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SECOND EUROPEAN SUMMER SCHOOL on MICROSCOPIC QUANTUM MANY-BODY THEORIES and their APPLICATIONS

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QUANTUM SIMULATIONS
Bloch Transition (1929)

Part II

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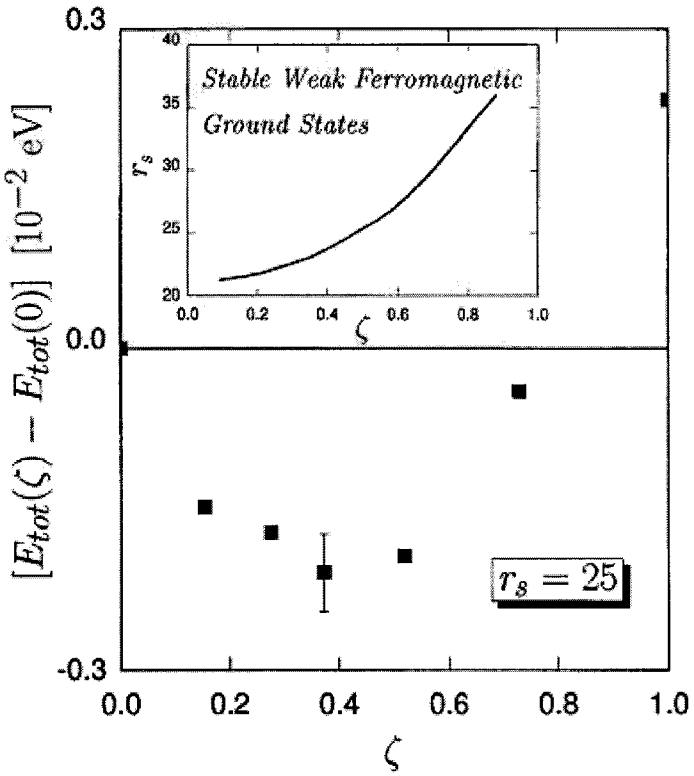
Bloch Transition (1929)

- Exchange favors spin alignment at large coupling r_s
- Thus Hartree-Fock predicts a transition from para- to ferro-magnetic fluid at high density:
  - $r_s^B = 5.5$ in 3D and $r_s^B = 2.0$ in 2D
- Correlation effects move the transition at much lower density:
  - away from metals in 3D
  - possibly in regimes that are nowadays achievable in 2D in semiconductor heterostructures
- Is the transition first or second order?
- Is it observable?
- Is incipient ferromagnetism related to the metal insulator transition in 2D systems with disorder?

3D electron gas, according DMC (T = B = 0)

- Ceperley-Alder (1980) : $r_s^B \approx 75$
  - However if a partial polarization is allowed the transition might move at $r_s^B \approx 20$ (Ceperley et al, 1982)



- Ortiz, Harris and Ballone (PRL 82 5317, 1999)
  Predict a continuous transition at $20\pm5 \le r_s \le 40\pm5$

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

$$\frac{4\pi (r_s a_B)^3}{3} = \frac{N}{V}$$

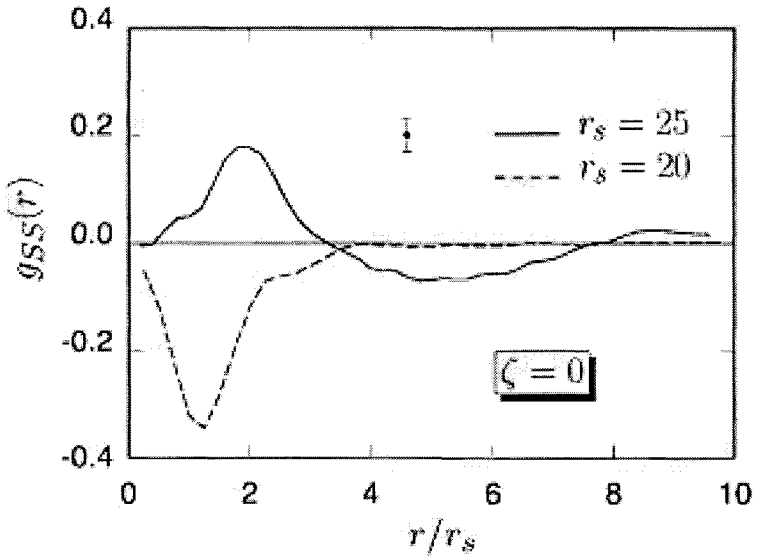


FIG. 3. Spin-spin correlation function (VMC) near the magnetic instability. A typical error bar is reported.

$$g_{ss}(r) = 2[g_{\uparrow\uparrow}(r) - g_{\uparrow\downarrow}(r)]$$

- Any relation to the experiment of Young et al (Nature 397 412, 1999) on $La_xCa_{1-x}Ba_6$?
- It is unlikely! Band structure and temperature effects cannot be neglected.
- Electrons (holes) in 2D … are a different story!

