Quantum Monte Carlo methods as an exact route to correlated regimes in 1D systems.

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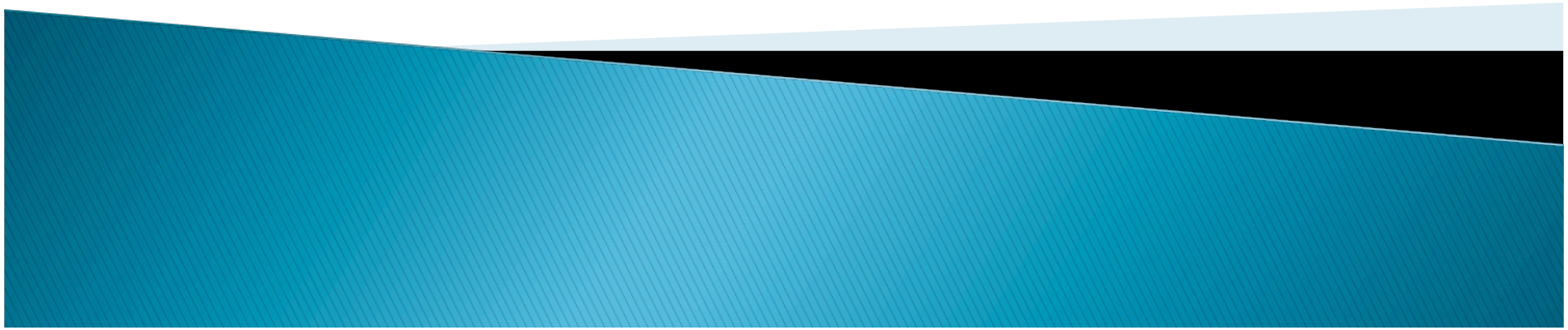


Why exact? No sign problem!

- Diffusion Monte Carlo (DMC) (Reynolds *et al.,* JCP **77**, 5593 (1982)) and Lattice Regularized Diffusion Monte Carlo (LRDMC) (Casula *et al.,* PRL **95**, 100201(2005))
- Wave function projection using imaginary time propagator

$$\left|\psi(\tau+\delta\tau)\right\rangle = e^{-\hat{H}\delta\tau}\left|\psi(\tau)\right\rangle = \sum_{i=0}^{\infty} c_i e^{-\varepsilon_i \delta\tau}\left|\phi_i\right\rangle$$

- Initial state (trial wave function) product of a determinant of plane waves and a 2-body Jastrow factor

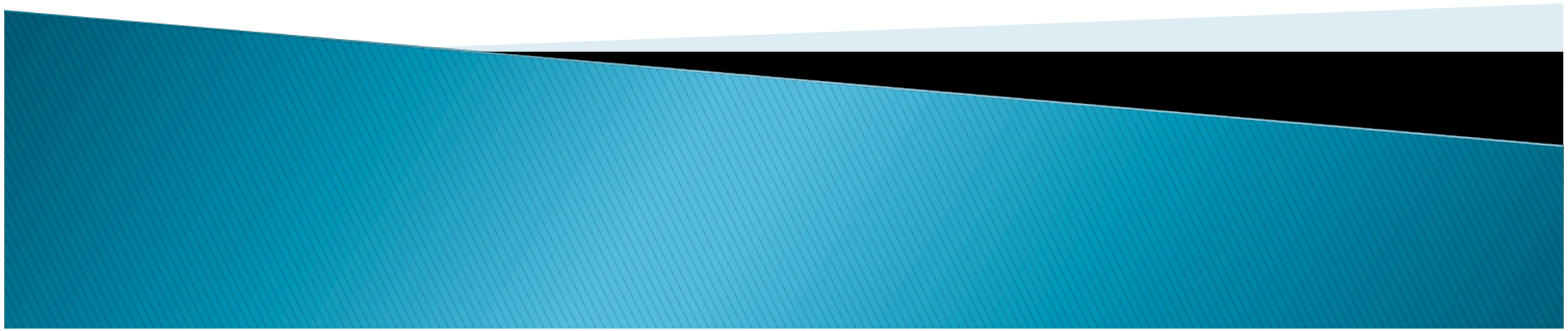
$$\left|\Psi_T\right\rangle = D^{\uparrow}D^{\downarrow}\exp(-\sum_{i<j} u(x_{ij})) \qquad D^{\sigma} = \prod_{1\le i<j\le N^{\sigma}} \sin(G(x_i^{\sigma} - x_j^{\sigma})/2)$$

- Fermion sign problem: constrain the diffusion within the nodal pockets of the trial wave function
  - In 1D the nodes are known exactly and given by $x_i^{\sigma} = x_j^{\sigma}$
  - **Ground state properties can be computed without bias in 1D** (the only error comes from statistical fluctuations of the sampling)

Outline

- **Properties of the 1D homogeneous electron gas (1DEG)**
  - *Onset of long-range charge order* in the 1DEG: localization transition in experiments and liquid-to-quasi-crystal crossover
  - *Effect of screening* on the onset of crystal-like correlations
  - *Spin and charge velocities* in quantum wires
- **Properties of a trapped Gaudin gas**
  - Experimental realization of the model
  - Phase diagram from Thomas-Fermi approximation
  - *Zero and finite temperature* results from QMC

Ground state and thermodynamic properties of the 1DEG



Long-range charge order in 1D

- Condition for the presence of charge order in 1D electron gas depending on the **long distance behavior of the interparticle potential**[1]: $V(r) \propto 1/r^n$
  - $n < 1 \rightarrow$ crystallization is possible
  - $n = 1 \rightarrow$? (border line difficult case)
  - $n > 1 \rightarrow$ no long-range order
- $n = 1$

  Luttinger liquids with long range 1/r interactions have **quasi** long-range correlations[2]

$$\langle \rho(x)\rho(0)\rangle = A_1 \cos(2k_F x)\exp(-c_2\sqrt{\ln x})/x + A_2 \cos(4k_F x)\exp(-4c_2\sqrt{\ln x}) + \cdots$$

$$S(k = 4k_F) = \int_a^L dx \exp(-4ik_F x)\langle \rho(x)\rho(0)\rangle = aL\exp\left(-4c\sqrt{\ln L}\right) + b$$

$4k_F$ periodicity of mean interparticle distance in case of unpolarized Fermi system

[1]Mermin, PR **176**, 250 (1968)
[2]Schulz, PRL **71**, 1864 (1993)

Long-range charge order in 1D

- The **strength of the effective interaction** is set by r_s
  (Wigner-Seitz radius: $2\, r_s a_0$ mean interparticle distance)
  r_s= potential energy / kinetic energy
  What is the role of the density in the stabilization of the quasi Wigner order? (in the Luttinger picture is left undetermined)

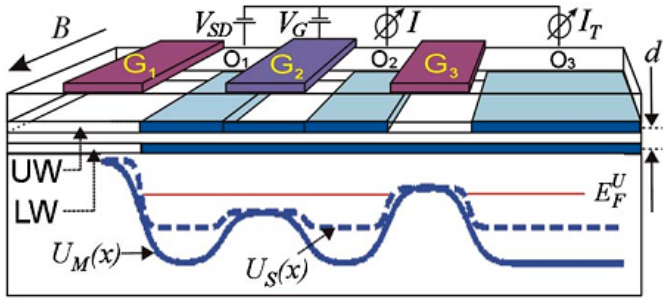
- Are the **$4k_F$ correlations** always present as soon as the interaction is switched on? Is there any crossover density?

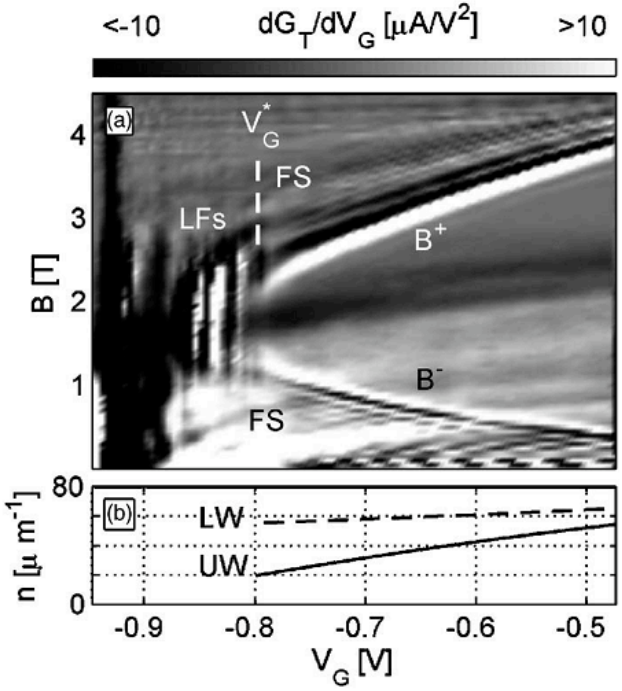
- In 1D **strong quantum fluctuations**
  What is the role of quantum fluctuations in the stabilization of the long-range order and what is the interplay with the range of the interaction?

Localization Transition in Experiments

- Parallel quantum wires with tunable density in upper wire realized with cleaved edge overgrowth of GaAs
- Electrons localize at low density **(below 20 μm^{-1})** tunneling changes character
- Extended tunneling in momentum space implies localization in real space; at the same density the conductance in the wire drops down
- Questions to be resolved: Is the observed effect due to disorder or intrinsic correlations? What is the role of screening?

Auslaender *et al.* Science **295**, 825 (2002)
Auslaender *et al.* Science **308**, 88 (2005)
Steinberg *et al.* PRB **73**, 113307 (2006)

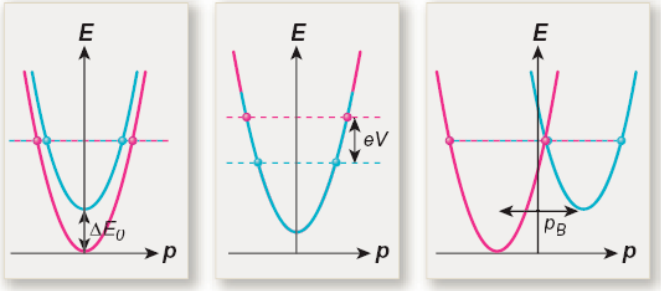


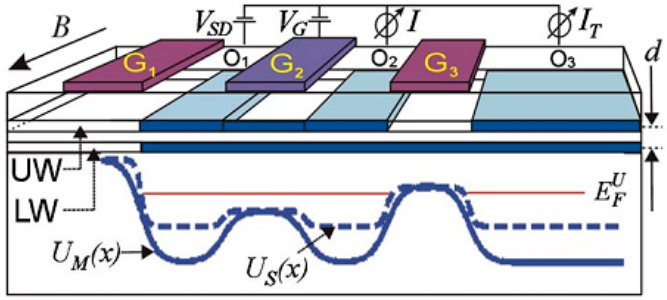


Spin-charge separation

Tunneling when Fermi point from one wire coincides with unoccupied states in the other

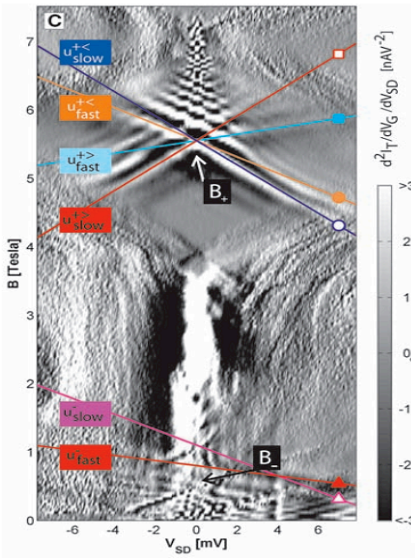
Zulicke, Science **295**, 810 (2002)

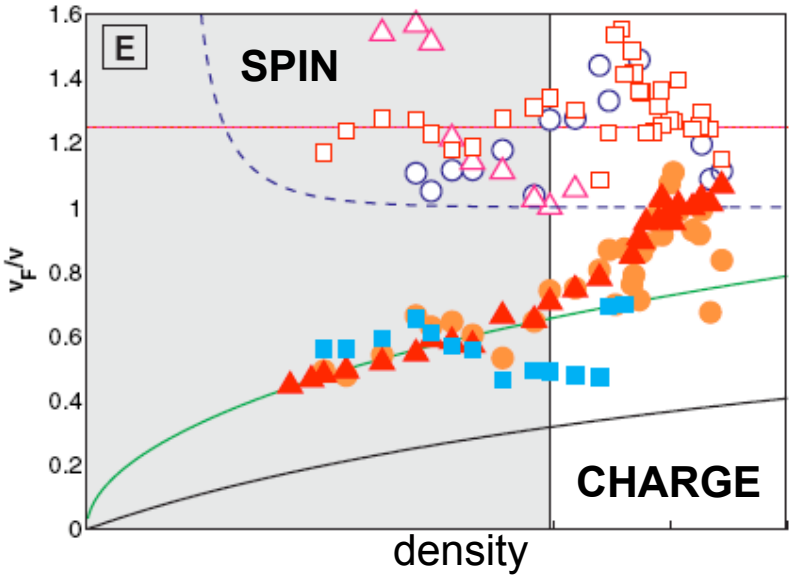




Strong renormalization of charge and spin velocities due to the interaction (for spin it is larger then expected)

Auslaender *et al.*, Science **308**, 88 (2005)





$$v_\sigma = \frac{\pi}{2} r_s J$$

from Heisenberg spin chain

$$\frac{v_F}{v_\rho} = \frac{1}{\sqrt{c + \frac{V(k \to 0)}{\pi k_F}}}$$

from RPA

Our model for the 1D homogeneous electron gas

- Strictly 1D electrons in a **neutralizing homogeneous background**

$$\hat{H} = -\sum_i \frac{\nabla_i^2}{2m} + \frac{1}{2}\frac{e^2}{\varepsilon}\sum_{i\neq j} V(x_i - x_j) + \hat{H}_{e-b}$$

- Effective 1D interparticle potential derived by assuming **harmonic confinement in the transverse direction**

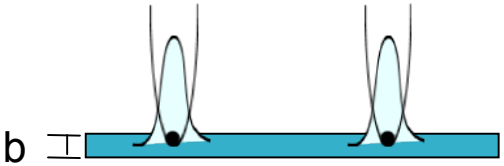
$$V_{\text{transverse}}(r_\perp) = \frac{r_\perp^2}{4b^4}$$

b is the thickness of the wire

and **single subband approximation** (only the lowest subband is occupied)

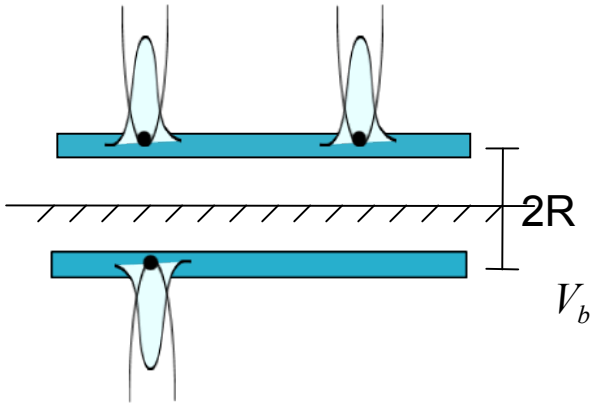
Model interactions

Unscreened

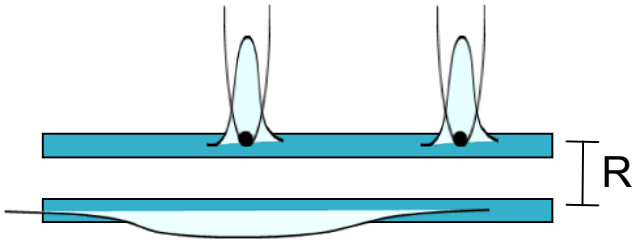


$$V(x) = \frac{\sqrt{\pi}}{b} e^{\frac{x^2}{4b^4}} erfc\left(\frac{|x|}{2b}\right)$$

