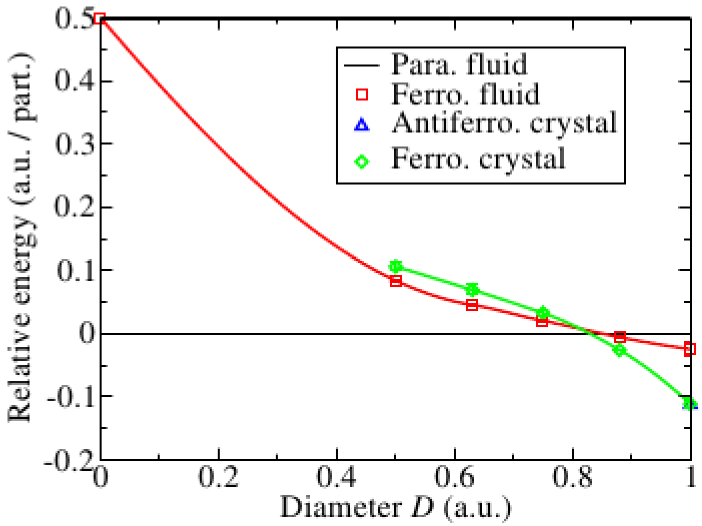
- 3D hard spheres

Energy vs polarization, S. Pilati et al. (2010)



- 2D hard spheres

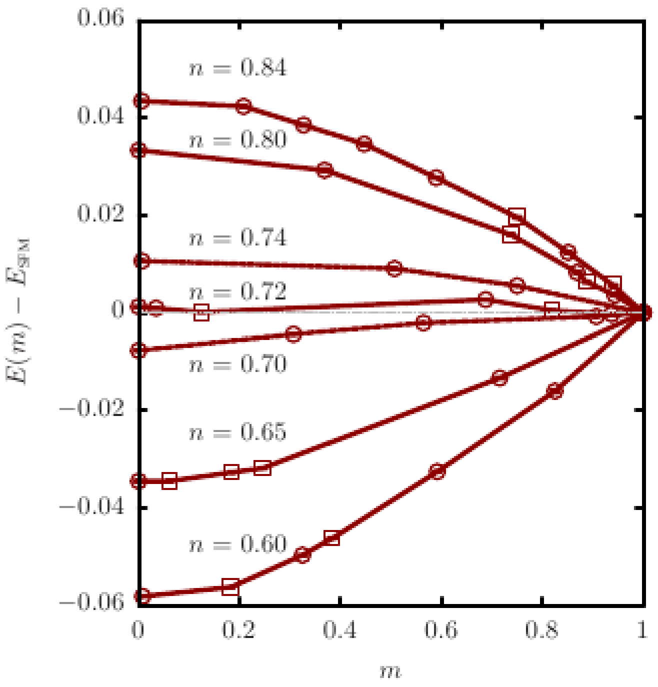
Phase diagram, N. Drummond et al., (2011)



Itinerant ferromagnetism

- Infinite-U Hubbard model

Energy vs polarization, G.Carleo et al. (2010)

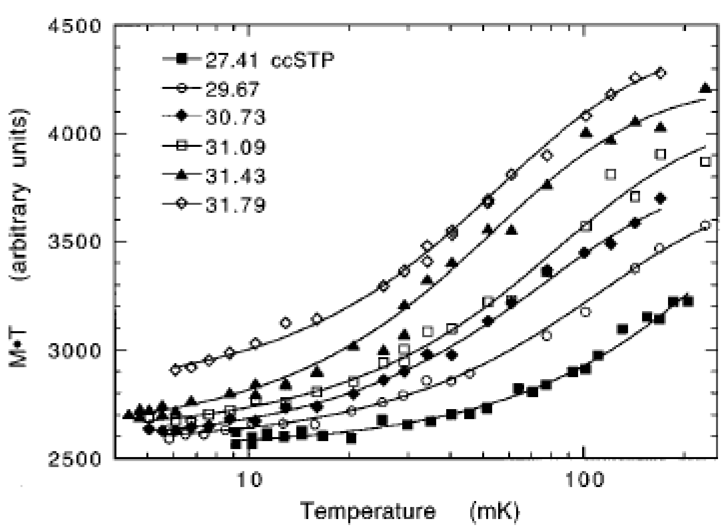


Liquid 3He is paramagnetic in both 3D and 2D

- how close to ferromagnetic?