DMC predictions for the 2D e-gas (T = B = 0)

- Tanatar and Ceperley (1989)
  - There is no stability range for the ferromagnetic fluid
  - All three phases (crystal, paramagnetic, and ferromagnetic fluid) meet at r_s=37±5

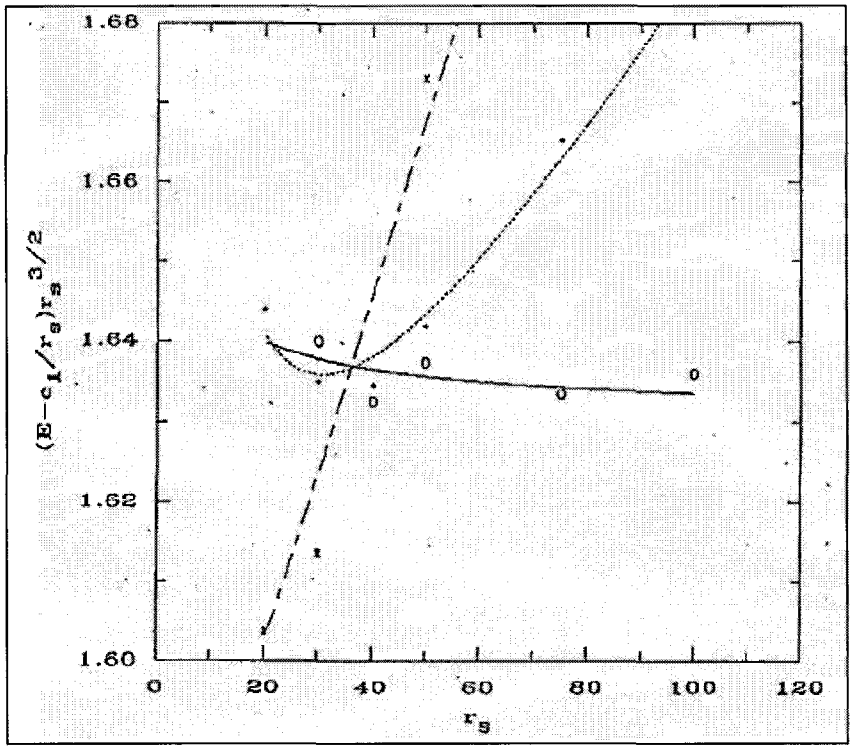
•Predictions not completely reproducible:

•Kwon, Ceperley, and Martin (PRB 48 12037, 1993)

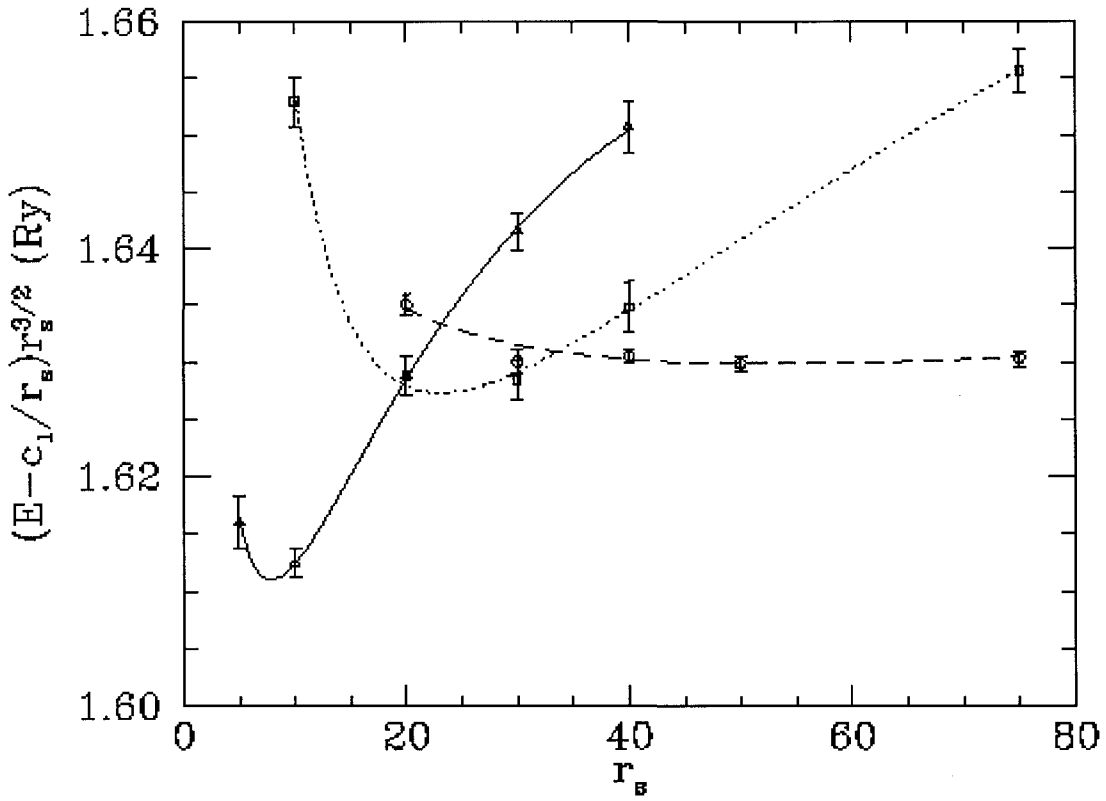
•Rapisarda and Senatore (Australian J. Phys. 13 12, 1996)