Gate screening

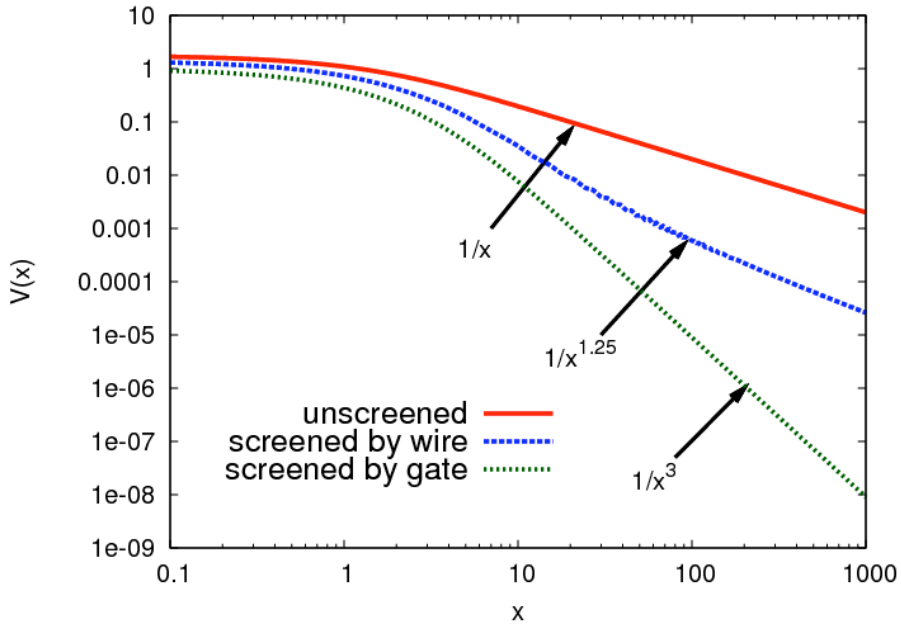


Wire screening



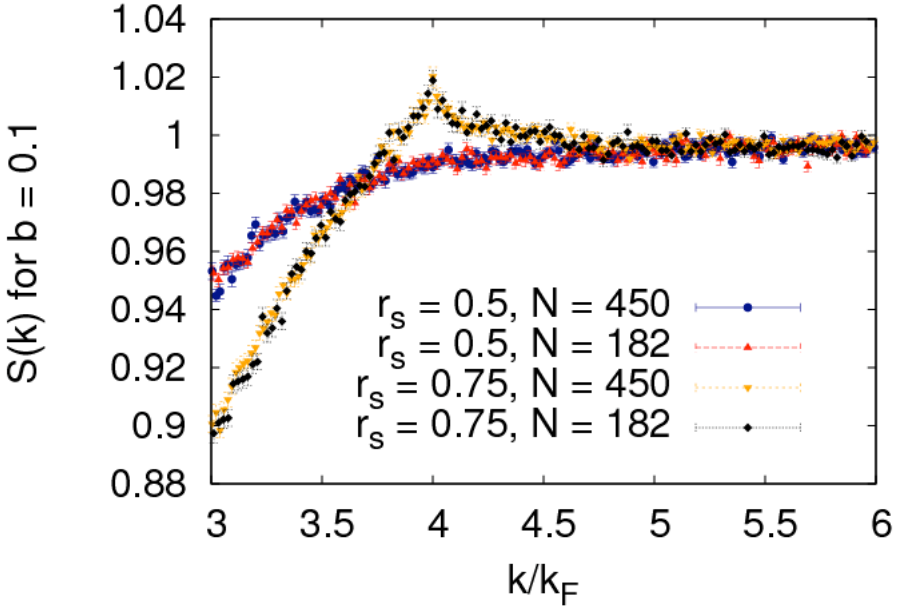
$$V_b(k,R) = V_b(k) + V_{\text{int}}(k,R)\chi(k)V_{\text{int}}(k,R)$$

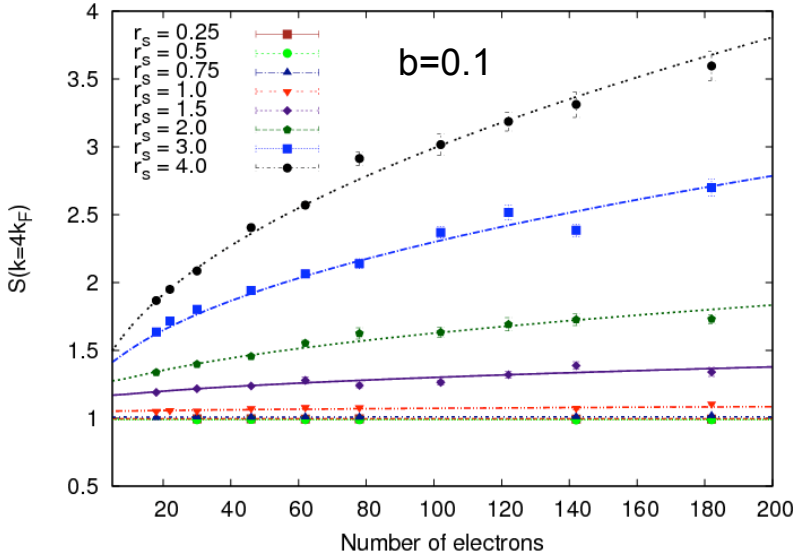
Linear response theory for the second wire



Quasi Wigner crystal

$4k_F$ peak of structure factor for V(x) ∝ 1/x





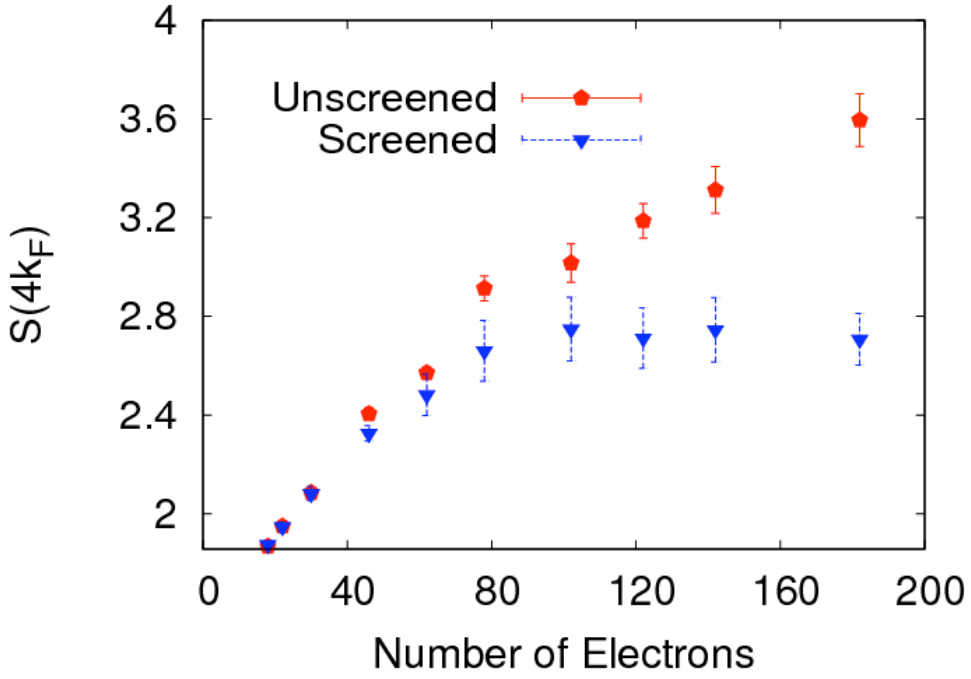
- **Sub-linear scaling** of $4k_F$ component of S(k) with particle number indicates presence of quasi Wigner crystal.
- Agrees with Luttinger liquid theory predictions in the Wigner phase:

$$S(k = 4k_F) = aL\exp\left(-4c\sqrt{\log L}\right) + b$$

- There is a **crossover density** $r_s^* = r_s^*(b)$ above which the system has only $2k_F$ correlations (no $4k_F$ peak)

Screening effects

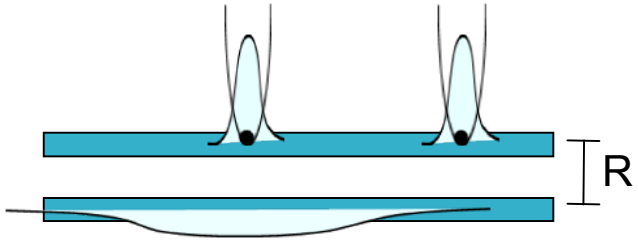
- Gate screening ($V(x) \propto 1/x^3$) destroys the quasi-order
- Quasi long-range order replaced by strong $4k_F$ correlations



b=0.1, r_s=4

Wire screening

- Electrons are confined to the wires by harmonic potentials as before
- Correlations are treated explicitly in one of the wires with the other wire treated as a screening medium
- Response of second wire is calculated using linear response with an RPA density-density response function
- GaAs parameters:
  $m^* = 0.067\ m_e$
  $\varepsilon = 13.1$
  $a_0 \sim 10$ nm
  $b = 0.707$
  $b' = 1.061$
  (radial root mean square equal to the lithographic thickness)

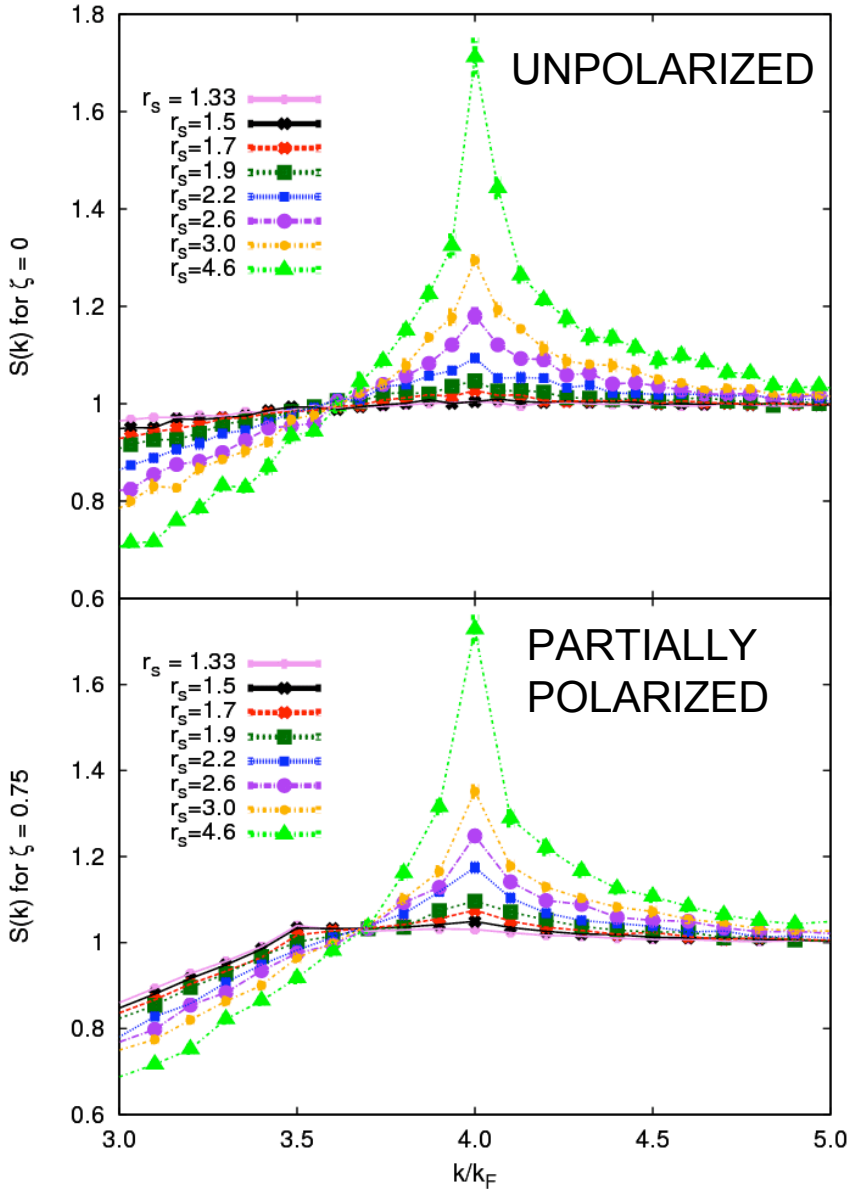


$$V_b(k,R) = V_b(k) + V_{\text{int}}(k,R)\chi(k)V_{\text{int}}(k,R)$$

$$\chi_{RPA} = \frac{\chi_0(k)}{1 - V_{b'}(k)\chi_0(k)}$$

$$\chi_0(k) = \frac{1}{\pi k}\ln\left|\frac{k-2k_F}{k+2k_F}\right|$$

Crossover with wire screening



- Unpolarized wire with screening coming from another parallel wire

- Crossover region is r_s= 1.9-2.2 in the unpolarized wire

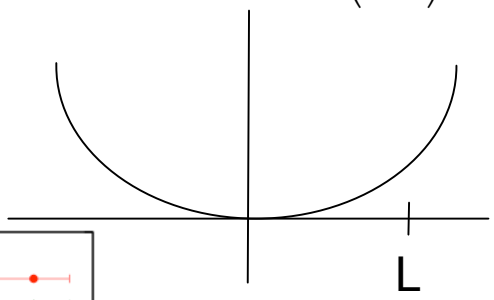
- **In the experiment the wire is in a quite strong magnetic field, which might induce a polarization**. We study the effect of the spin polarization in the crossover

- Crossover region is the same in the wire with polarization 0.75

- **$2k_F$-to-$4k_F$ crossover density is insensitive to the polarization in this regime**

Localization in finite wire

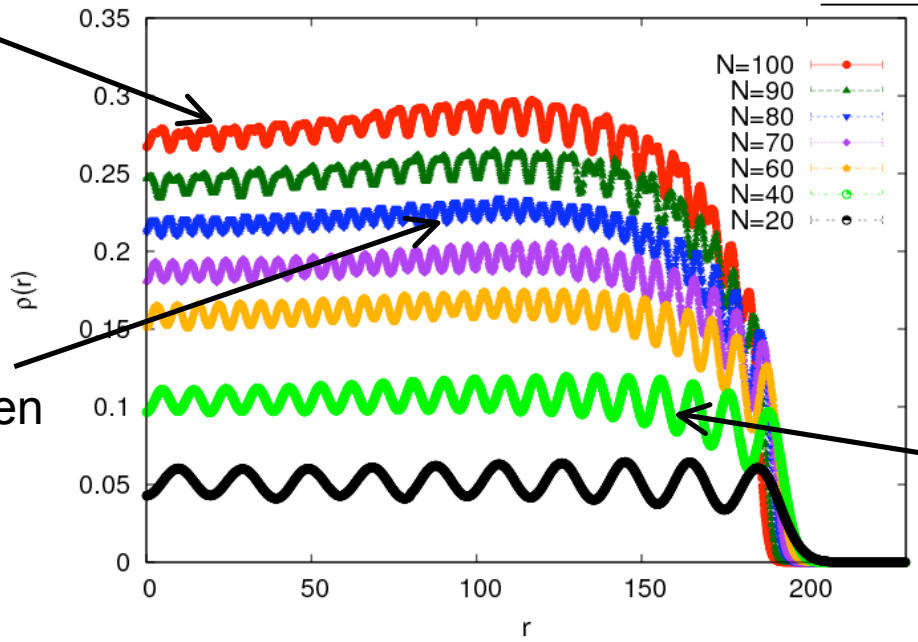
- Finite length wire realized with a soft longitudinal confinement $W(x) = E_F \left(\frac{2x}{L}\right)^8$
- Interactions are screened by the second wire
- Vary the number of electrons in the “trap”



Fiete et al.
PRB **72**, 045315 (2005)
Tserkovnyak et al.
PRB **68**, 125312 (2003)

Two electrons per peak

Density profile



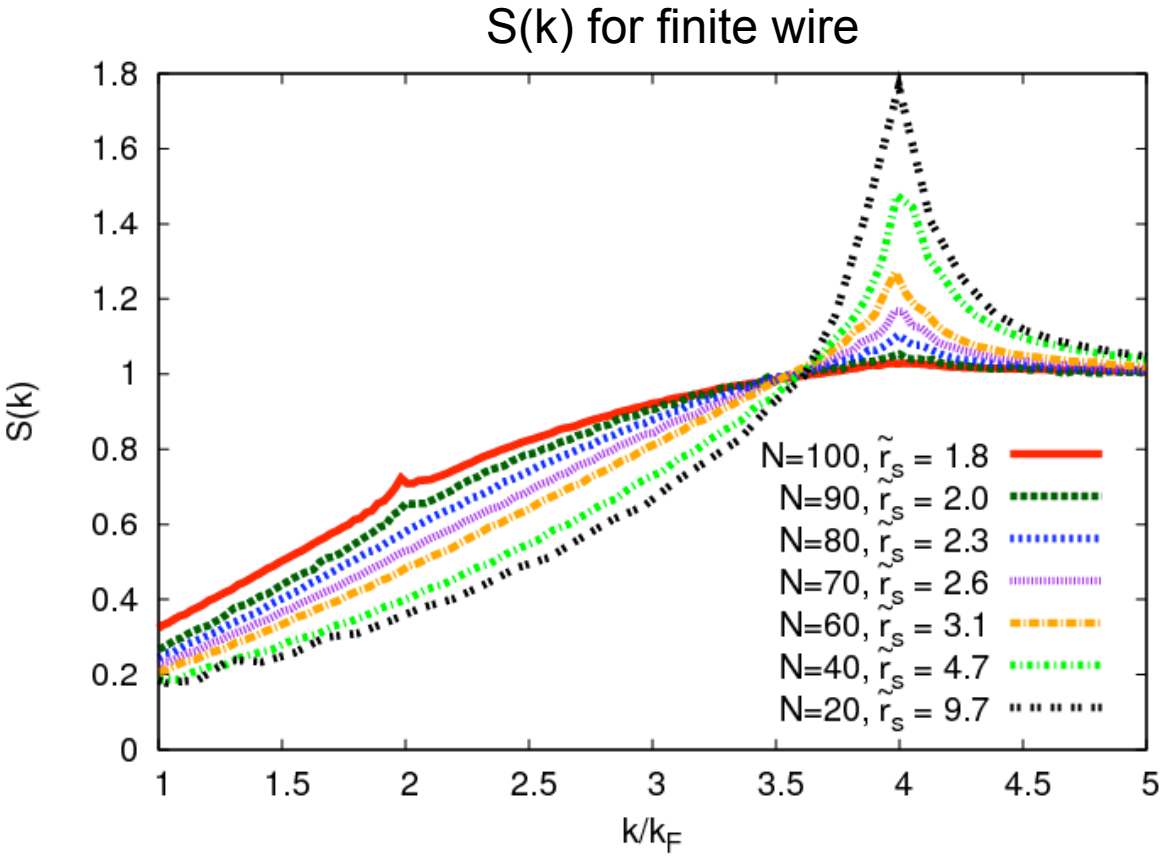
Peaks broaden

One electron per peak

- **Number of peaks per electron doubles as average density decreases (onset of $4k_F$ correlations and broken translational invariance joint together)**