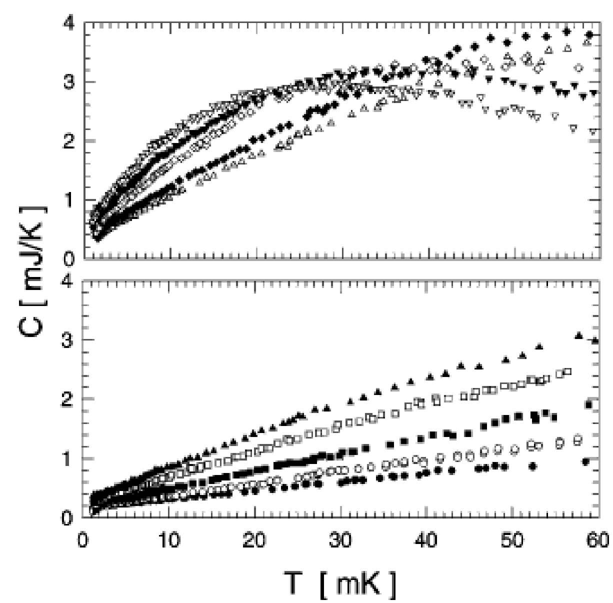
Measurements on 3He layers adsorbed on preplated graphite

Magnetization of II layer of 3He



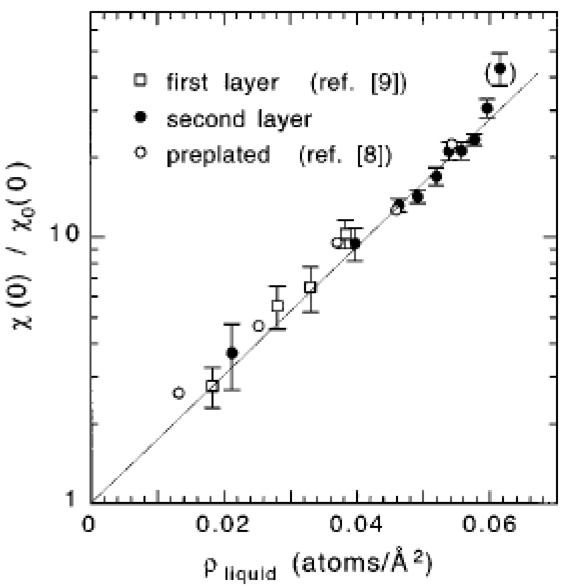
$$\chi = \frac{C_{\text{liquid}}}{\sqrt{T^2 + T_F^{**2}}}$$

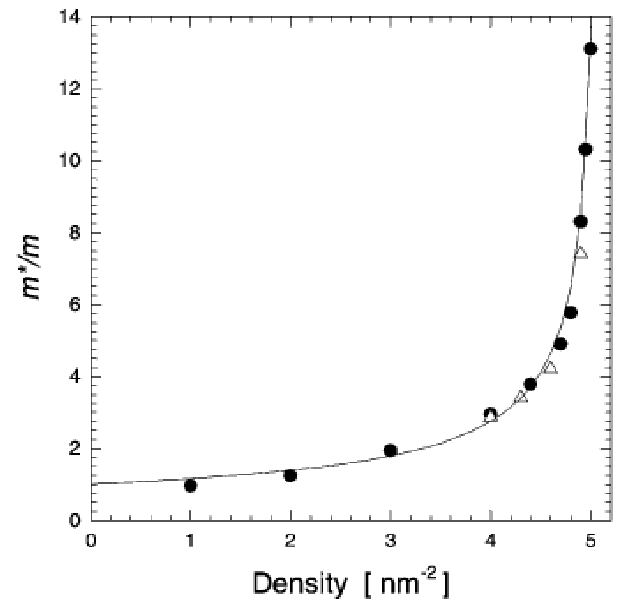
Specific heat of a 3He layer on HD bilayer

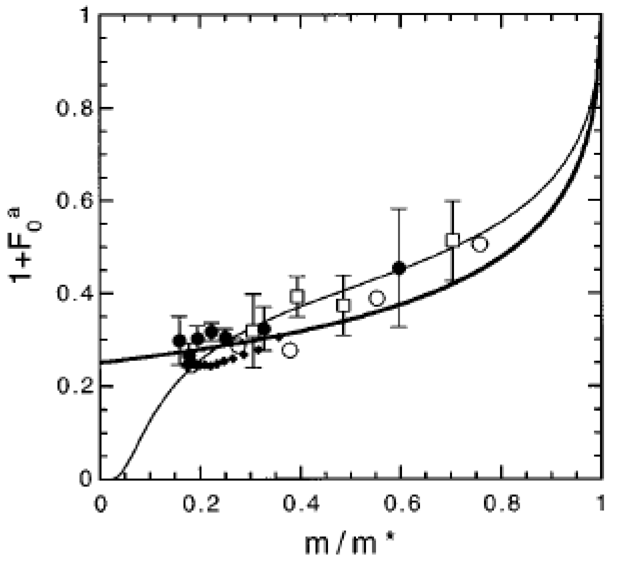


$$c = \beta + \gamma T + \Gamma_{2D} T^2$$

Measured properties are rather independent of substrate







Thick line: qualilocalized model, D. Vollhardt (1984)