•In 2D

$$\pi(r_s a_B)^2 = \frac{N}{V}$$



- Rapisarda and Senatore (Australian J. Phys. 13 12, 1996)
  - Crystallization at $r_s=34\pm4$
  - Stability range for the ferromagnetic phase $20\pm2 \leq r_s \leq 34\pm4$



Diffusion Monte Carlo fixed-node

- Imaginary time (τ) evolution, starting from a Trial wavefunction Ψ_T, to filter out higher energy components and sample the ground state Φ_0
- In practice, one works with $\Psi_T \Phi(\tau)$ and samples $\Psi_T \Phi_0$
- For Fermions, to obtain a stable algorithm one has to assume the nodes of Ψ_T (fixed-node approximation)
- Time evolution is implemented using random walks. In actual calculations:
  - The walkers' population N_W is large but finite
  - The number N of electrons can be large, but finite
  - The time step $\Delta\tau$ is small but finite
- In principle one should extrapolate in N_W, N, and $\Delta\tau$

- In practice, to date, fixed values of N_W and $\Delta\tau$ have been used and the N extrapolation has been borrowed from VMC simulations
- For the first time we systematically extrapolate in N_W and $\Delta\tau$, at each value of N
- We perform the N extrapolation directly on DMC simulations

- With Slater-Jastrow nodes we have studied
  - The dependence of the energy on ζ, at $r_s = 20, 30$

- We have checked the effect of improving the nodes (including backflow effects) for the paramagnetic and ferromagnetic fluids, again at $r_s = 20, 30$

Trial wavefunction and nodes

- The trial wavefunction:

$$\Psi_T(R) = D^{\uparrow} D^{\downarrow} \prod_{i<j} \exp[-u_{\sigma_i,\sigma_j}(x_{ij})]$$

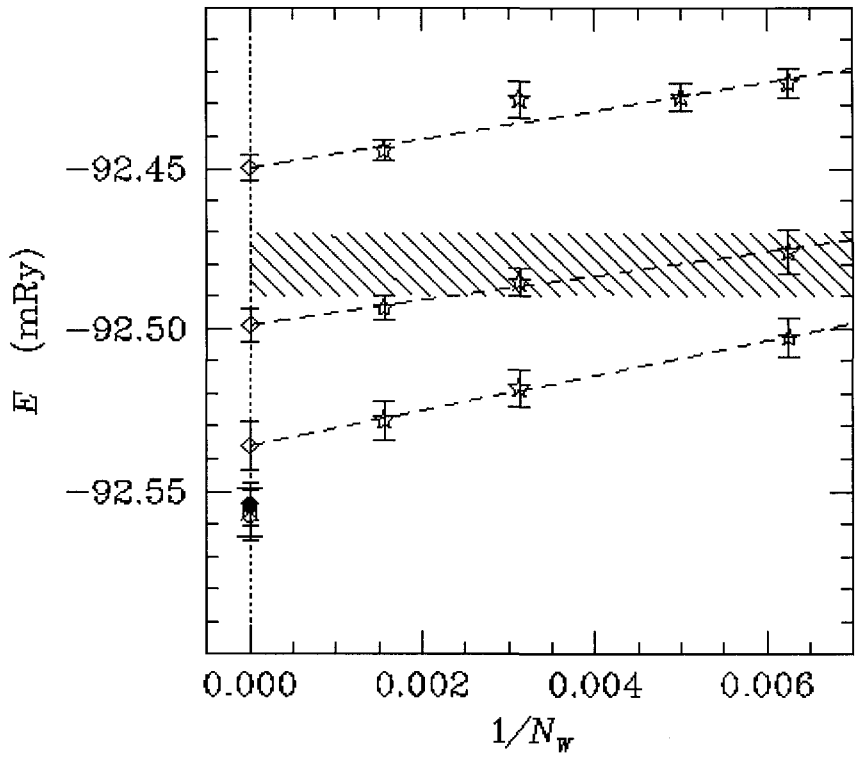
- D^s is a Slater determinant of one-particle orbitals ϕ_i; u(r) are pseudopotentials.
- Slater-Jastrow nodes: $\phi_\alpha(r_j)=\exp(ik_\alpha r_j)$
- Backflow nodes: $\phi_\alpha(s_j)=\exp(ik_\alpha s_j)$, with

$$\vec{s}_i = \vec{r}_i + \sum_{j\neq i}^{N} \eta(r_{ij})(\vec{r}_i - \vec{r}_j)$$

- Note: B=T=0.