Localization in finite wire

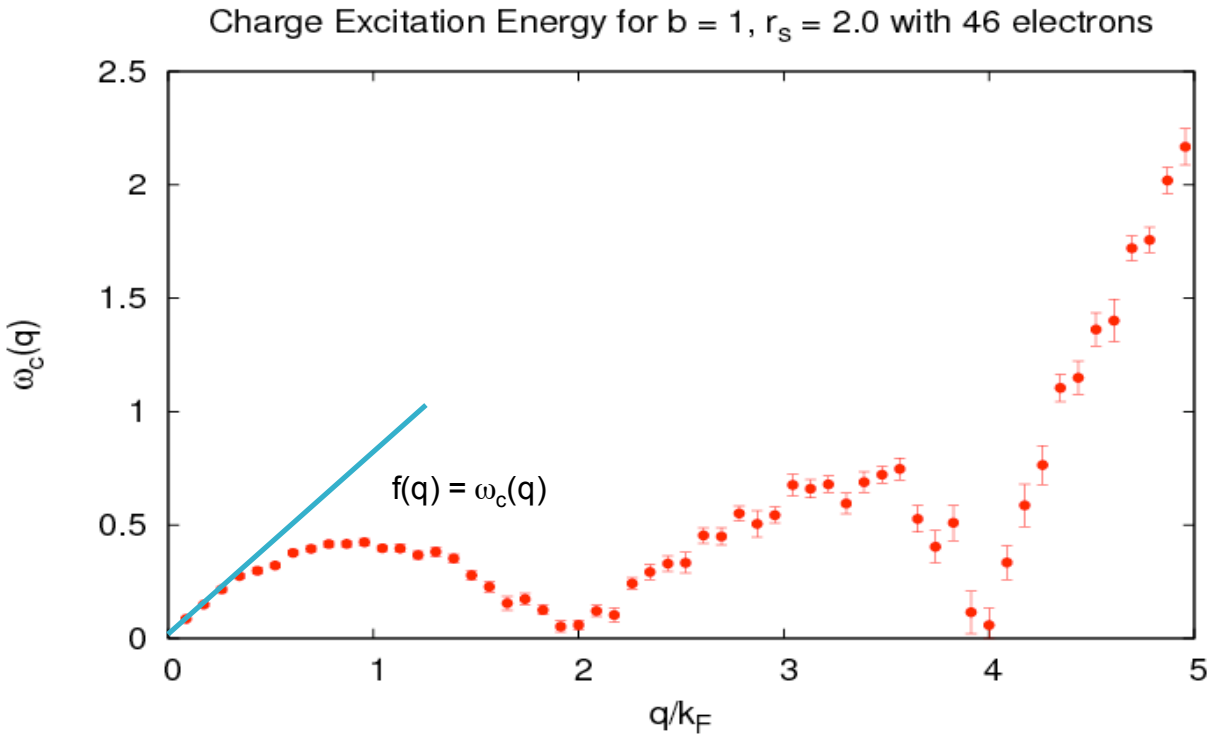
- Appearance of feature at $4k_F$ at same density as density profile changes
- Transition occurs between r_s = 2.0 and r_s= 2.3 giving a transition density of 22 μm^{-1}
- Remarkable agreement with experimental transition at 20 μm^{-1}
- The soft confinement does not change much the critical density for the crossover.



Correlations play a strong role in the localization transition

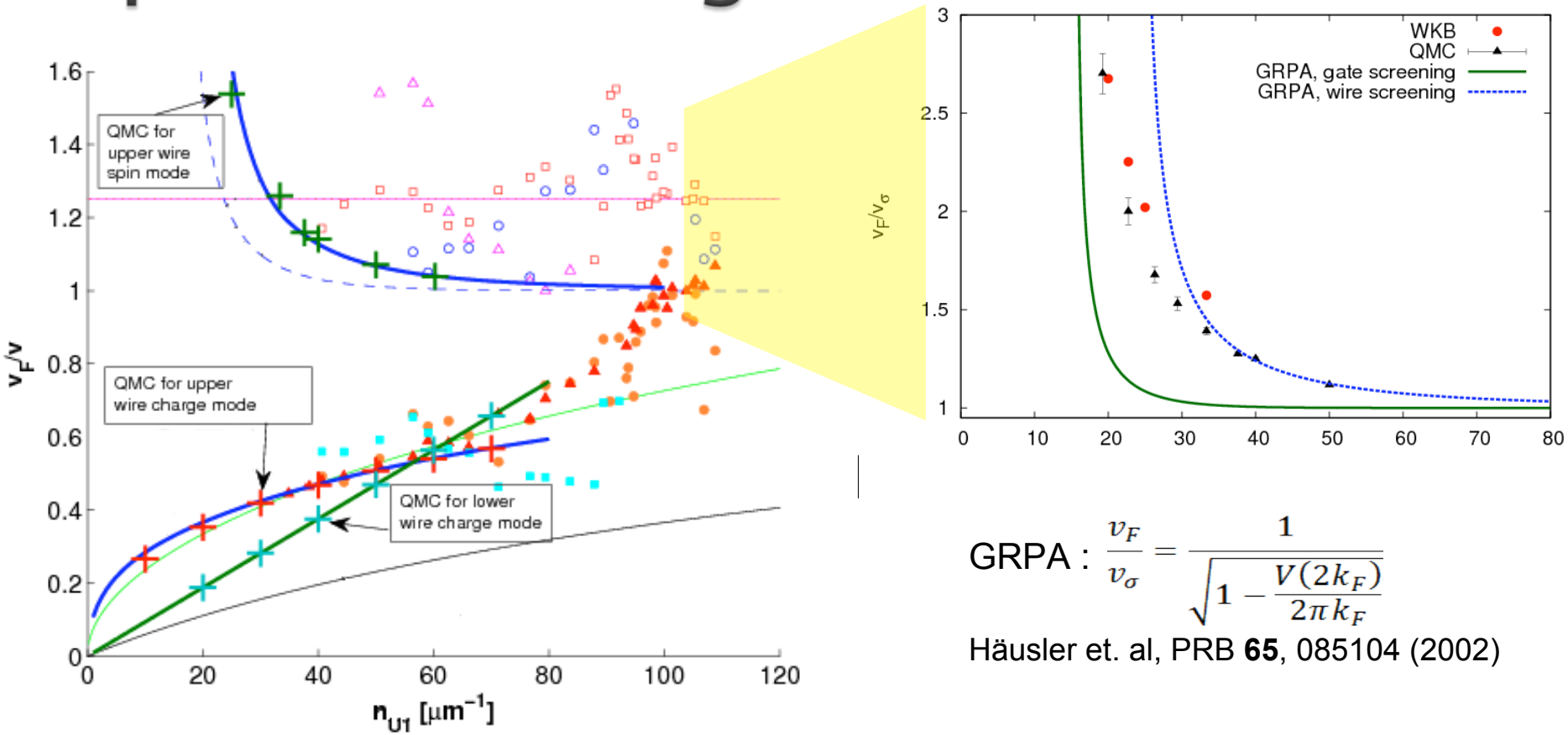
Momentum resolved excitation energies

- Trial wave function $\Psi_T(q) = \sum_j e^{iqr_j}\Psi_0$ best for small k (Feynman's ansatz)
- Slope of excitation spectrum at small q gives charge and spin velocities
- Excitation energy is gapless at $2nk_F$ due to continuous translational invariance



Reference for the method: D. M. Ceperley and B. Bernu, JCP **89**, 6316 (1988)

Spin and Charge Velocities



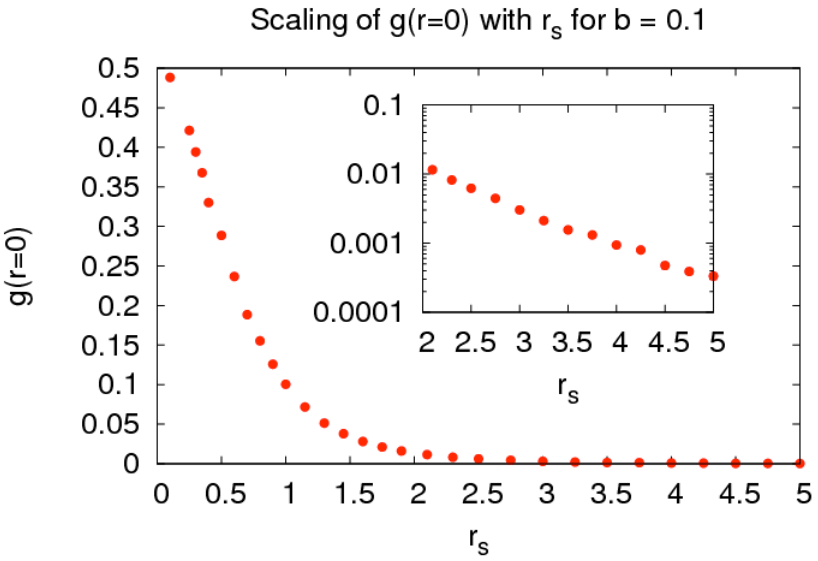
GRPA : $\frac{v_F}{v_\sigma} = \frac{1}{\sqrt{1 - \frac{V(2k_F)}{2\pi k_F}}}$

Häusler et. al, PRB **65**, 085104 (2002)

- Points from Auslaender *et al.*, Science **308**, 88 (2005), dispersion of the system with two parallel quantum wires

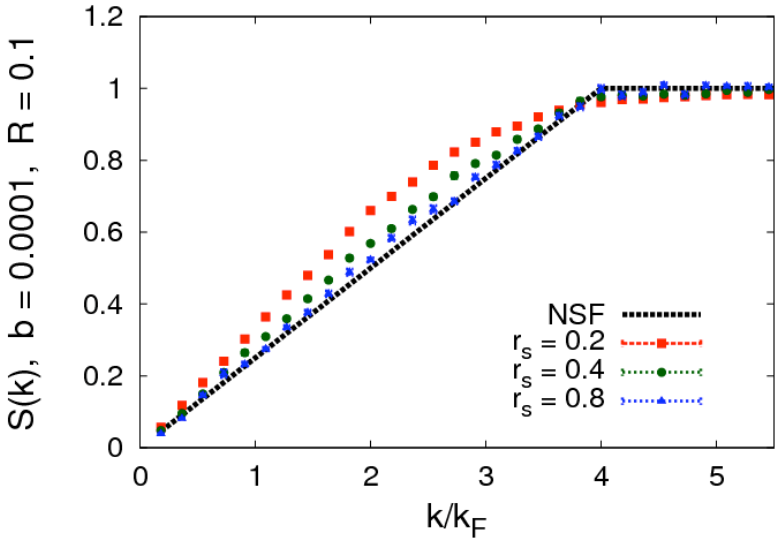
- Upper wire charge velocity in good agreement with the experimental data
- **Upper wire spin velocity strongly dependent on the screening** (spin sector very sensitive to the microscopic model)

Quasi Wigner Crystal to Impenetrable Particles Crossover



- Pair correlation function g(r) exponentially approaches 0 for r=0
- In low density limit g(r) becomes independent of spin → like spinless fermions

- For **screened interactions**, approach to noninteracting spinless fermion limit
- Structure factor goes to the non interacting spinless with $2k_f$-to-$4k_f$ mapping



Relation to Tonks-Girardeau

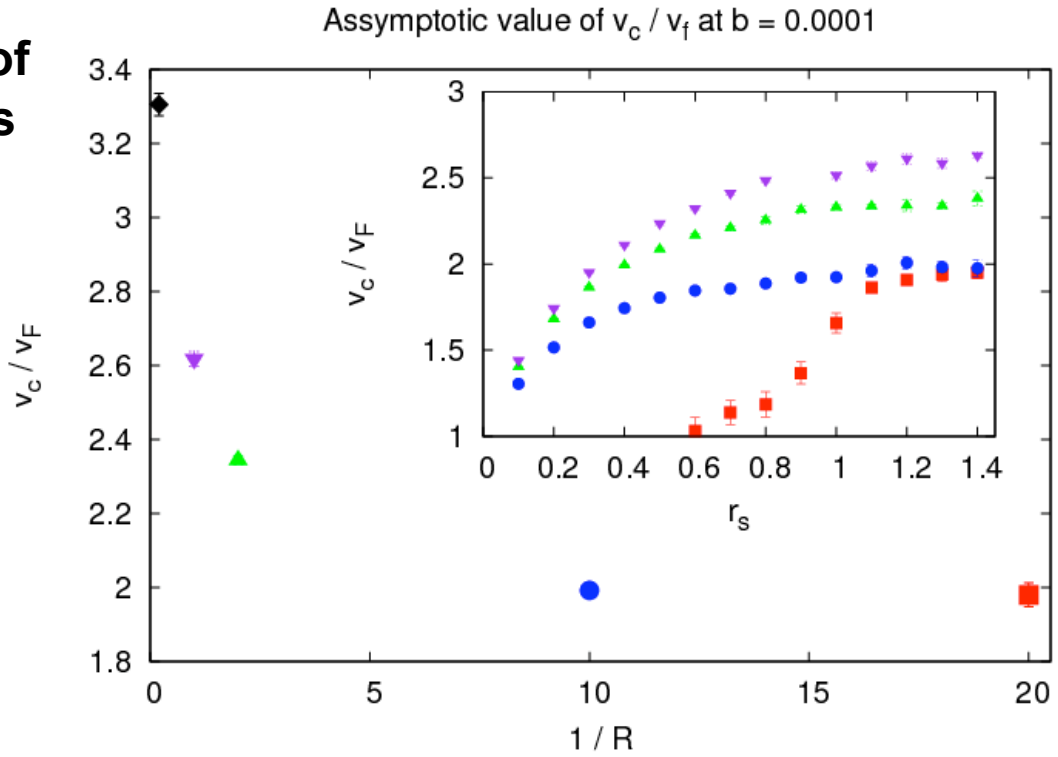
- Tonks and Girardeau physics of ***strongly interacting*** particles mapped into ***non interacting spinless fermions***
  - Contact interactions assumed
  - Particles become impenetrable
  - $v_c \rightarrow 2v_F$ (spinless non interacting physics)

As screening shortens range of interaction, electrons act as noninteracting spinless fermions

To get a Tonks-Girardeau behavior we need:

1. small thikness (small b)
2. strong coupling (large r_s)
3. large screening (small R)

$$b << 1 \qquad r_s >> 8R^2/\pi$$



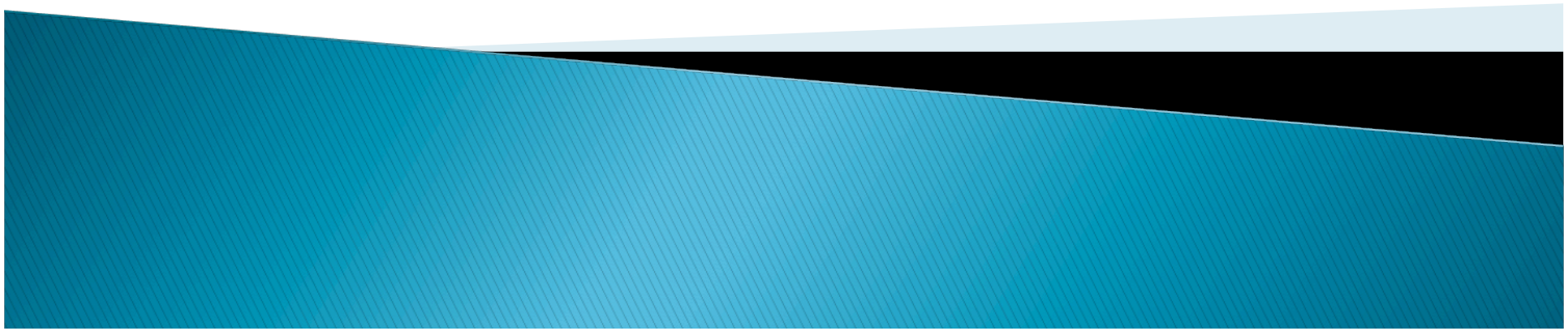
Summary

- Performed exact quantum Monte Carlo calculations of 1D electron gas
  - Onset of quasi Wigner crystal correlations as density decreases
  - Screening destroys long range correlations
- Developed model to study parallel wire experiments
  - Localization transition in quantitative agreement with experiment
  - Velocities of spin and charge excitations computed in QMC