Thin line: paramagnon model, M. T. Beal-Monod (1980)

Problems with fixed-node QMC:

3D 3He with 3-body backflow

PHYSICAL REVIEW B **74**, 104510 (2006)

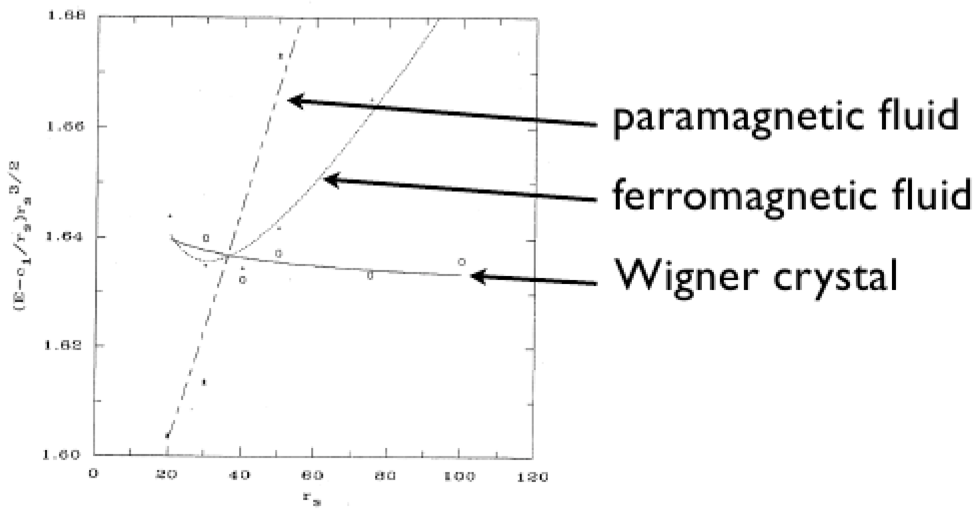
Many-body wavefunctions for normal liquid ^{3}He

Markus Holzmann,[1] Bernard Bernu,[1] and D. M. Ceperley[2]

TABLE III. Magnetic susceptibility χ/C in K^{-1}, where C is the molar Curie constant, estimated from the DMC calculations using the 3BF4 wave function; experimental values (Ref. 33) at densities ρ_{exp} are given for comparision.

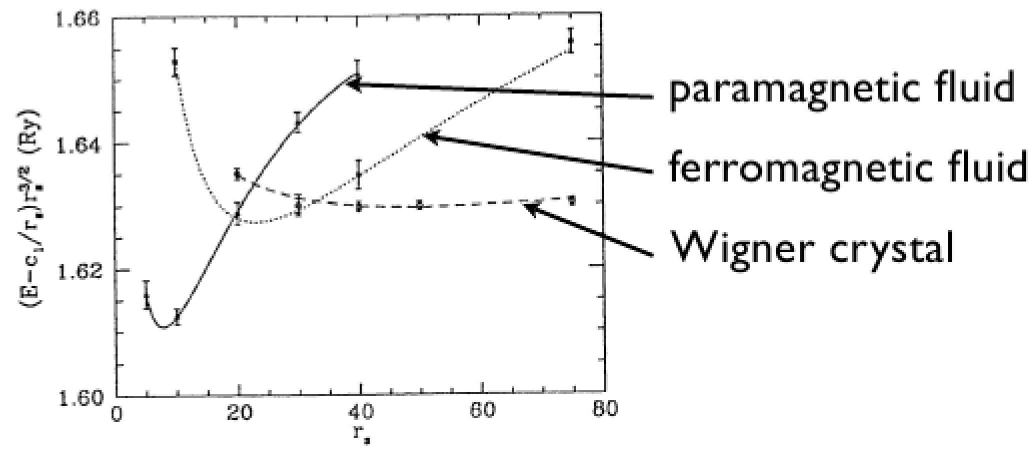
ρ (nm^{-1})	χ/C (K^{-1}) BF3	χ/C (K^{-1}) BF4	ρ_{exp} (nm^{-3})	χ_{exp}/C (K^{-1})
16.35	8(2)	4.5(5)	16.37	3.0
19.46	5(2)	8(3)	19.44	4.0
23.80		$\lvert\chi/C\rvert \gtrsim 14$	23.45	6.1