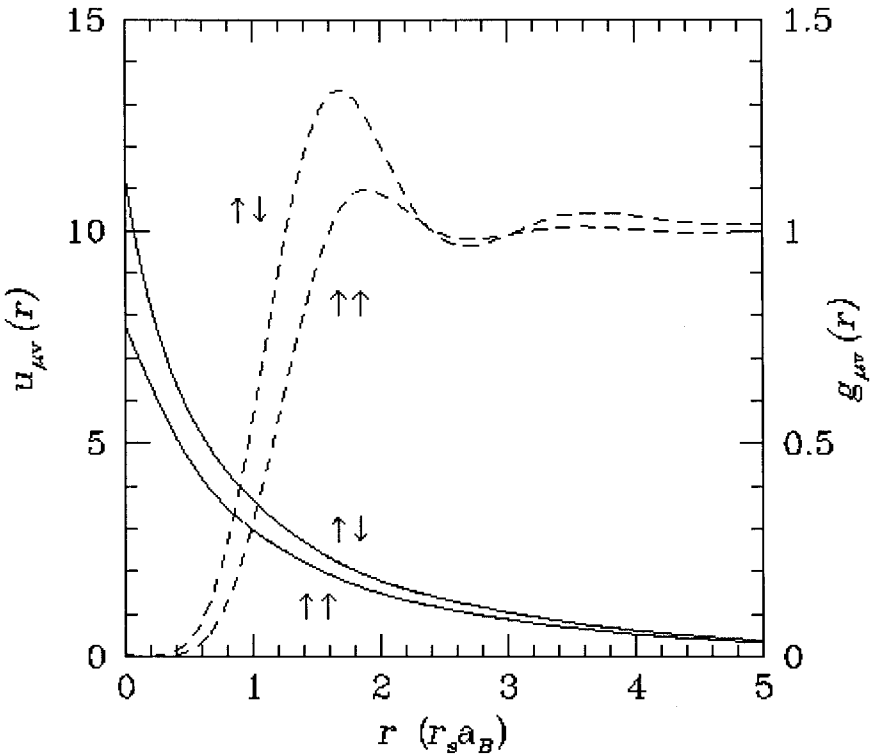
Extrapolation in N_W and $\Delta\tau$

- Results for 3 value of $\Delta\tau$
- $r_s = 20$, $N = 58$



Spin correlations (VMC)

- Like spin pseudopotentials are less repulsive than for unlike spins
- No magnetic instability is evident, however, at variance with 3D
- $r_s = 20$, $N = 58$