Some reference:

M. Casula, S. Sorella, and G. Senatore, PRB **74**, 245427 (2006)
L. Shulenburger, M. Casula, G. Senatore, and R. M. Martin, PRB **78**, 165303 (2008)
L. Shulenburger, M. Casula, G. Senatore, and R. M. Martin, J. Phys. A: Math. Theor. **42**, Issue 21, 214021 (2009)
Güçlü, Umrigar, Jiang, Baranger, arXiv:0807.4292

Ground state and thermodynamic properties of a trapped Gaudin gas

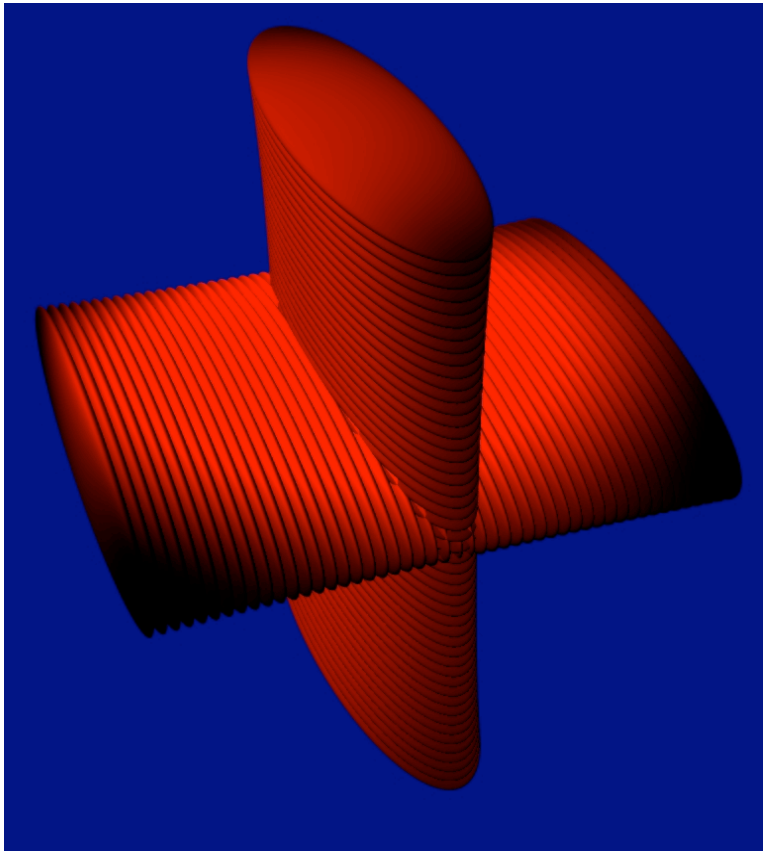


Realizing a 1D Fermi gas

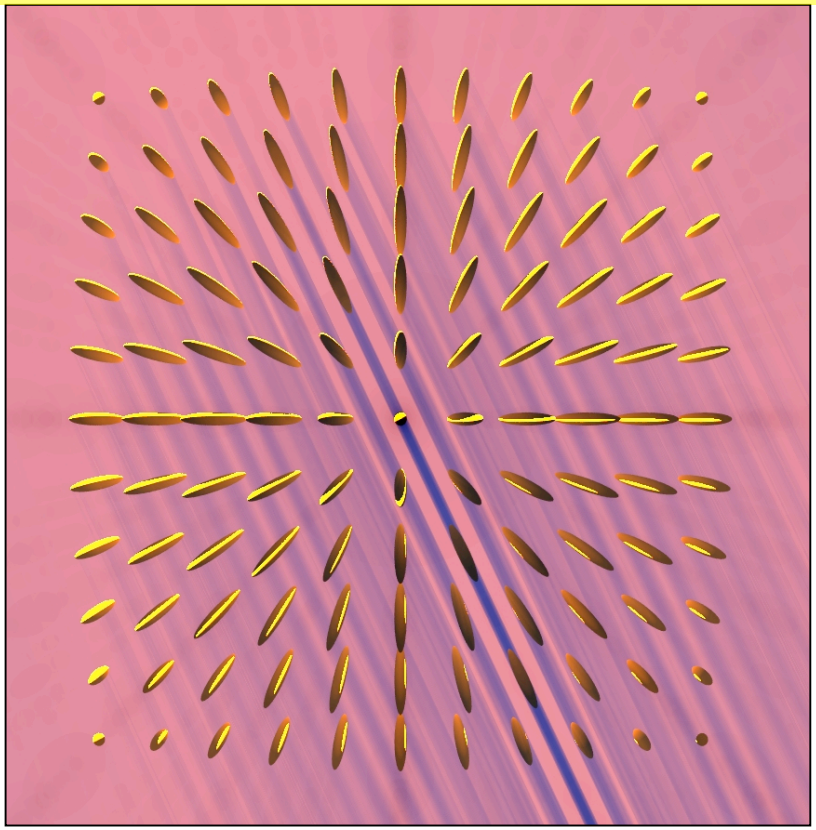
Going on experiment by Randy Hulet at Rice University

Ultracold ^{6}Li atoms trapped in an optical lattice created by orthogonal laser beams

Total number of atoms: 500,000



- Elliptically focused crossed beam trap (aspect ratio ~ 6:1)
- Produces an array of long narrow tubes (tube size ~ 0.5 μm x 300 μm)
- Central tubes contain ~300 atoms



1D Fermions with attractive contact interaction

For a **single tube**, with a single subband occupied (large transverse frequency), the Hamiltonian is

$$H = -\frac{\hbar^2}{2m}\sum_i \frac{\partial^2}{\partial x_i^2} - \sum_{(i,\uparrow)(j,\downarrow)} g\,\delta(x_i^{\uparrow} - x_j^{\downarrow}) + \sum_i \frac{1}{2} m\omega^2 x_i^2$$

We use units $\hbar = m = \omega = 1$

The pair binding energy is $\frac{g^2}{4}$

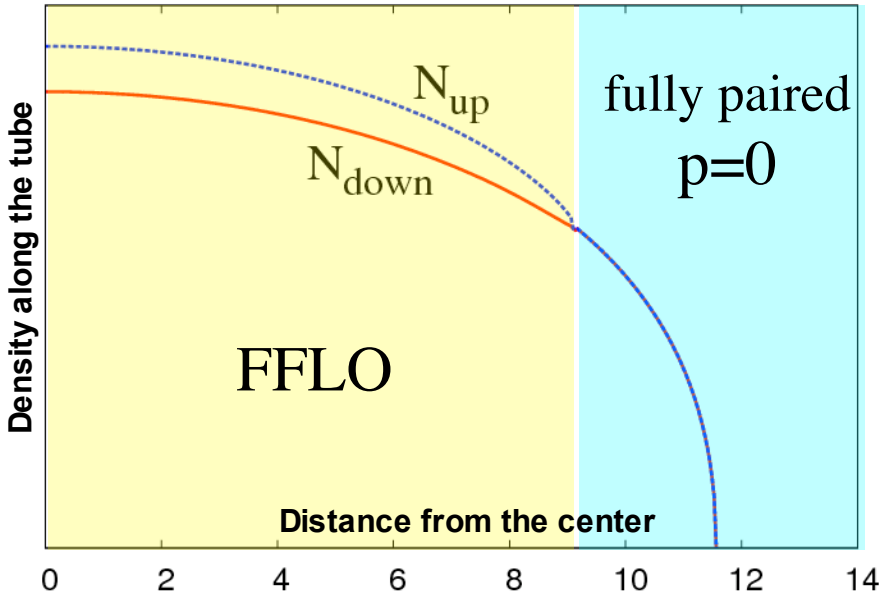
Fermi level $\mu_{\updownarrow} = N_{\updownarrow}$

Ratio gives **effective coupling** $\frac{g}{2\sqrt{N}}$

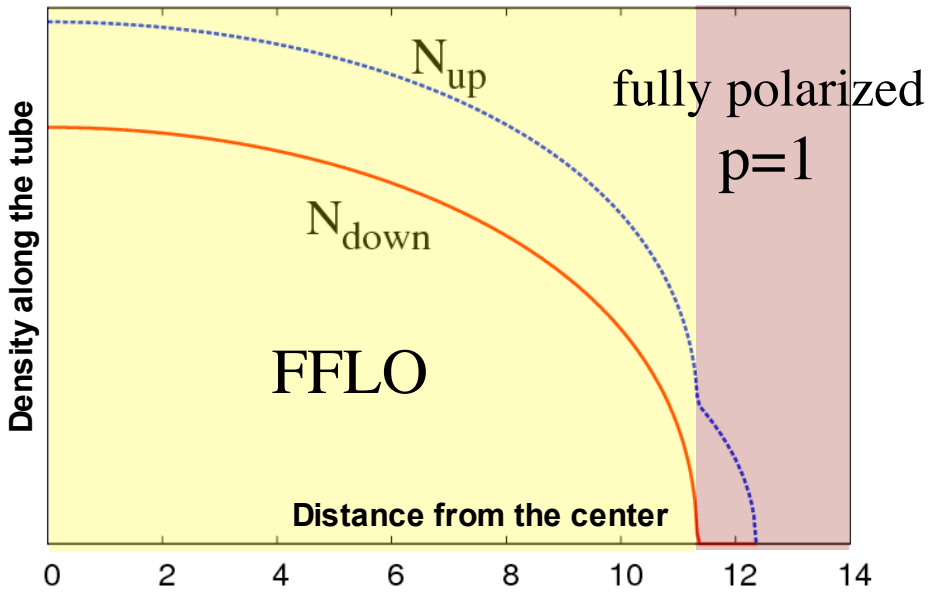
Thomas-Fermi phase diagram

Local density approximation based on the **Bethe ansatz** solution for the homogeneus system

G. Orso, *Phys. Rev. Lett.* **98**, 070402 (2007)



Strong coupling,
small spin imbalance

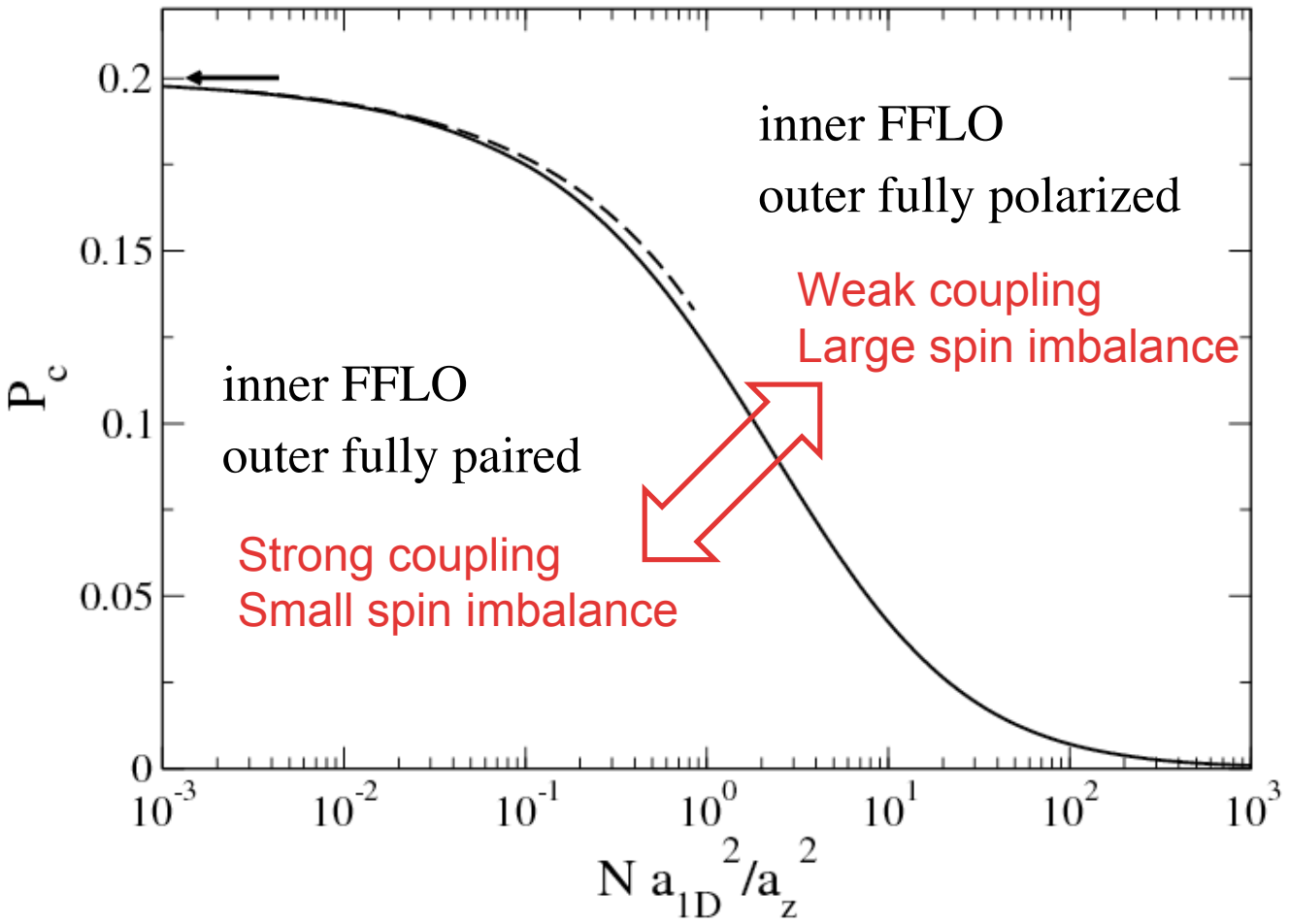


Weak coupling,
large spin imbalance

<u>Phase separation experimentally detectable by imaging the cloud</u>

“Critical” polarization (T=0)

G. Orso, *Phys. Rev. Lett*. **98**, 070402 (2007)



$$a_z = \sqrt{\hbar / m\omega_z} = 1$$

$$a_{1D} = -2\hbar^2 / mg = -2/g$$

Trial wave function for VMC and DMC

Slater-Jastrow form $\Psi = D^{\uparrow} D^{\downarrow} J$

Antisymmetric product of **Hermite polynomials**

$$D^{\sigma} = \det(H_i(x_j^{\sigma})) = \prod_{1 \le i < j \le N^{\sigma}} (x_i^{\sigma} - x_j^{\sigma})$$

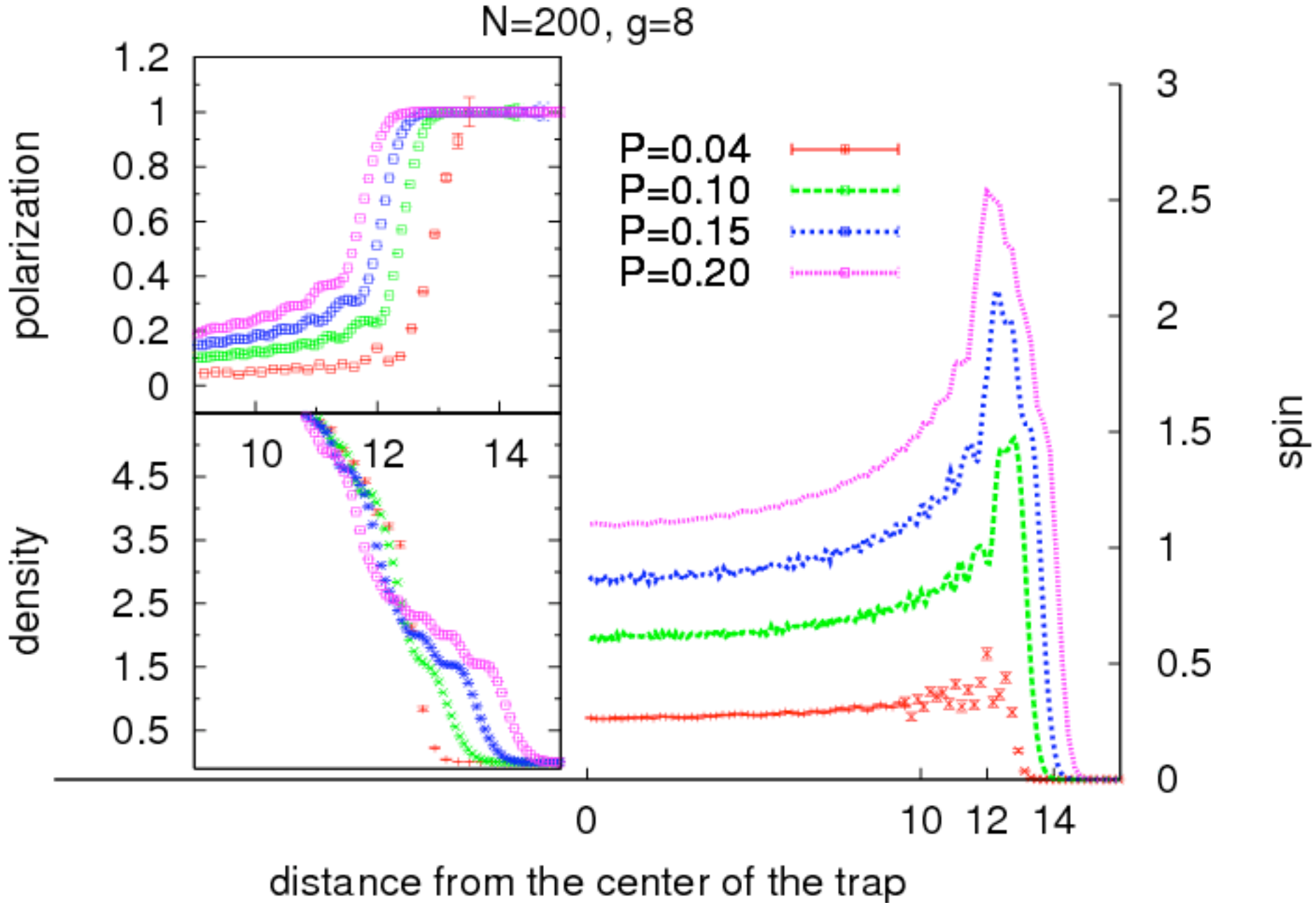
one-body, two-body, and three-body Jastrow factor J