2D electron gas: Fixed-node calculations



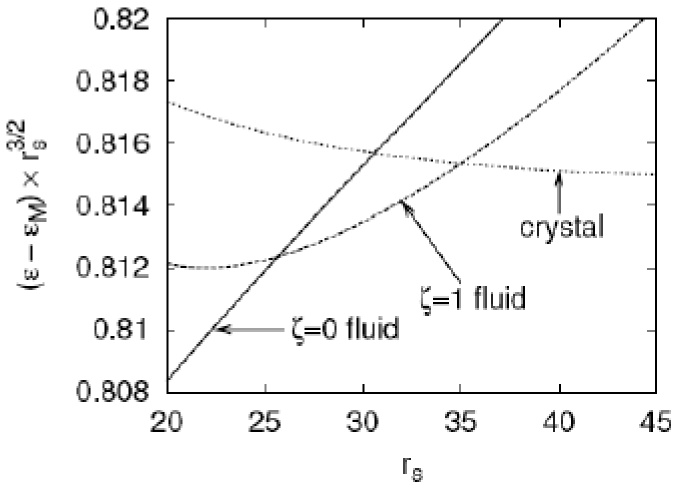
Tanatar and Ceperley (1989) - plane wave nodes

2D electron gas: Fixed-node calculations



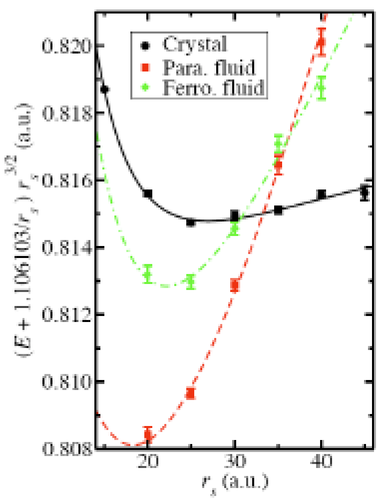
Rapisarda and Senatore (1996) - plane wave nodes

2D electron gas: Fixed-node calculations



Attaccalite et al. (2002) - backflow nodes

2D electron gas: Fixed-node calculations



Drummond and Needs (2008) - better backflow nodes

Unbiased fermionic ground state as an excitation

Dynamical properties in bosonic systems

A familiar example:

$$F(\mathbf{q},t) = \frac{1}{N}\langle \rho_{\mathbf{q}}(t)\rho_{-\mathbf{q}}(0)\rangle$$

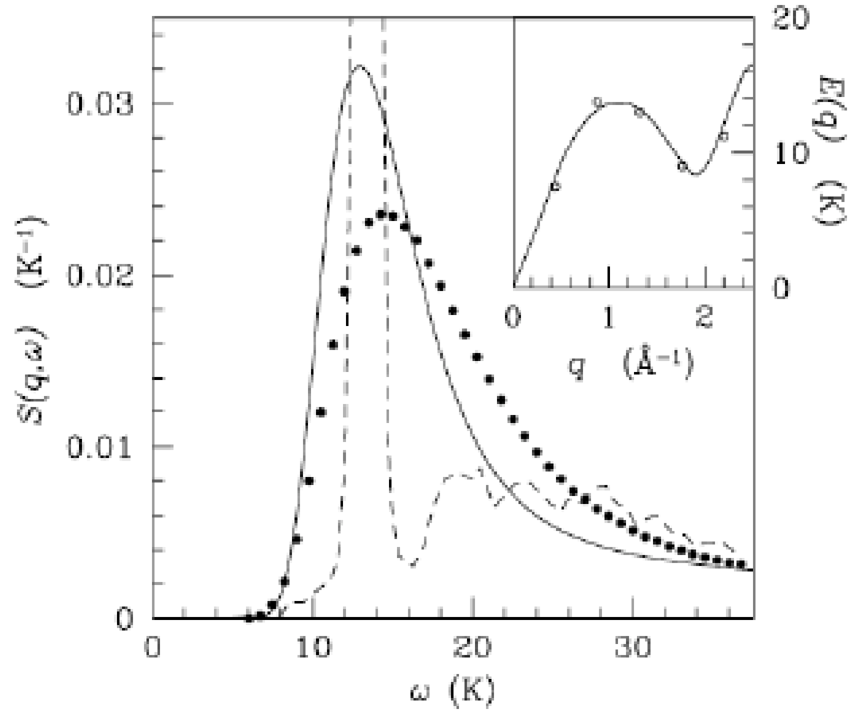
$$F(\mathbf{q},t) = \int d\omega e^{i\omega t} S(\mathbf{q},\omega)$$