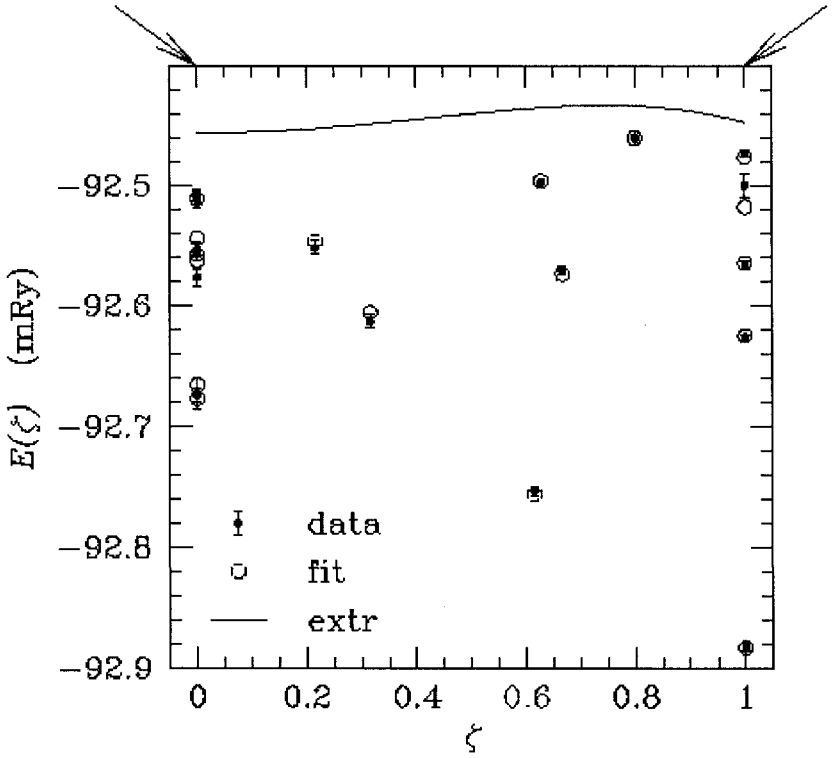
DMC energy at r_s=20

- The N-extrapolated energy is given by

$$E(\zeta) = E(\zeta=0) + \beta\,\zeta^2 + \gamma\,\zeta^4$$

- In units of 10^{-5}Ry,

$$\beta = 8.22 \text{ and } \gamma = -7.34$$



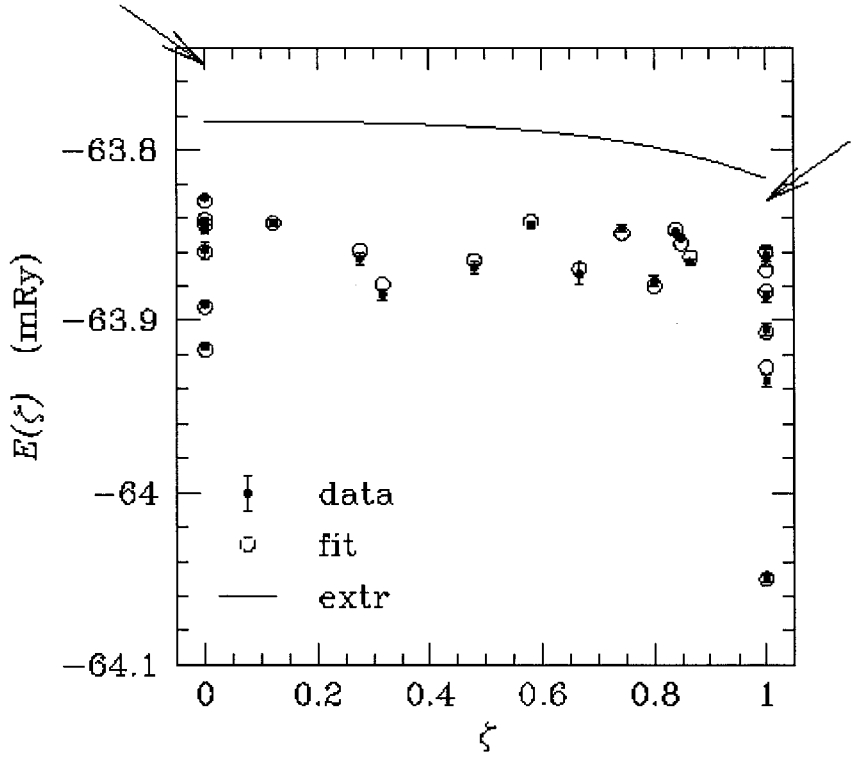
DMC energy at r_s=30

- Note that an absolute minimun at $0 < \zeta < 1$ requires

  $\beta < 0$, $\gamma > 0$, and $\gamma > -\beta/2$

- In units of 10^{-5}Ry

  $\beta = -0.64$ and $\gamma = -2.72$



Spin-polarizations transition

- The transition appears to be first order
- The new results have minor differences from those of i) Rapisarda and Senatore and ii) Kwon et al; they disagree from those of iii) Tanatar and Ceperley. Note that all 3 calculations are nominally equivalent.
- Thus, with Slater-Jastrow nodes, the ferromagnetic phase is confirmed stable for r_s between 20 and 30.
- At $r_s = 20$, the spin susceptibility is greatly enhanced. We estimate $\chi_s = 30\chi_{Pauli}$
- Could experiments measure the susceptibility enhancement of the 2D electron gas?

DMC calculations with backflow-nodes

- BackFlow nodes (BFN) are the most accurate ansatz for the electron gas to date
- In cases where it has been feasible to check it, the energy predictions of DMC simulations with BFN essentially coincide with exact transient estimates.

- We have performed calculations at $r_s = 20, 30$ for $\zeta = 0, 1$

- At $r_s = 20$, the paramagnetic phase is stabilized by backflow
- However at $r_s = 30$ the ferromagnetic phase remains stable
- An r_s stability window of the ferromagnetic phase should remain before the Wigner crystal sets in

Static spin response of the 2D e-gas at T=0

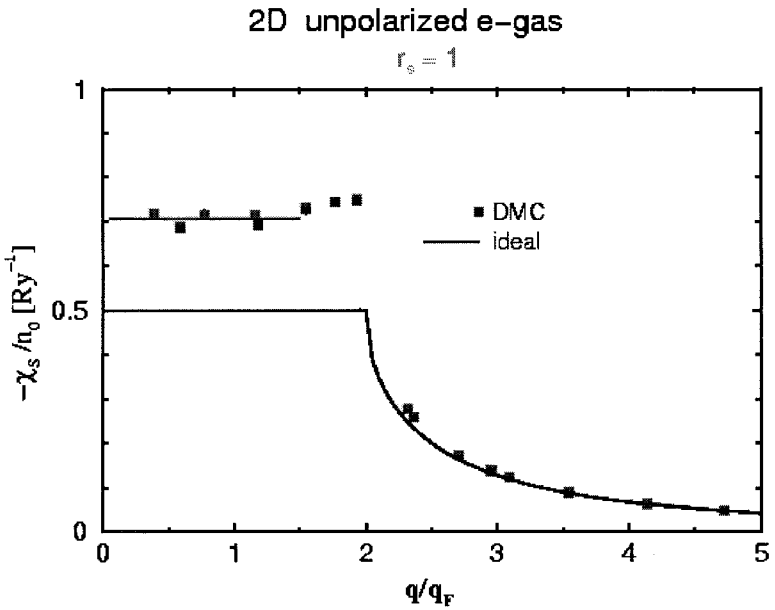
- Recently we have calculated, with DMC, the static spin response $\chi_s(q)$, at $r_s = 1, 2, 5, 10$

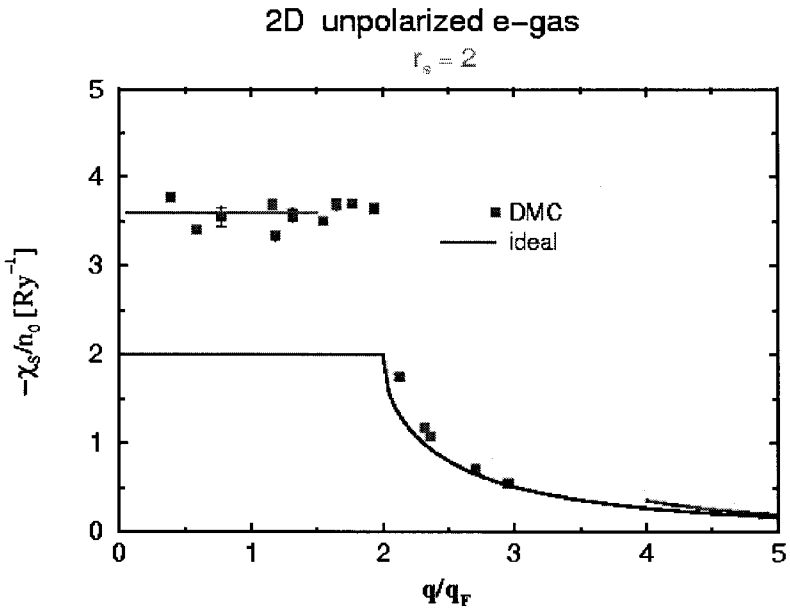
- Extrapolating our results at zero wavevector, we can estimate the enhancement of the spin susceptibility and combine these results with those of the energy calculations at $r_s = 20$