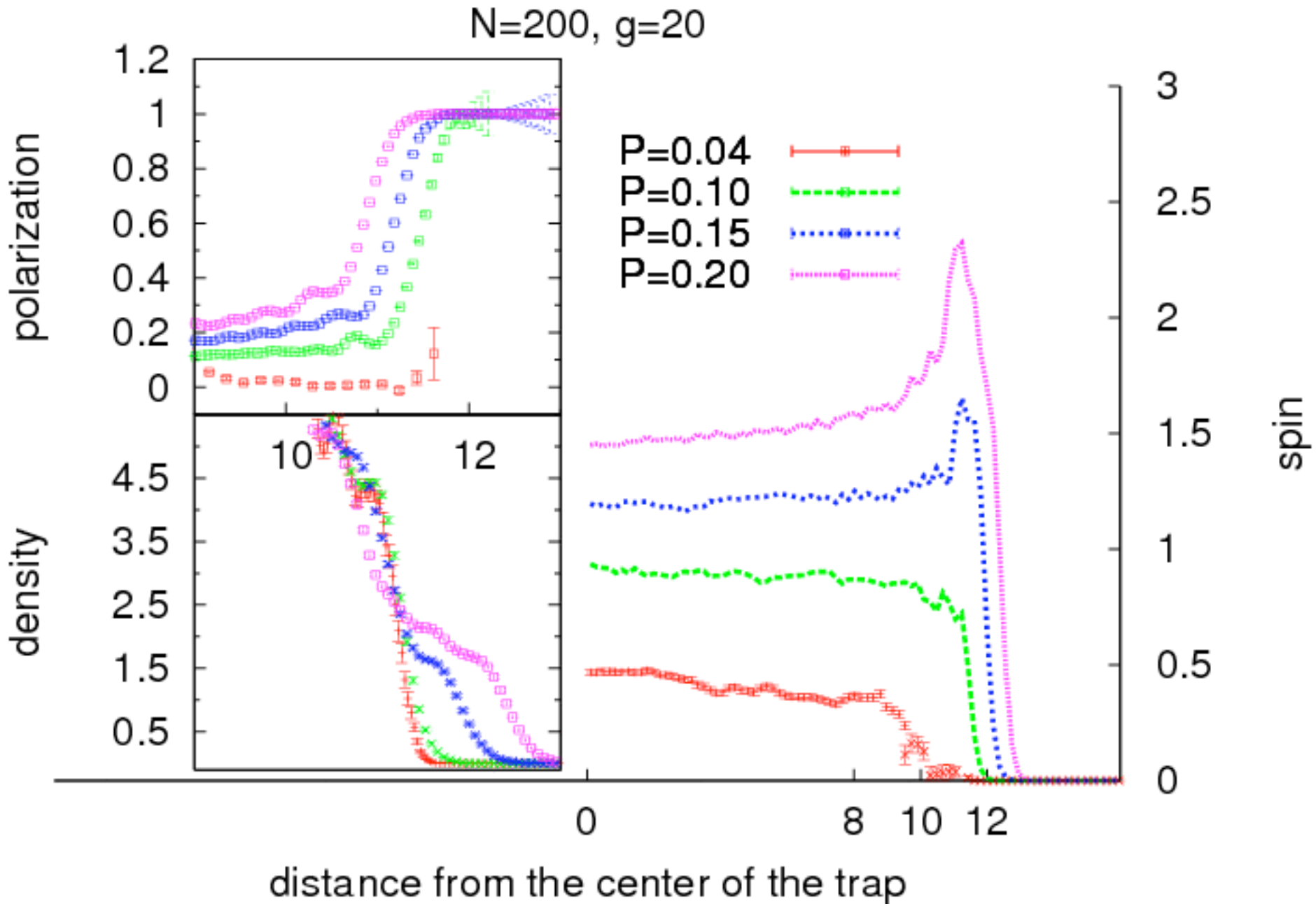
delta function potential handled with **cusp conditions**

$$V(x = x_1^{\uparrow} - x_2^{\downarrow}) = -g\ \delta(x) \quad \Rightarrow \quad \frac{d}{dx} J^{\uparrow\downarrow}(|x|)\Big|_{x=0} = -\frac{g}{4}$$

30 independent variational parameters

Stochastic reconfiguration method to minimize the energy


N=200, g=8
polarization
density
spin
P=0.04
P=0.10
P=0.15
P=0.20
distance from the center of the trap
1.2
1
0.8
0.6
0.4
0.2
0
4.5
3.5
2.5
1.5
0.5
10
12
14
3
2.5
2
1.5
1
0.5
0
0
10
12
14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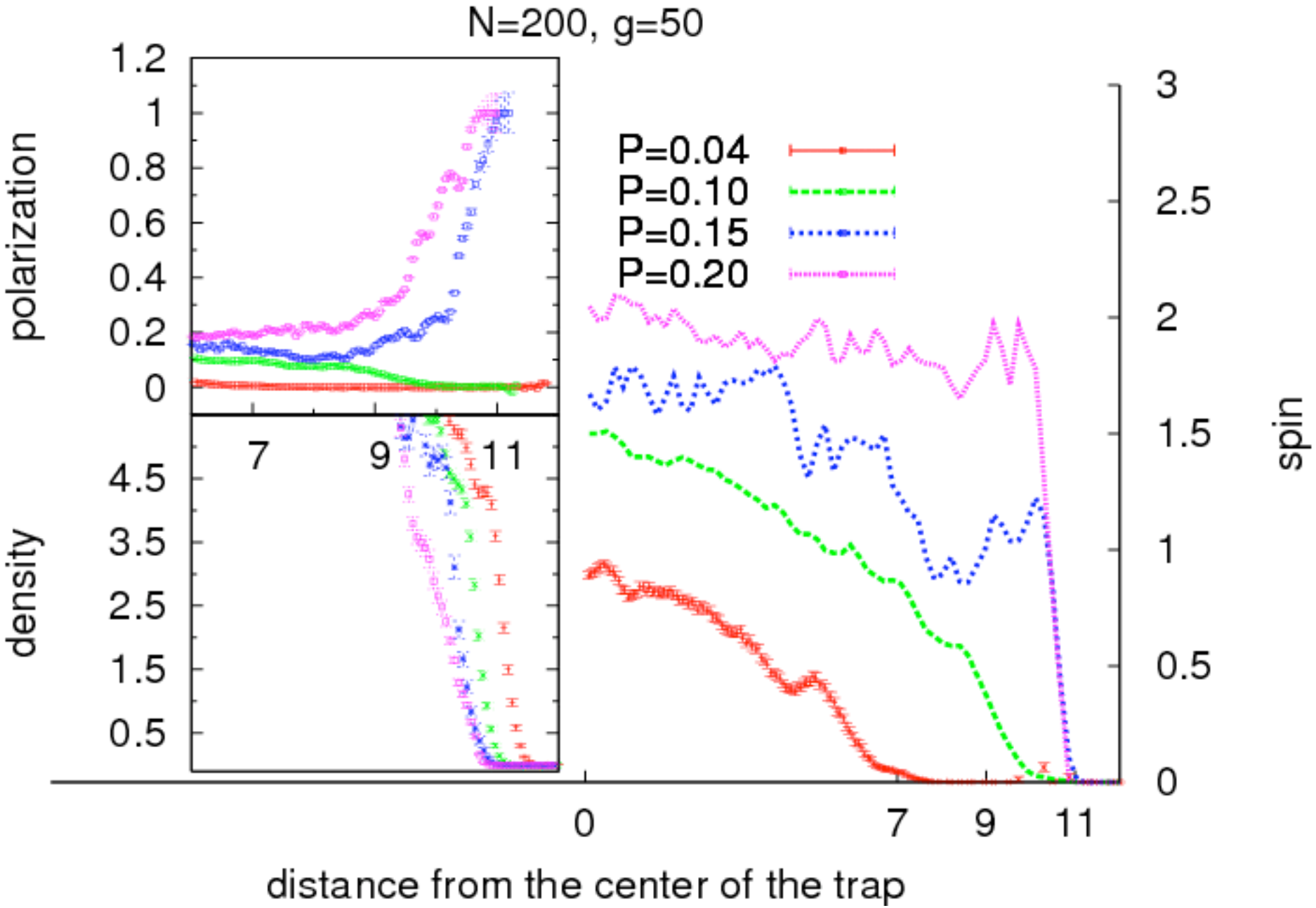
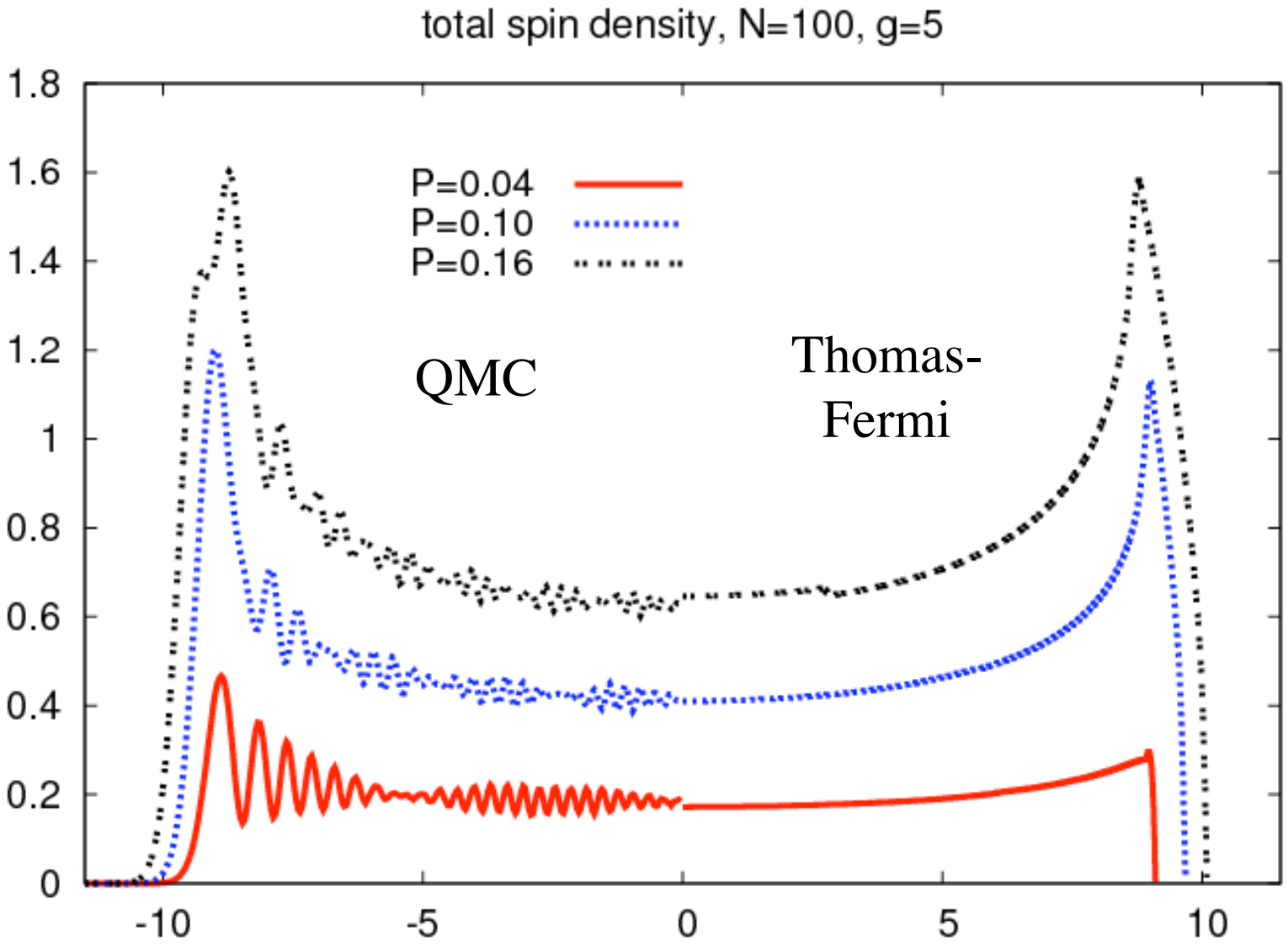
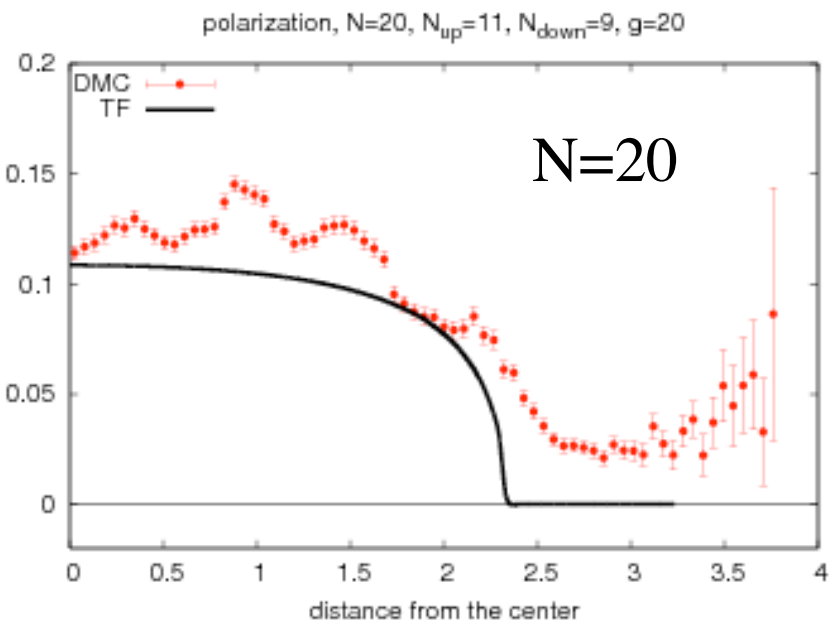
2.5
1.5
0.5
10
12
3
2.5
2
1.5
1
0.5
0
0
8
10
12

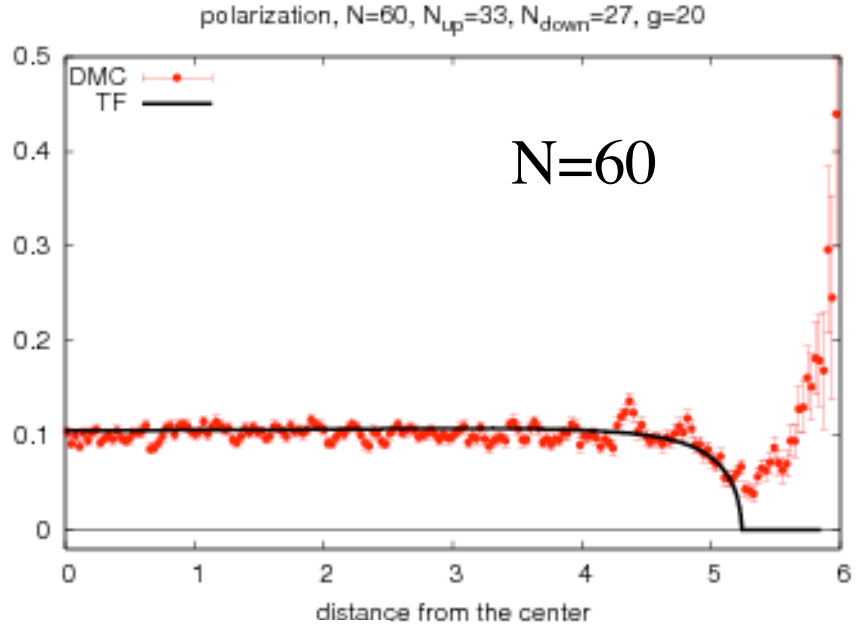

N=200, g=50
polarization
density
spin
distance from the center of the trap
P=0.04
P=0.10
P=0.15
P=0.20
1.2
1
0.8
0.6
0.4
0.2
0
4.5
3.5
2.5
1.5
0.5
7
9
11
3
2.5
2
1.5
1
0.5
0
0
7
9
11