In imaginary time:

$$F(\mathbf{q},\tau) = \frac{1}{N}\langle \rho_{\mathbf{q}}(\tau)\rho_{-\mathbf{q}}(0)\rangle$$

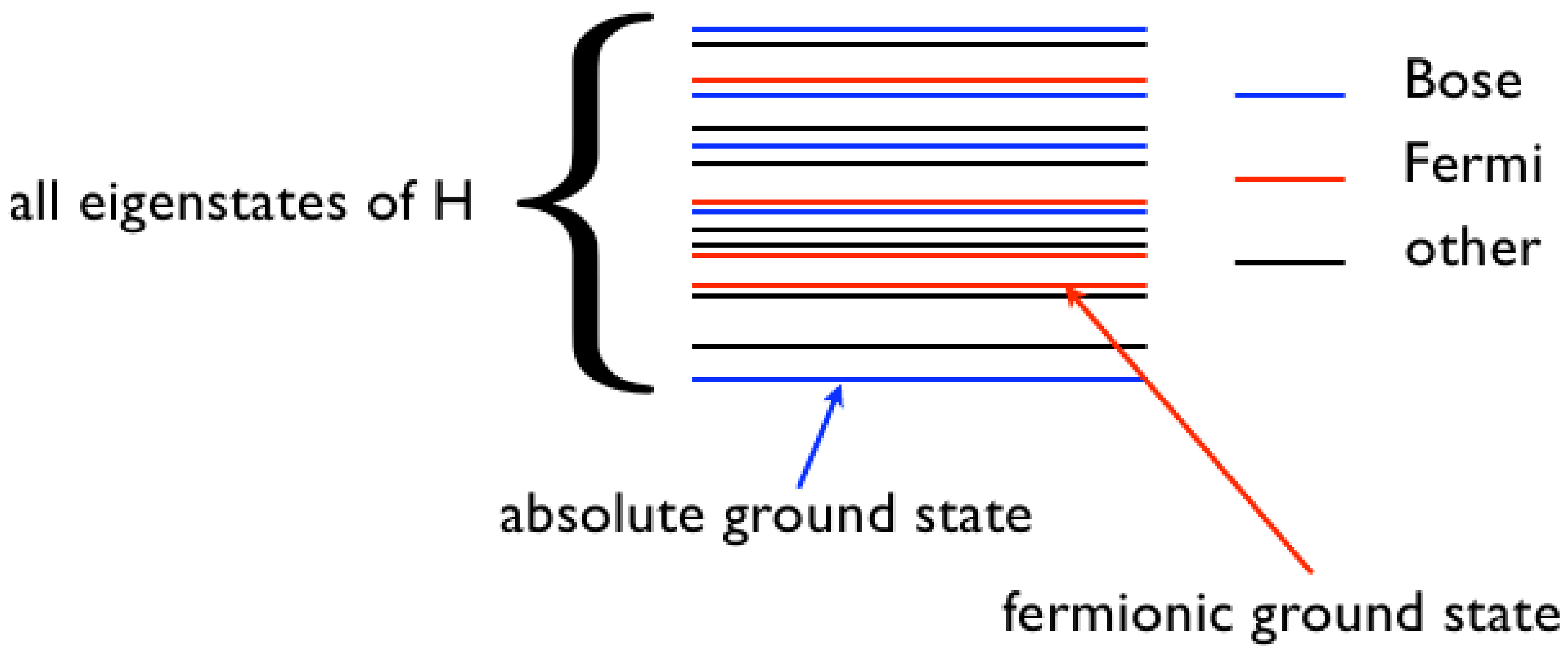
$$F(\mathbf{q},\tau) = \int d\omega e^{-\omega\tau} S(\mathbf{q},\omega)$$

Dynamical properties in bosonic systems



Spectral reconstruction and phonon-roton dispersion in 4He

Fermionic states as excitations from a Bosonic ground-state



Fermionic energies from imaginary-time correlation functions

$$
\begin{aligned}
c(\tau) &= \langle D(\tau) D^*(0) \rangle \\
&= \langle D e^{-\tau H} D^* \rangle \\
&= \sum_i |\langle \Phi_0 | D | \Psi_i \rangle|^2 e^{-\tau E_i}
\end{aligned}
$$

Φ_0	bosonic ground state
$\Psi_i, \quad E_i$	fermionic eigenstates and their energies
D	a Slater determinant

When does this work?