- The results for the spin response, combined with those for the charge response, which we have also calculated, allow one to construct effective electron-electron interactions *a la* Kukkonen-Overhouser

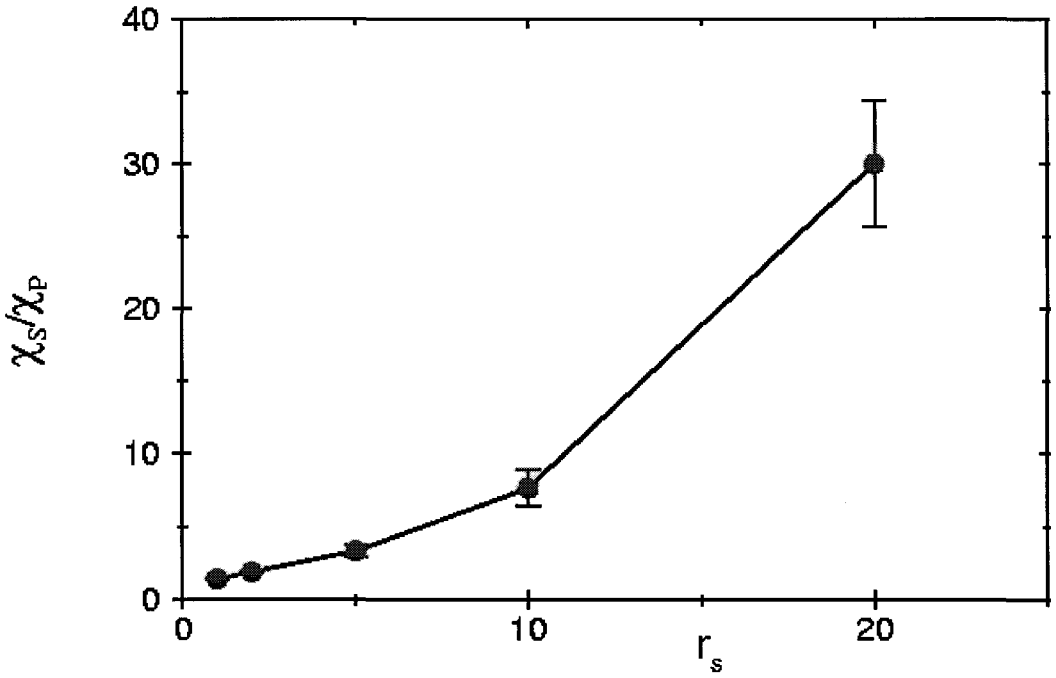
Spin response

- Full response compared with ideal response (the response of non interacting Fermions)





Spin susceptibility enhancement



Model quantum wire

- Quasi one dimensional motion [parabolic confinement].
- One dimensional [projected] pair potential:

$$\mathrm{v}(x) = e^2 \frac{\sqrt{\pi}}{2b} \exp[(x/2b)^2] Erfc[|x|/2b]$$

- Strictly 1D treatment: nodes are exactly known, results are exact!
- The trial wavefunction:

$$\Psi_T(R) = D^{\uparrow} D^{\downarrow} \prod_{i<j} \exp[-u_{\sigma_i,\sigma_j}(x_{ij})]$$

- D^s a Slater determinant of one-particle orbitals, and u(r) the RPA pseudopotential.
- Beware: B=T=0; $r_s = (L/N)/(2a_B)$