Spin density profile



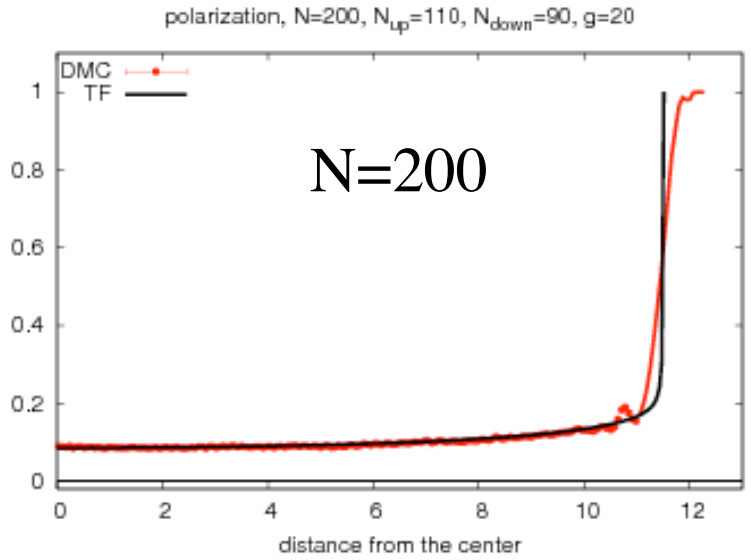
Dependence on N





Spin imbalance 10%
g=20

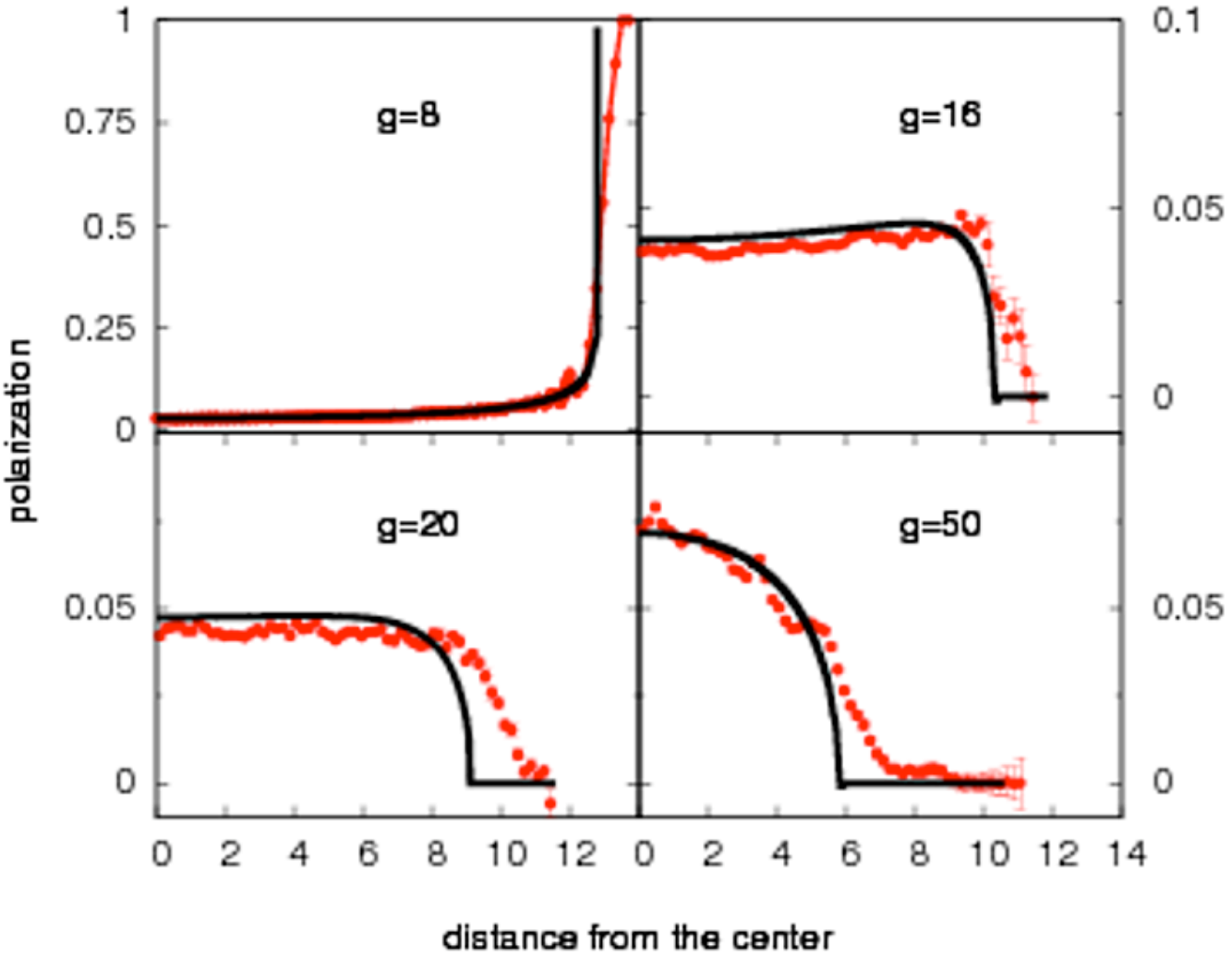
Polarization
$(n^{\uparrow} - n^{\downarrow})/(n^{\uparrow} + n^{\downarrow})$



For N>100, good agreement with Thomas-Fermi

Dependence on g

Spin imbalance 4% N=200



Finite temperature simulations (PIMC)

Thermal density matrix $\rho = \rho_{harmonic}\ \rho_{Fermi}\ \rho_{\text{interaction}}$

$$\rho_{\text{harmonic}}(x,x') = (4\pi\,\lambda\,\tau)^{-N/2} \exp\left(-\sum \frac{(x_i - x_i')^2}{4\lambda\tau}\right)\ \exp\left(-\frac{\tau}{2}\sum (x_i^2 + x_i'^2)\right)$$

with $\lambda = \hbar^2/2m$

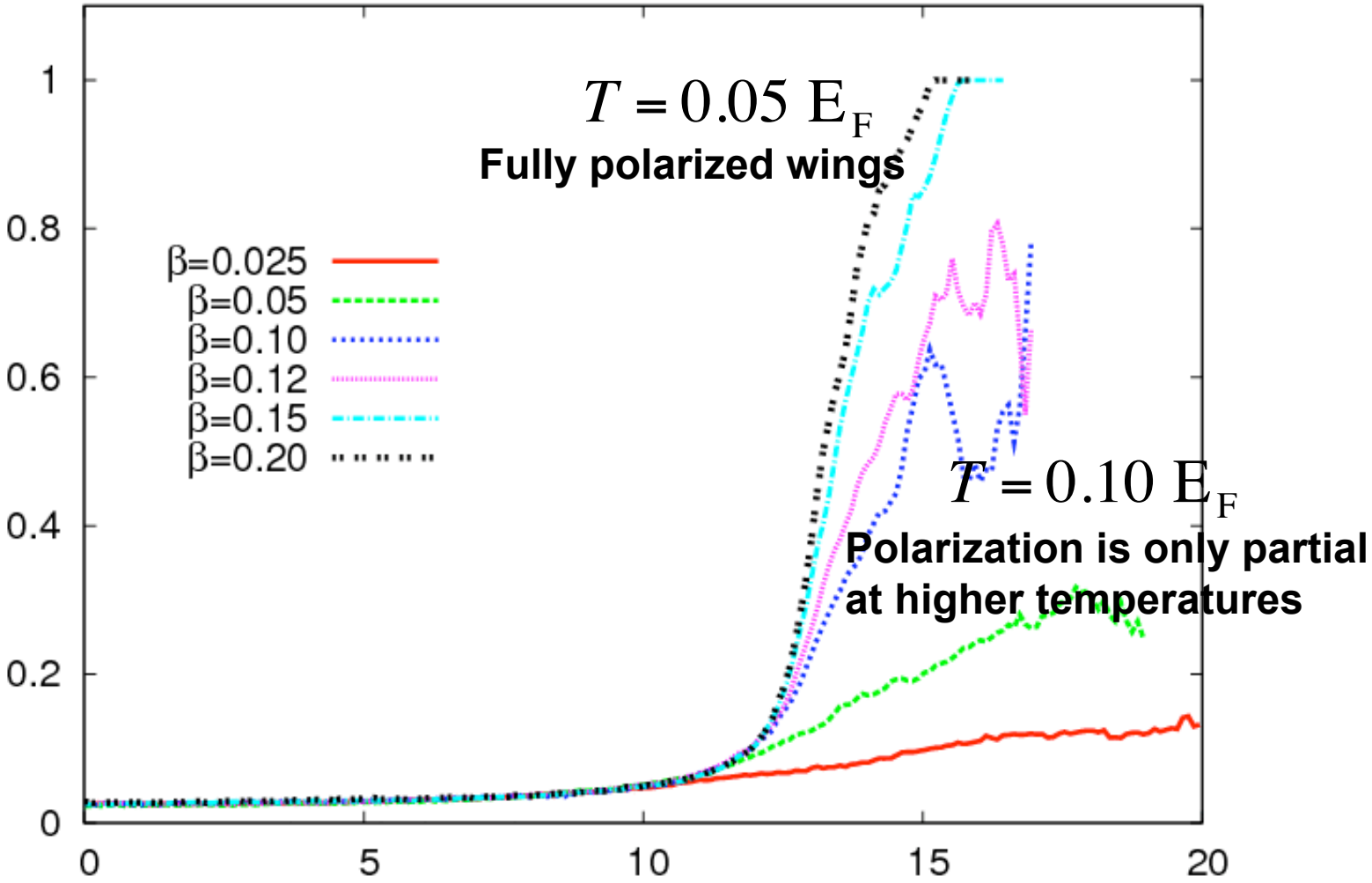
$$\rho_{\text{Fermi}}(x,x') = \prod_{i=2}^{N}\left[1 - \exp\left(-\frac{(x_i - x_{i-1})(x_i' - x_{i-1}')}{\tau}\right)\right]$$

$$\rho_{\text{interaction}}(x,x') = \prod_{i,j}\left[1 - f(x_i, x_j, x_i', x_j')\right]$$

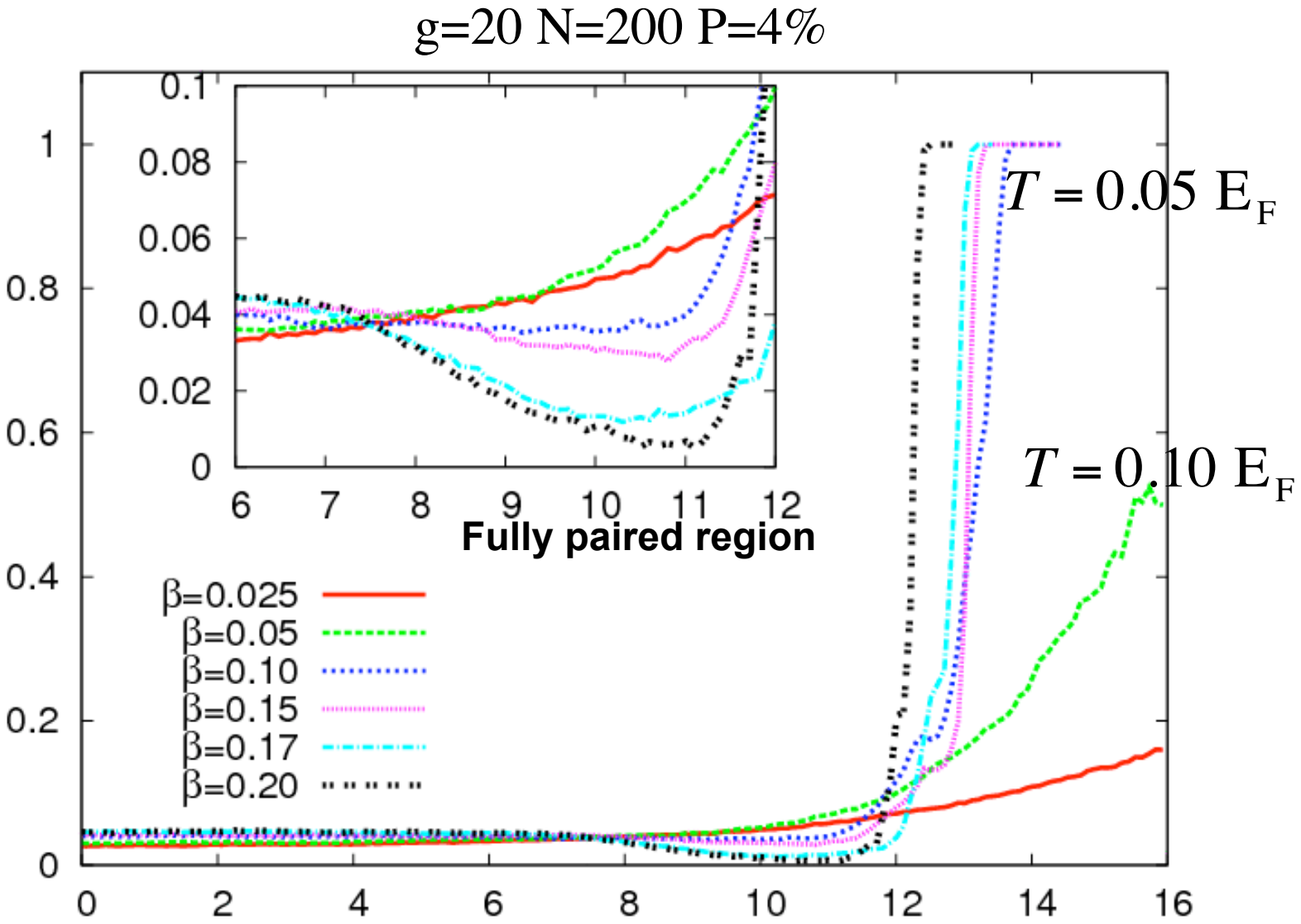
See Bernard Gaveau and Lawrence Schulman, J. Phys. A, **19** 1833-1846 (1986)

Dependence on T

g=8 N=200 P=4%



Dependence on T

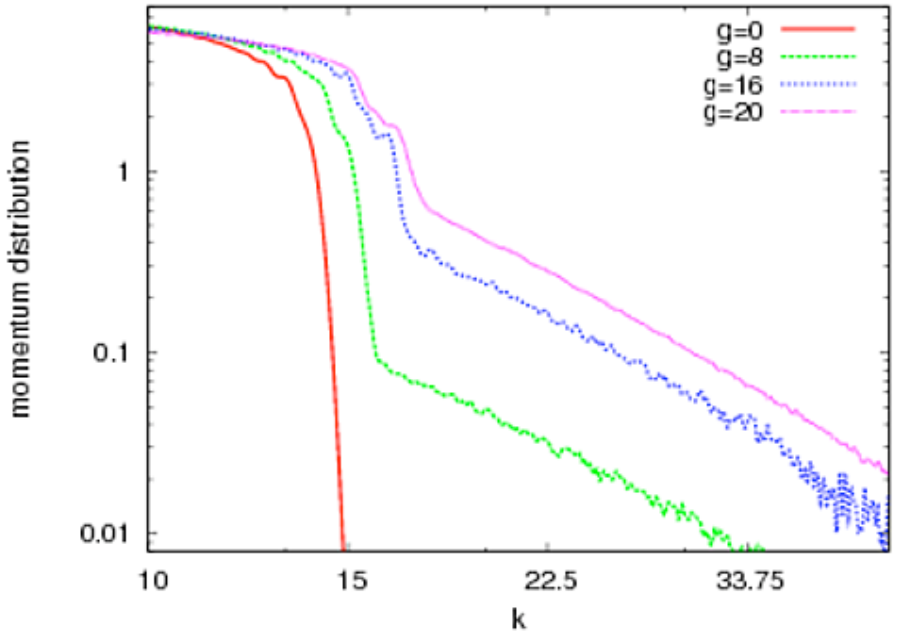


Momentum and pair momentum distribution

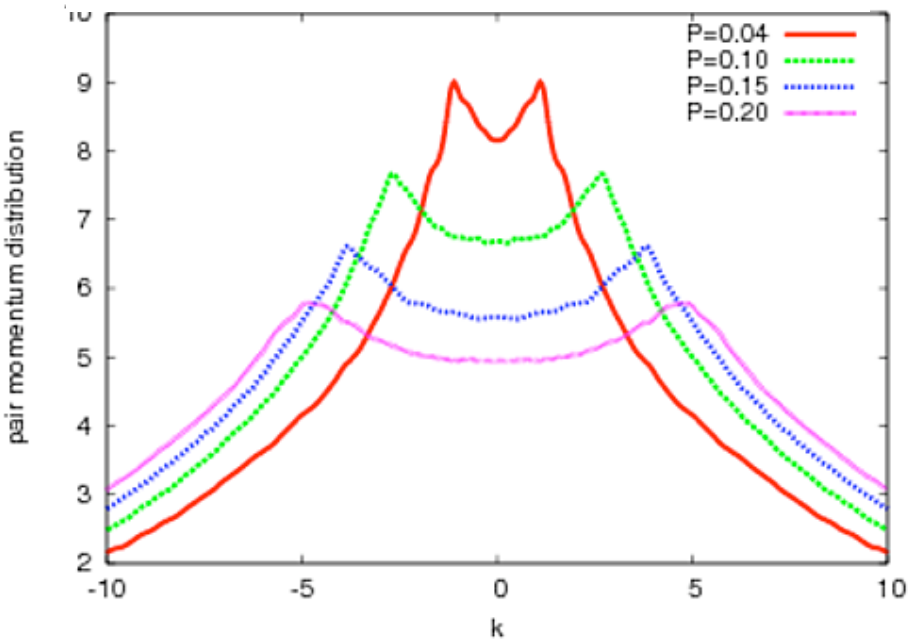
$$n(k) = \int dr \int dr'\ \rho(r,r')\ \exp(-ik(r-r'))$$

$$\rho(x,y) = \int dx_2 \cdots dx_N \Psi(x,x_2,\cdots,x_N)\Psi(y,x_2,\cdots,x_N)$$

$$\rho_{\text{pair}}(x,y) = \int dx_3 \cdots dx_N \Psi(x^{\uparrow},x^{\downarrow},x_3,\cdots,x_N) \times \Psi(y^{\uparrow},y^{\downarrow},x_3,\cdots,x_N),$$