- Fermionic gap not much smaller than the Fermi-Bose gap

  - relatively small systems

  - strong correlations

- Good trial functions

(similar to Transient Estimate)

Closely related to:

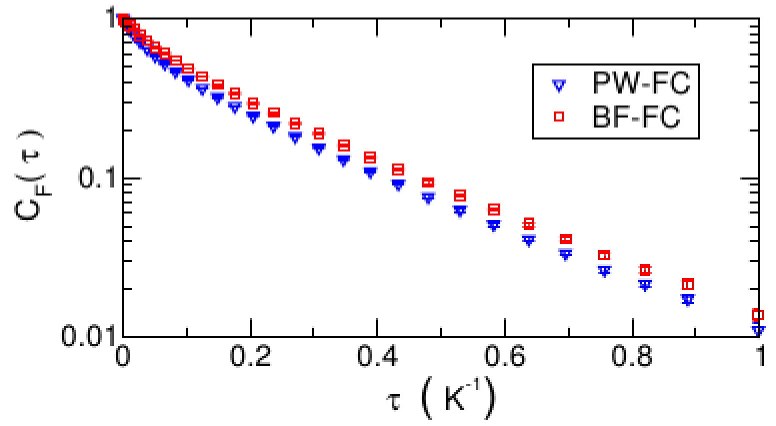
J. Chem. Phys., Vol. 97, No. 11, 1 December 1992

A Bayesian analysis of Green's function Monte Carlo correlation functions

M. Caffarel[a] and D. M. Ceperley

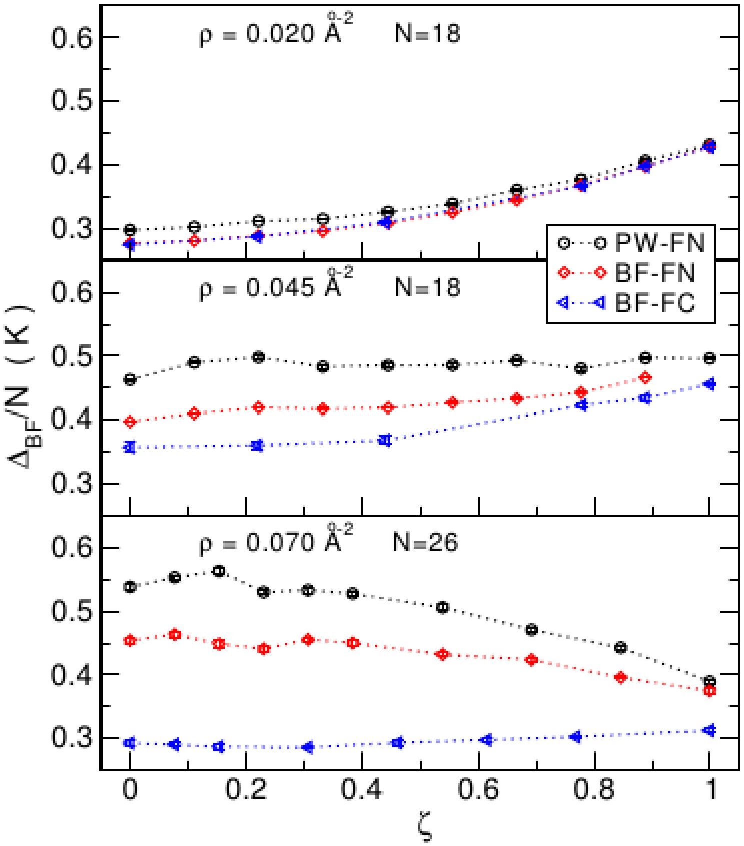
$$h^{(k)}(t) = \langle \Psi_T | H^k O(t) | \Psi_T \rangle \quad \text{where } k = \{0,1,2\}$$