The energy

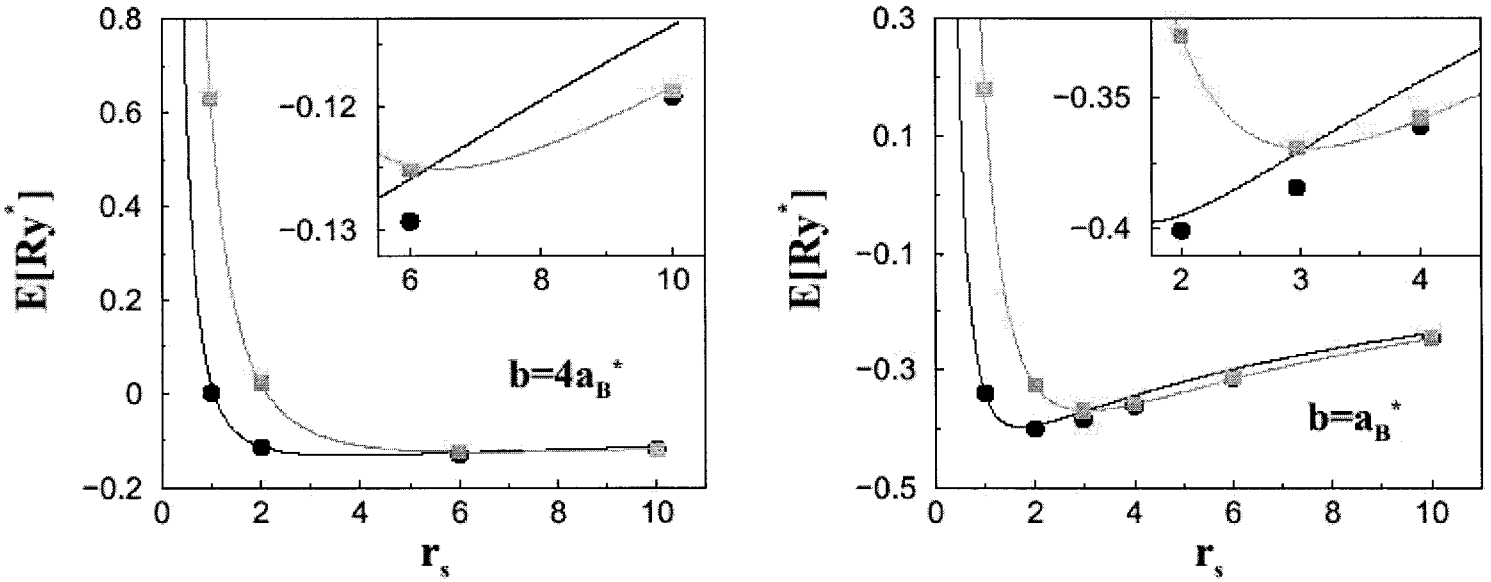


Figure 1: DMC ground state energy per particle, in $Ry^* = e^2/2\epsilon a_B^*$, of the paramagnetic (squares) and ferromagnetic (circles) fluids, in the thermodynamic limit $N = \infty$. The error bars are much smaller than the symbols. The predictions of STLS are given by the black and gray line, respectively for the paramagnetic and ferromagnetic phase. The insets show the Bloch instability yielded by the STLS scheme but not by our DMC simulations.

The structure

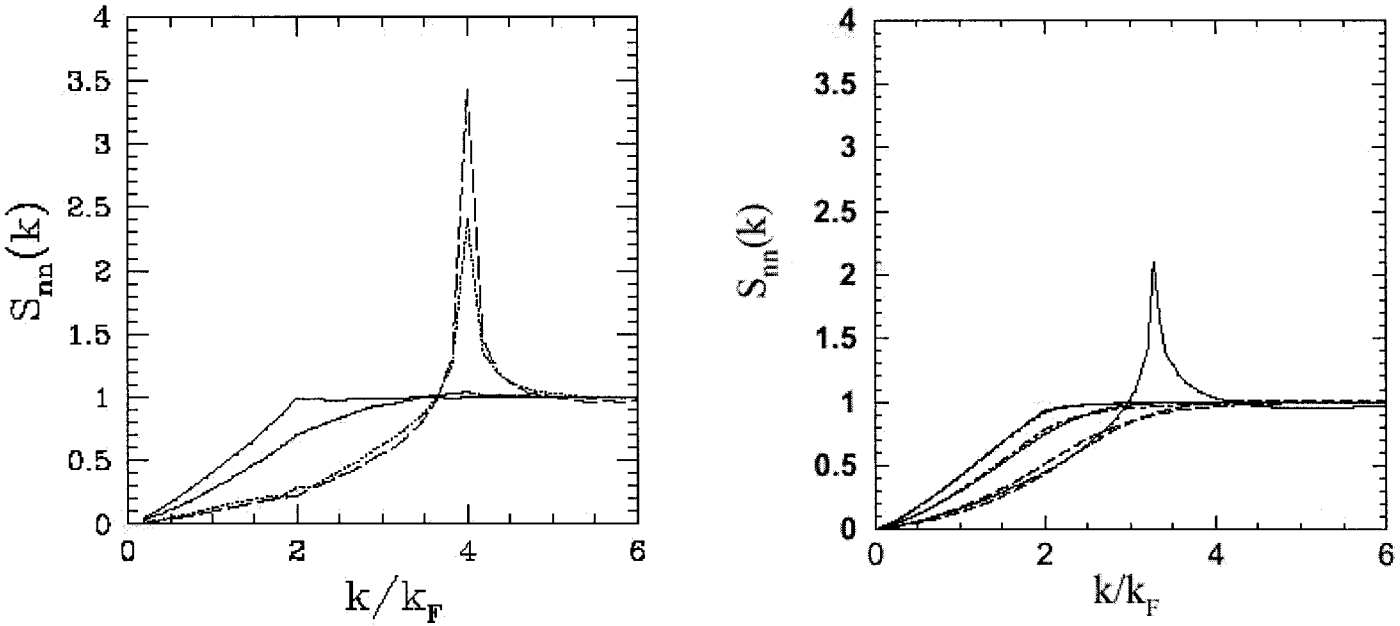


Figure 2: Static structure factor of the paramagnetic fluid. The left panel gives extrapolated DMC estimates for 22 particles and $b = a_B^*$, at $r_s = 1, 2, 6, 10$; the errors are not visible on this scale. The right panel gives the predictions of STLS (dashed curves) and DSTLS (full curves). In all cases a decreasing slope at the origin corresponds to increasing r_s. Also, for the DSTLS only results for r_s up to 6 are shown.