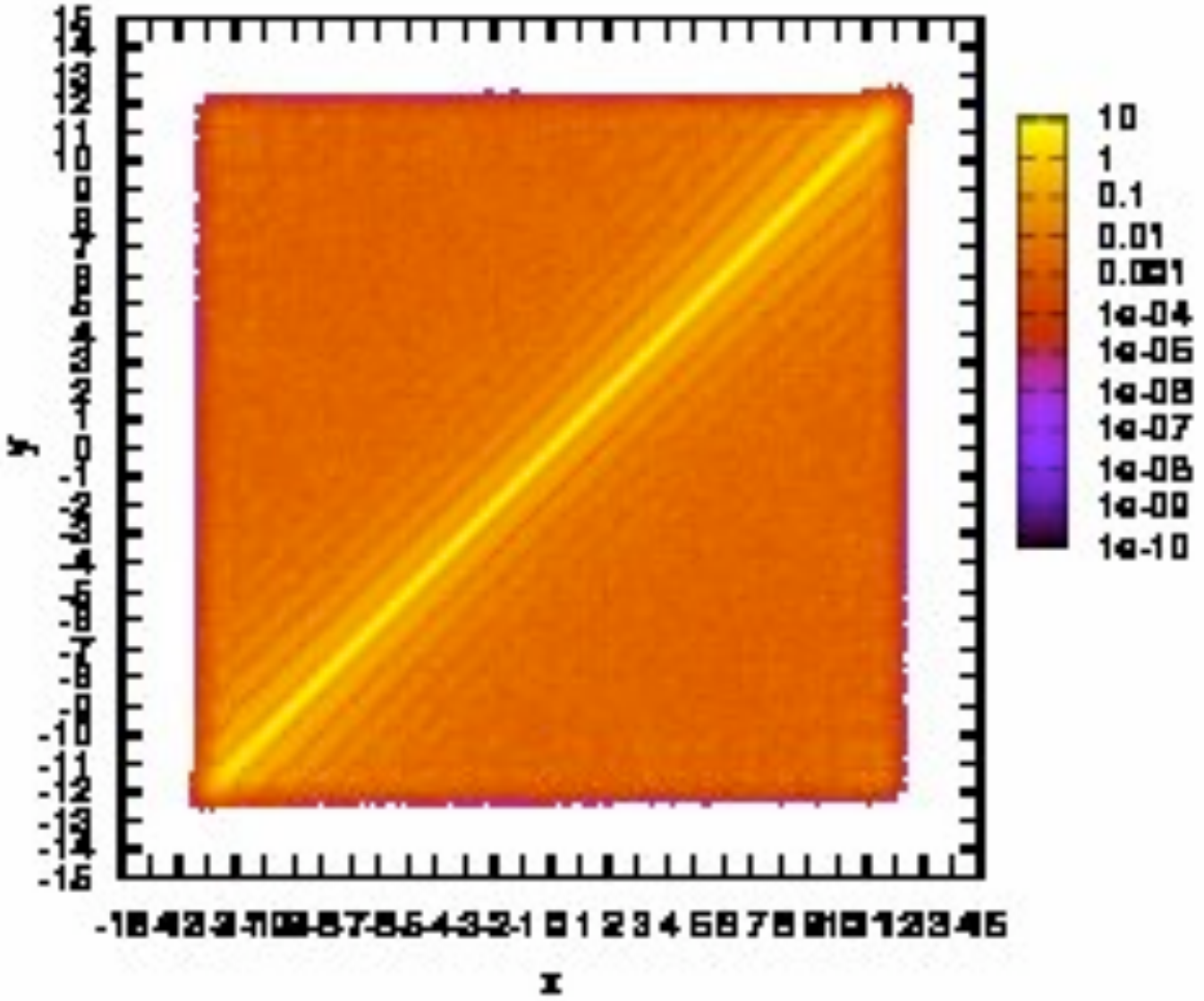
Momentum distribution
N=200, fixed polarization 4%
Dependence on the coupling
$1/k^4$ decay due to cusp



Pair momentum distribution
N=200, fixed coupling g=20
Dependence on the polarization
Peak at $\left|k_F^{\uparrow} - k_F^{\downarrow}\right|$
Signature of FFLO!

Pair momentum distribution

Pair two-body density matrix N=200, g=20, P=0.10%



Summary

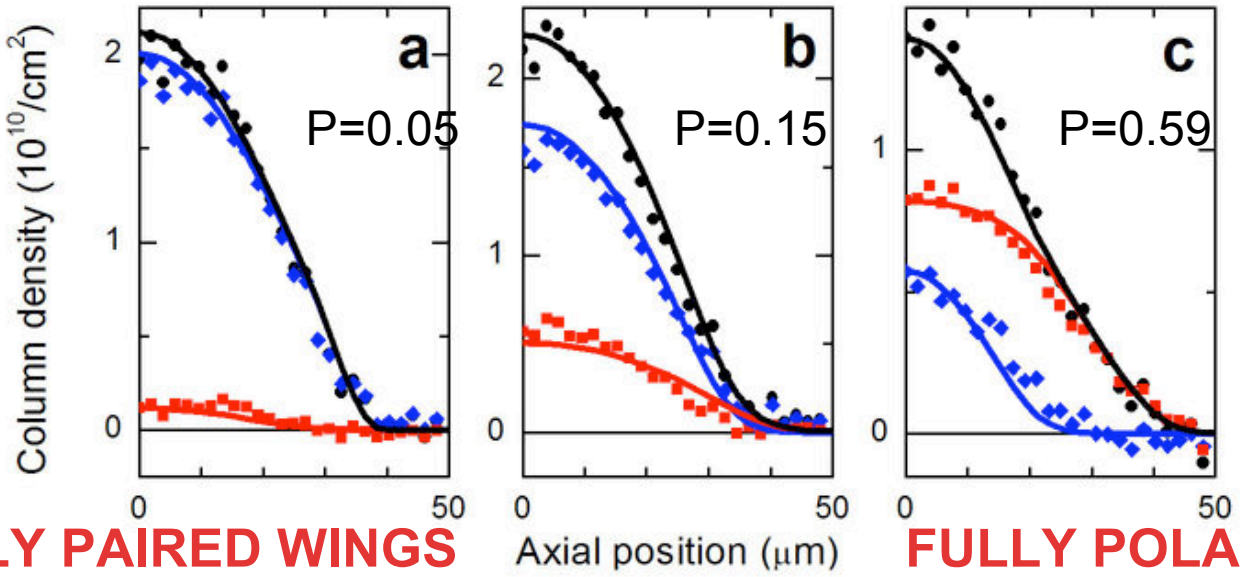
- **Weak coupling** (g ~ 8, N=200)
  spin density profile shows a beating structure reminiscent of the non interacting behavior
  phase separation is between fully polarized wings and a FFLO state in the central part of the cloud
- **Intermediate coupling** (g ~ 16, N=200)
  polarization with P=4% shows clearly fully paired wings
  pairing mechanism seems to involve only one or few particles at the edge of the cloud
- **Strong coupling** (g ~ 50, N=200)
  both polarizations with P=4% and P=10% feature fully paired wings
  LDA overestimates the extension of the fully paired region, particularly for a small number of particles

Some reference

Casula, Ceperley, Mueller, PRA **78**, 033607 (2009)
Batrouni, Huntley, Rousseau, Scalettar, Phys Rev Lett **100**, 116405 (2008)

Very recent developments

Outcome of the Hulet experiment: arXiv:0912.0092



T=0.05~0.10 T_F
N~250

FULLY PAIRED WINGS **FULLY POLARIZED WINGS**

Author: Liao *et al.*
Figure 2

DMRG study of the wings (up to N=160 with some difficulty…)
arXiv:1001.4720: F. Heidrich-Meisner, G. Orso, and A.E. Feiguin

General conclusions

- **QMC gives benchmark results** useful to model and understand the experiment.
- **Ideal tool to study one dimensional systems** (no sign problem) and go beyond the mean field methods or the low energy models like the Luttinger liquid.
- **Non homogeneous and finite size effects** can be consistently taken into account.
- **Static correlation functions** easily accessible.
- **Some limitations**

  Dynamic correlation functions difficult to compute (analitic continuation is necessary)

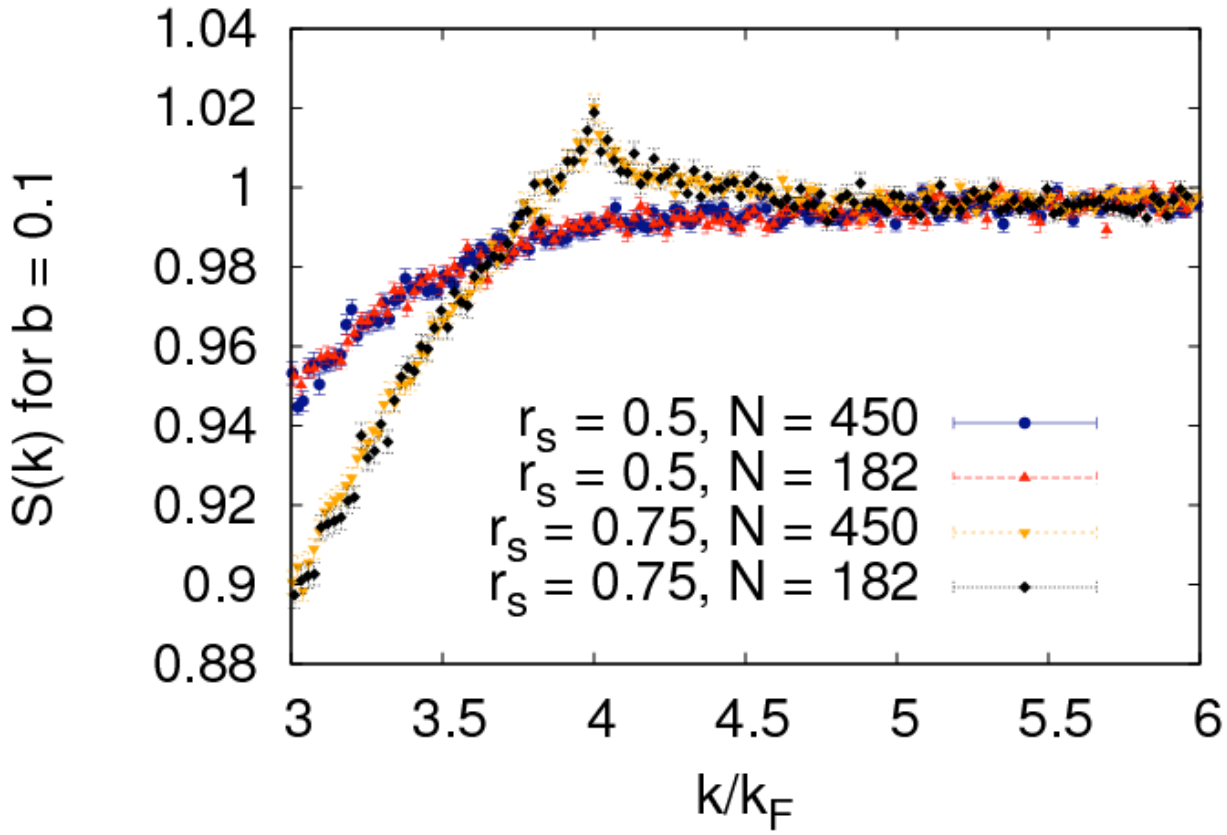
  Ergodicity problems at strong coupling in QMC simulations

Acknowledgements

- Funding via NSF grants DMR-0404853, the Materials Computation Center DMR-0325939, and the DARPA-OLE project
- Computational resources from the Turing Cluster at UIUC and at the NCSA

Onset of $4k_F$ correlations

- Presence of peak in structure factor signals onset of $4k_F$ correlations
- **Crossover density seems "robust" in the thermodynamic limit**
  (finite size scaling analysis necessary because in QMC one works with a finite number of particles in periodic boundary conditions)

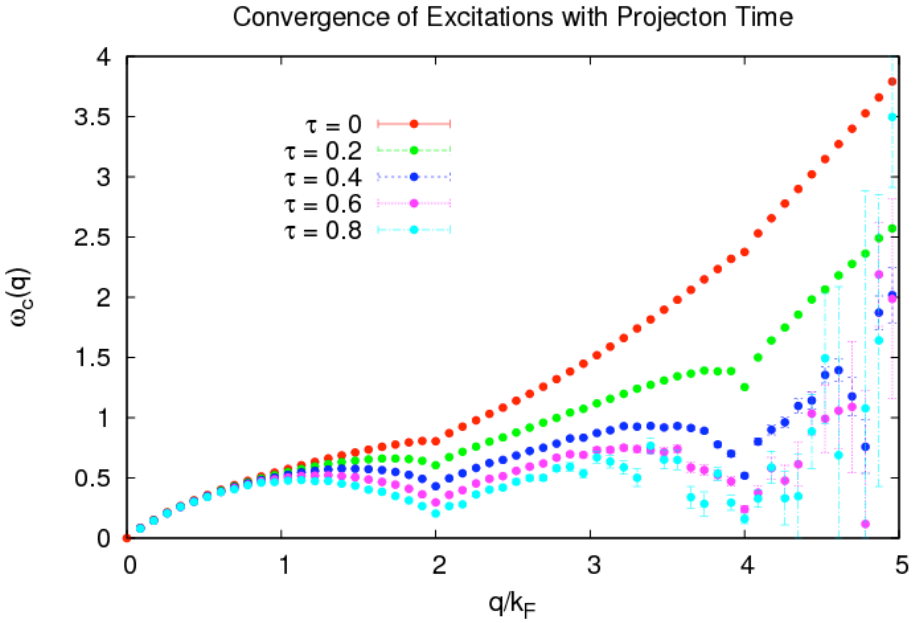


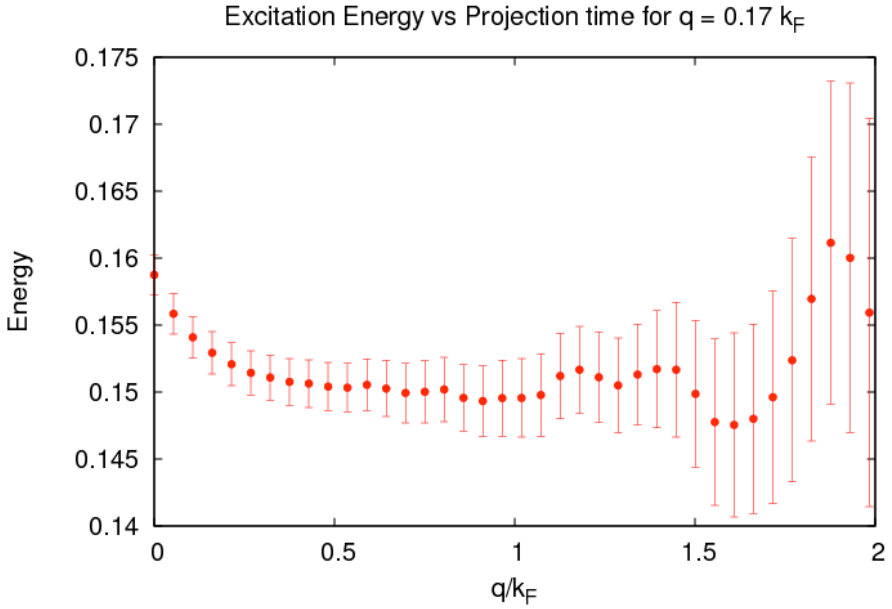
Momentum Resolved Excitation Energies

- A trial wavefunction for the excited state with a given momentum is projected in imaginary time
- The Feynman ansatz is used for the trial wavefunction
- Results are upper bounds on the excitation energies
- Sign problem causes infinite variance at large projection times
- Excitations with q small converge quickly due to more accurate trial wavefunction

$$\Psi_T(q) = \sum_j e^{iqr_j}\Psi_0$$

Reference for the method: D. M. Ceperley and B. Bernu, JCP **89**, 6316 (1988)