- Fit the long-time exponential tail of the correlation function

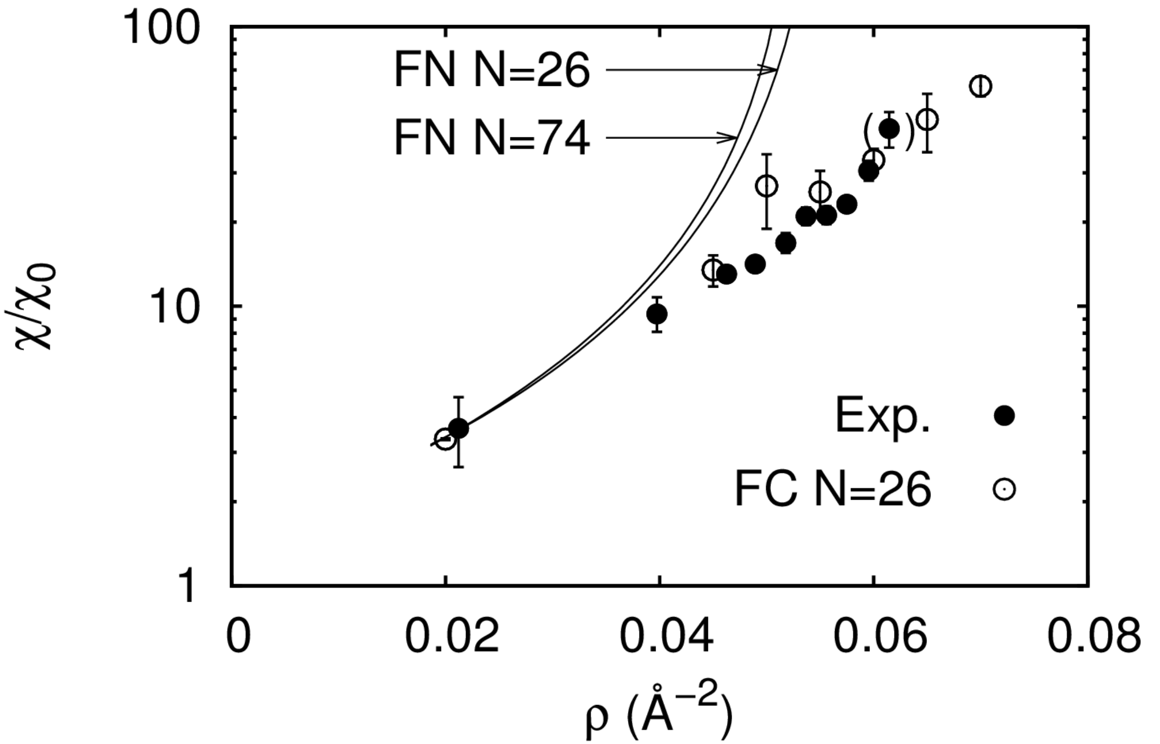


- Same result for PW or BF determinant

Energy vs polarization for various densities



- Results for the spin susceptibility



Excitation spectrum:

$$c(\tau) = \langle D(\tau)\rho_q(\tau)\rho_{-q}(0)D^*(0)\rangle$$

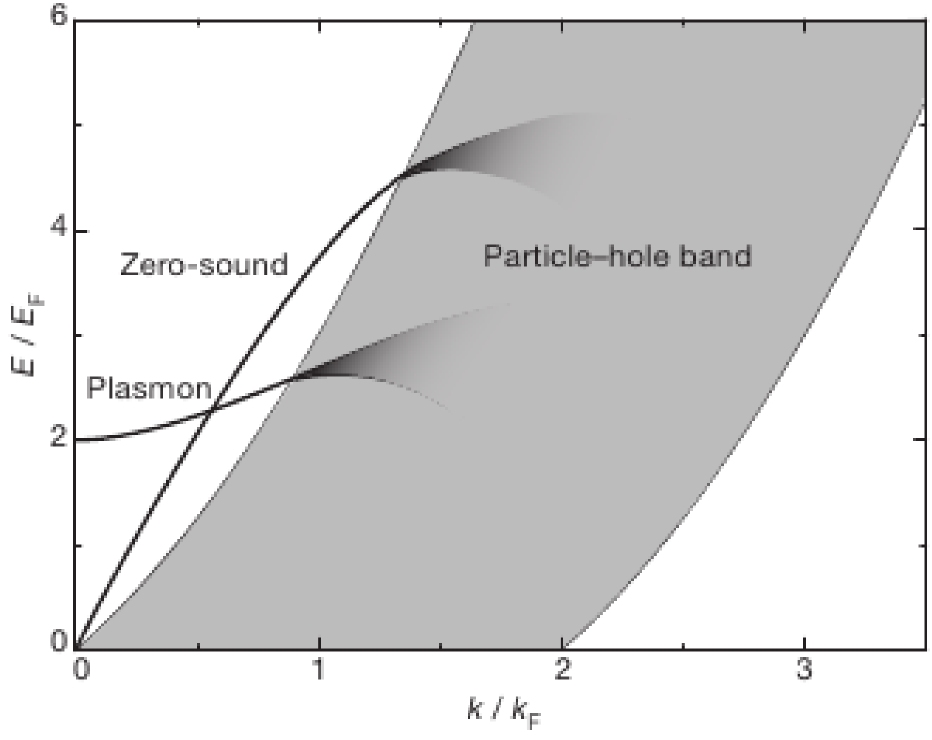
- Need a correction for the spectral weights, e.g.