Luttinger liquid predictions

- Similar potential:

$$v(x) = e^2 / \sqrt{x^2 + d^2}$$

- Linear dispersion of the kinetic energy and Bosonization technique
- Asymptotic correlations:

$$g_{nn}(x) \approx A_1 \frac{\cos(2k_F x)}{x} e^{-c_2\sqrt{\ln|x|}} + A_2 \cos(4k_F x) e^{-4c_2\sqrt{\ln|x|}}$$

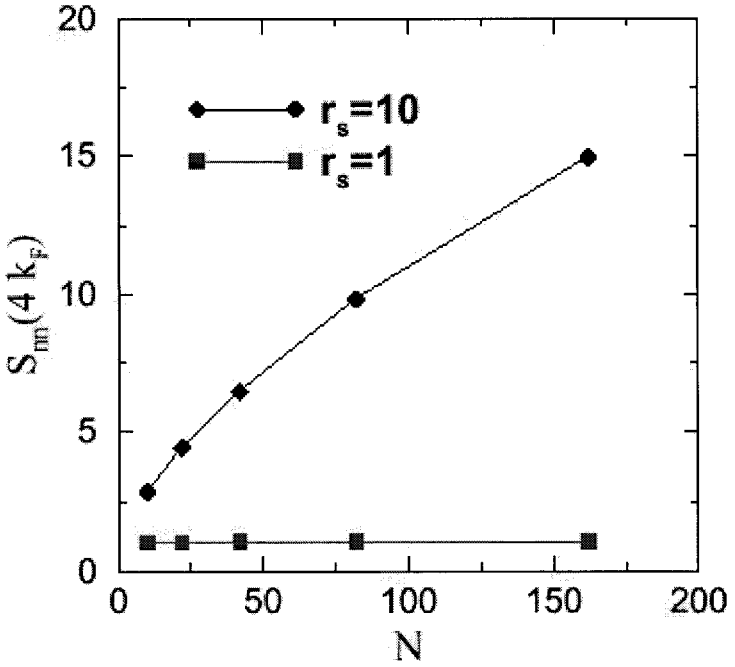
$$g_{mm}(x) \approx B_1 \frac{\cos(2k_F x)}{x} e^{-c_2\sqrt{\ln|x|}}$$

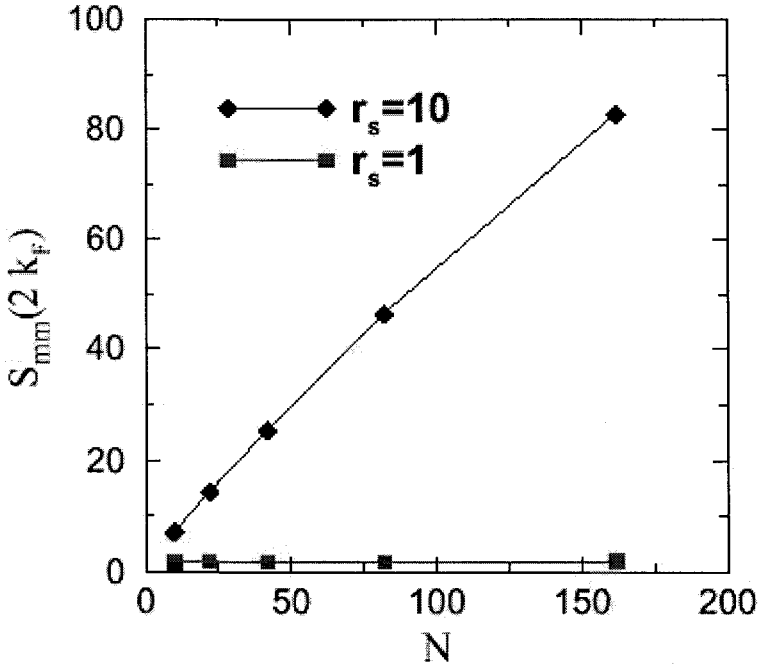
- A_1, A_2, B_1 are interaction (r_s) dependent
- In k space peaks at $2k_F$ and $4k_F$:

  $S_{nn}(4k_F)=\infty$ but $S_{nn}(2k_F)<\infty$ and $S_{mm}(2k_F)<\infty$

Peaks height

- DMC N dependence





- Wire width: $b=0.1a_B$

Conclusions: 2D e-gas

- We have performed DMC calculations of unprecedented accuracy for the 2D e-gas
- We have determined the ζ dependence of the ground state energy of the 2D e-gas at $r_s = 20, 30$
- We find that the polarization transition is first order, from the paramagnetic to the ferromagnetic fluid
- At the transition the magnetic susceptibility is greatly enhanced (by a factor 30!): this could be checked experimentally
- Using our previous results for the spin and charge response we have calculated effective inter-electronic interactions in the range $1 \leq r_s \leq 10$
- We have not considered spin or charge density waves

Conclusions: quantum wire

- DMC energies yield no surprises: the Lieb-Mattis theorem is of course satisfied and there is no Bloch instability, in contrast with results from approximate treatments.
- Pair correlation may become extremely strong, though no crystallization takes place.
- The N behaviour of the peaks in the structure factors are at variance with the predictions of Luttinger Liquid theory: more investigations both with DMC and with the bosonization technique are called for.