Momentum Resolved Excitation Energies

- Transient Estimate

$$S(k,\tau) = \frac{\left\langle \Psi_T | \rho(k,0) e^{-\tau H} \rho(-k,0) | \Psi_0 \right\rangle}{\langle \Psi_T | e^{-\tau H} | \Psi_0 \rangle}$$

- Use forward walking to calculate the matrix element
- S(k,τ) can be expanded in terms of energy eigenstates

$$S(k,\tau) = \sum_i a_i e^{-\epsilon_k^i \tau}$$

- At large τ an upper bound for the energy given by the imaginary time derivative

$$-\frac{d \ln S(k,\tau)}{d\tau} > \epsilon_k^0$$

- Correlation Function Monte Carlo

$$E(k,\tau) = \frac{1}{S(k,\tau)} \frac{\langle \Psi_T | \rho(k,0) e^{-\tau H} H \rho(-k,0) | \Psi_0 \rangle}{\langle \Psi_T | e^{-\tau H} | \Psi_0 \rangle}$$

- More accurate energies by considering the matrix element of the Hamiltonian

$$\frac{\int dr_1 dr_2 \ \rho(-k) G(r_1, r_2, \tau) E_L(k, r_2) \rho(k) P(r_2)}{\int dr_1 dr_2 \ \rho(-k) G(r_1, r_2, \tau) \rho(k) P(r_2)}$$

where

$$E_L(k,r) = \frac{H\rho(k)\Psi_T(r)}{\rho(k)\Psi_T(r)}$$

Charge Compressibility

- Sum rules relate long wavelength excitations to charge compressibility (A. Gold and L. Calmels, PRB **58**, 3497 (1998))

$$\lim_{q\to 0}\omega_c(q) = v_F|q|\sqrt{\rho_F V(q) + \frac{\chi_0}{\chi_c}}$$

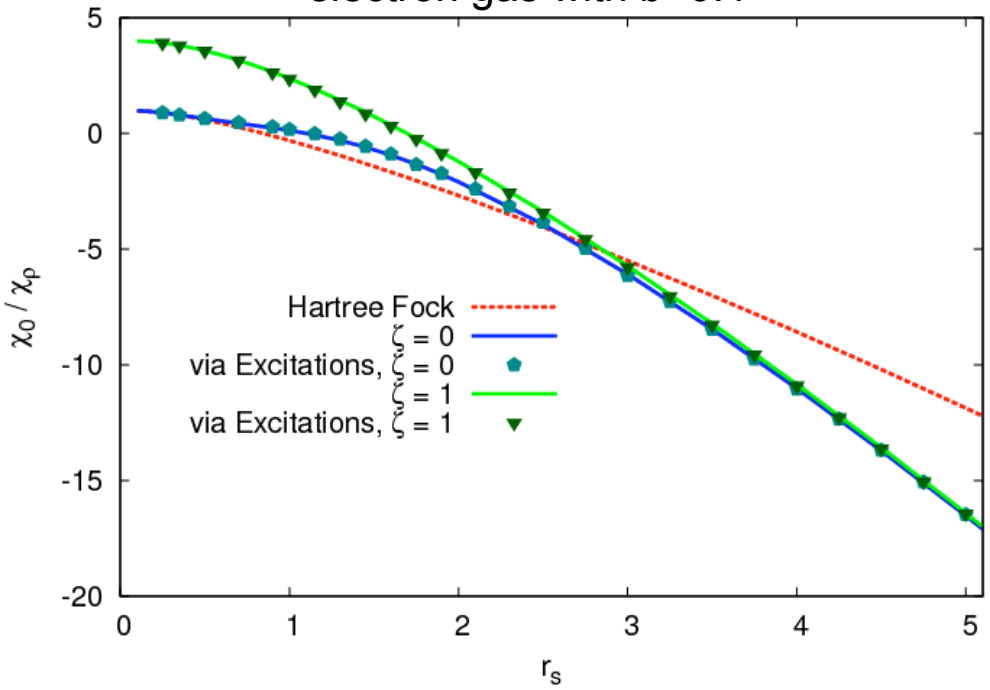
- Compressibility from ground state energy $1/\frac{\partial^2\varepsilon}{\partial r_s^2} = \frac{\chi_0}{\chi_c}$

- Parametrization of energy from Casula *et al.*, PRB **74**, 245427 (2006)

- Finite size effects much smaller in excitation energies due to cancellation of errors

- Charge compressibilities for unpolarized and polarized systems merge in the dilute limit

Charge compressibility of unscreened electron gas with b=0.1

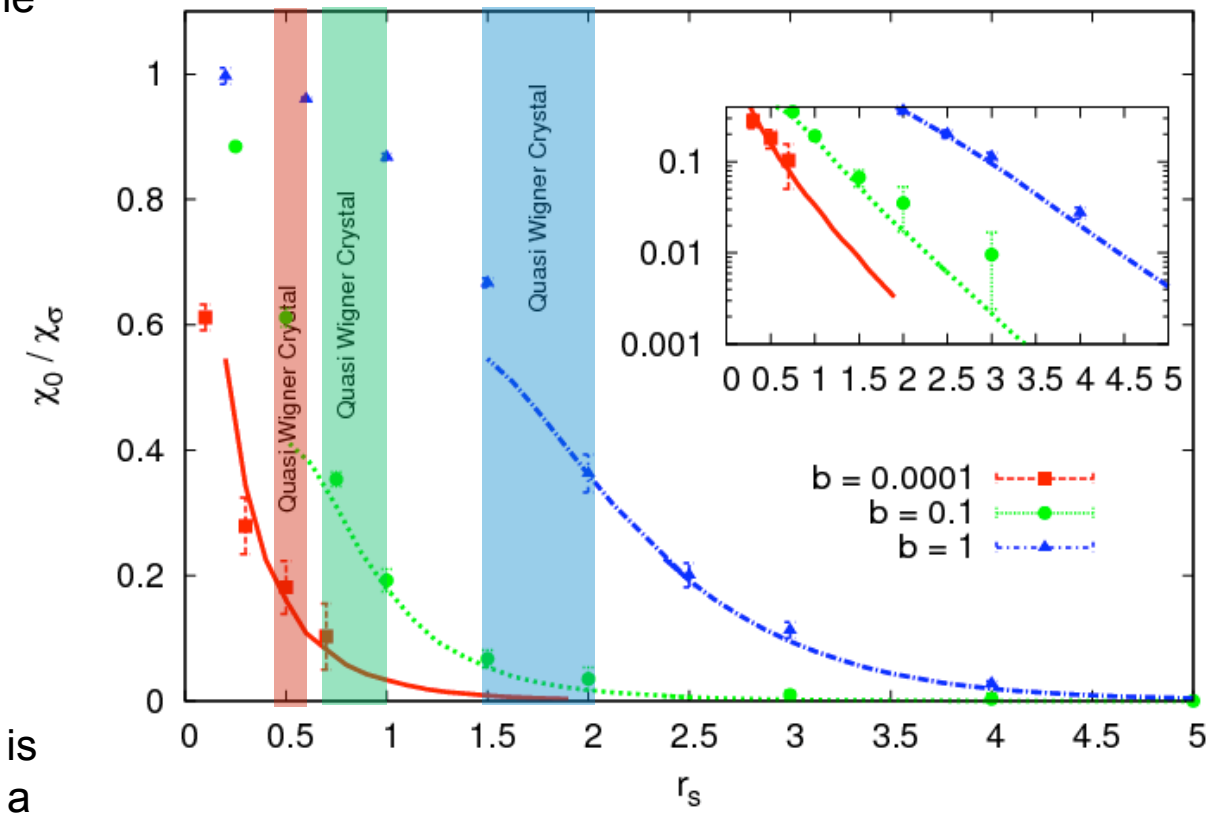


Spin Susceptibility

- Sum rules relate long wavelength excitations to the spin susceptibility
  (A. Gold and L. Calmels, PRB **58**, 3497 (1998))

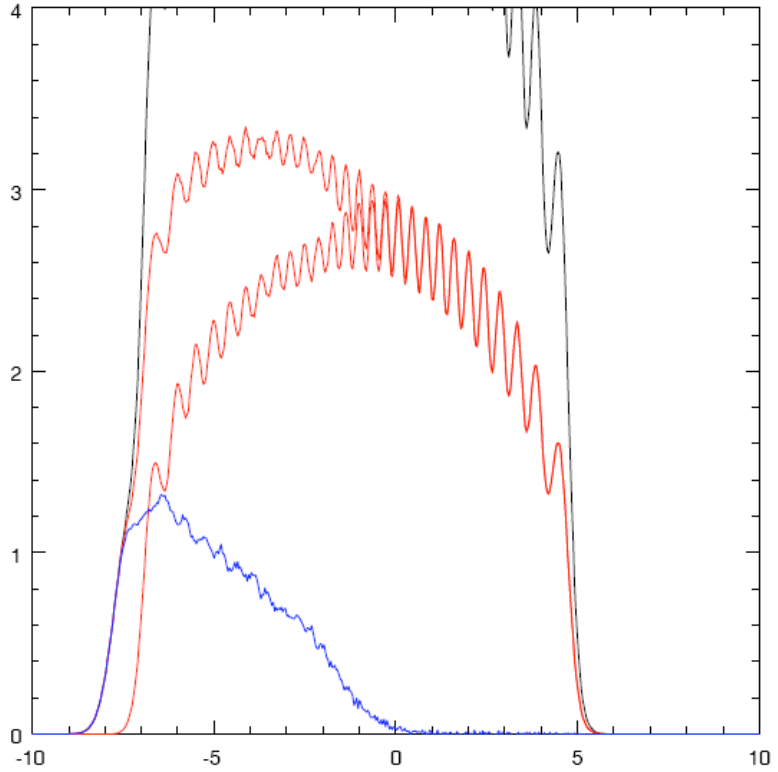
$$\lim_{q\to 0}\omega_s(q) = v_F|q|\sqrt{\frac{\chi_0}{\chi_s}}$$

- Spin susceptibility increases exponentially as density decreases (it is proportional to $1/J^{2)}$
- The blow up of the spin scusceptibility in the large r_s is the signature of the onset of a **spinless (or quasi spinless) regime**



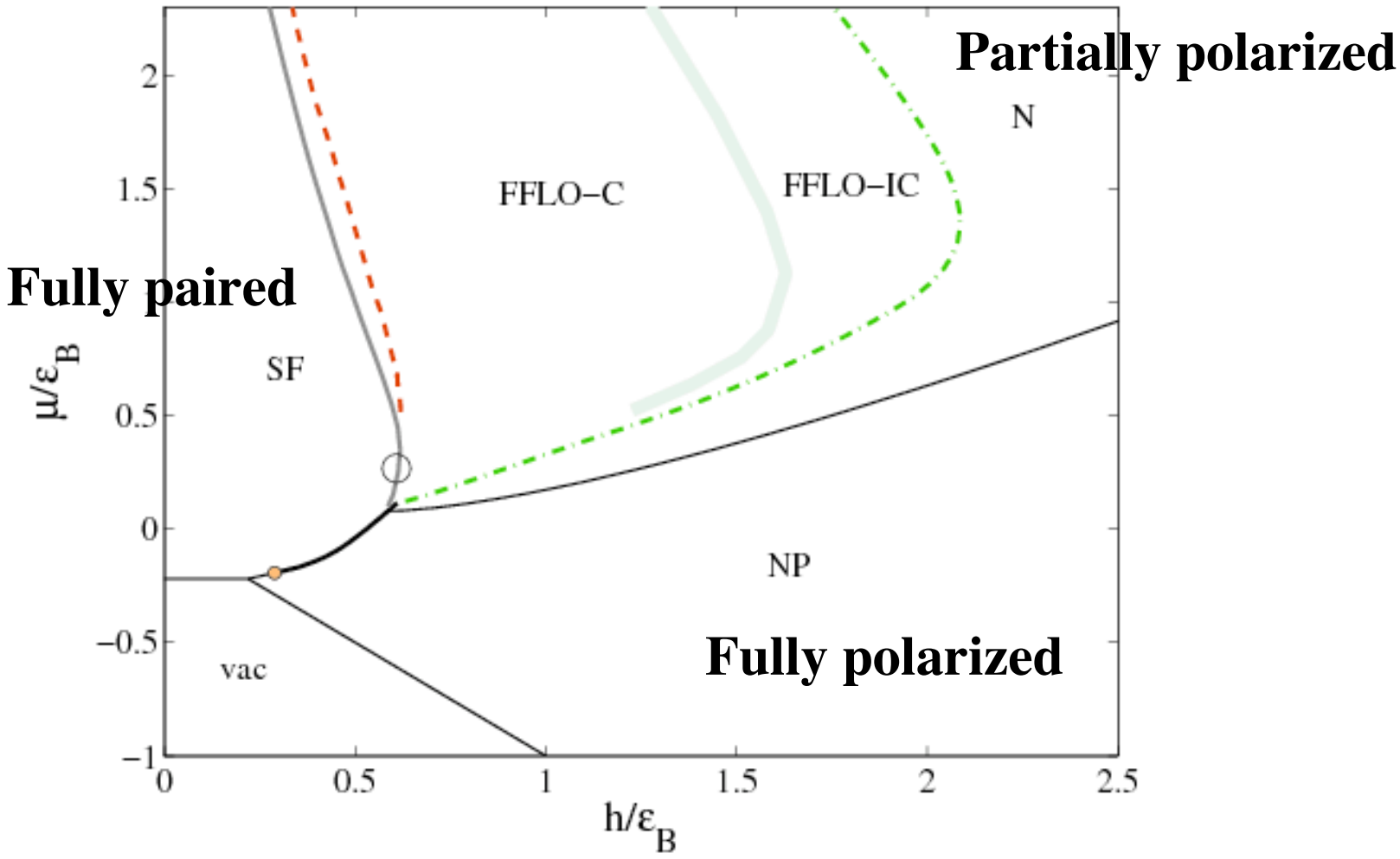
Ergodicity problem

- At strong coupling, it is hard for an unpaired atom to pass through pairs.
- Is this a physically observable effect?
- DMC seems to be more efficient than PIMC (trial wave functon helps)
- Need of better moves in PIMC



g=15 Nup=33, Ndown=27, T=0.5

Quasi 1D effects on the phase diagram



Meera M. Parish, Stefan K. Baur, Erich J. Mueller, David A. Huse, Phys. Rev. Lett. **99**, 250403 (2007)

Methods: Quantum Monte Carlo

- Diffusion Monte Carlo (DMC) and Lattice Regularized Diffusion Monte Carlo (LRDMC)
  - Determine ground state of Hamiltonian by projecting trial wave function in imaginary time

$$\left|\psi(\tau+\delta\tau)\right\rangle = e^{-\hat{H}\delta\tau}\left|\psi(\tau)\right\rangle = \sum_{i=0}^{\infty} c_i e^{-\varepsilon_i \delta\tau}\left|\phi_i\right\rangle$$

  - Recast projection as an integral

$$\left|\psi(\mathbf{R}',\tau+\delta\tau)\right\rangle = \int d\mathbf{R} G(\mathbf{R}',\mathbf{R},\tau)\left|\psi(\mathbf{R},\tau)\right\rangle$$

    where $G(\mathbf{R}',\mathbf{R},\tau) = \left\langle \mathbf{R}'\left| e^{-\tau(\hat{H}-E_T)}\right|\mathbf{R}\right\rangle$

  - The two methods principally differ in how they sample the Green's function

Methods: Quantum Monte Carlo

- Diffusion Monte Carlo
  - Observables are now calculated as:

$$\langle \psi_T | O | \psi_0 \rangle = \frac{\int \Psi_T(\mathbf{R}) \Psi_0(\mathbf{R}) \frac{O(\mathbf{R}) \Psi_T(\mathbf{R})}{\Psi_T(\mathbf{R})} d\mathbf{R}}{\int \Psi_T(\mathbf{R}) \Psi_0(\mathbf{R}) d\mathbf{R}}$$

  - The distribution sampled must be positive or the denominator will be 0, leading to exponentially large fluctuations
  - Fixed node approximation:
    - Use zero's of the trial wave function to restrict random walk
    - Exact nodes make this approximation exact
    - Nodes are known in 1D!