$$\Psi_0/\Phi_0 \simeq \Psi_T/\Phi_T$$

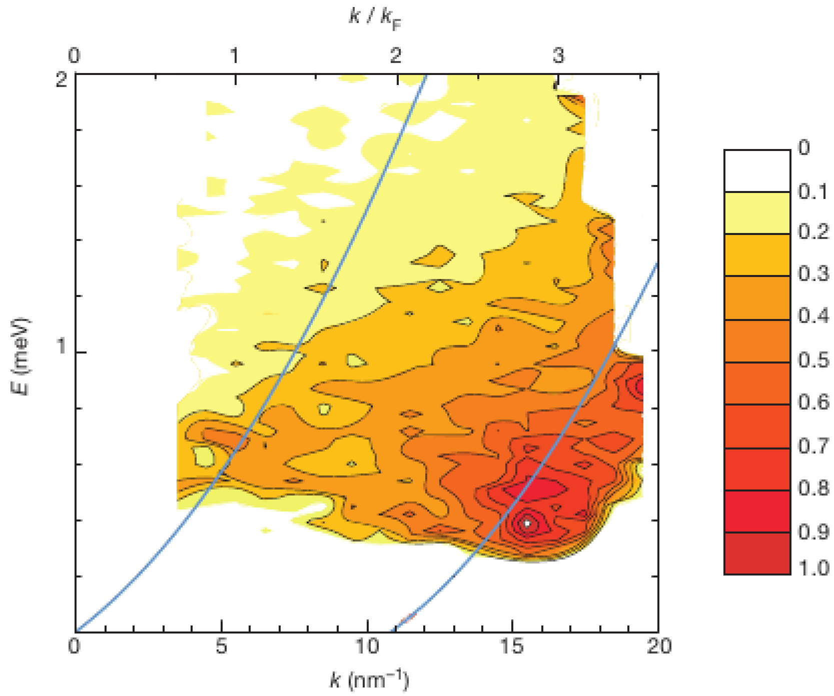
- Inverse Laplace transform:

  GIFT algorithm, Vitali et al. (2010)

Schematic picture of the FL excitation spectrum

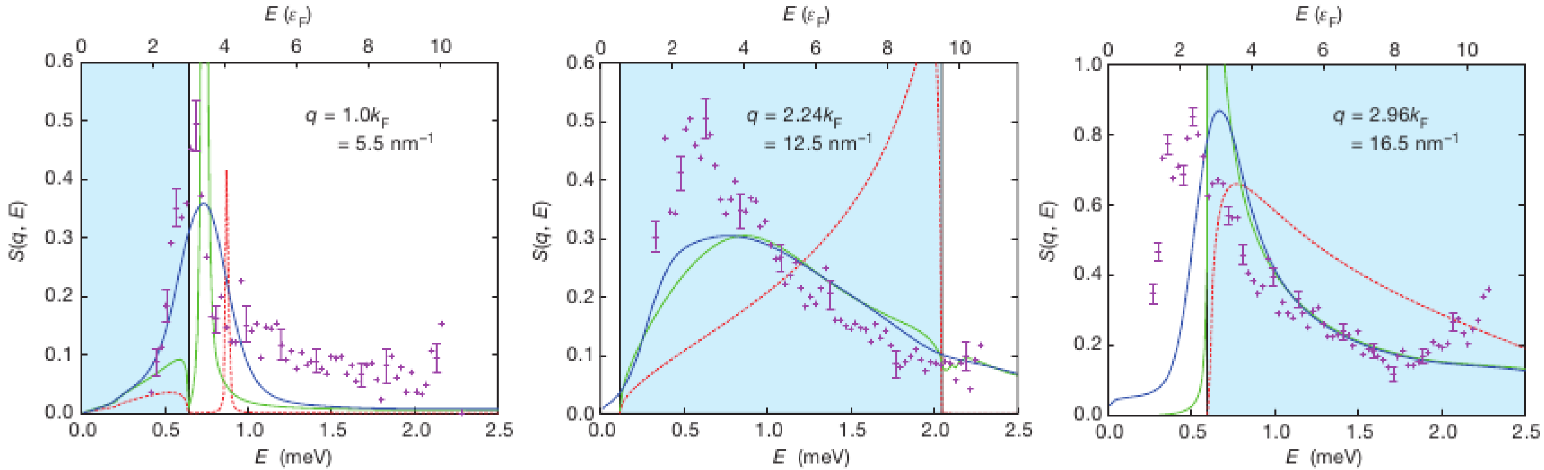


experimental dynamic structure factor



H. Godfrin et al., 5 7 6 | N AT U R E | VO L 4 8 3 | 2 9 M A R C H 2 0 1 2

- Neutron scattering data from second ^{3}He layer



red dashed, RPA

green, DMBT

blue, DMBT+experimental resolution

dynamic structure factor: simulation vs experiment