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

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Collaborators:
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

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

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

\[ |\Psi_T\rangle = D^\dagger D^\dagger \exp(-\sum_{i<j} u(x_{ij})) \quad D^\sigma = \prod_{1\leq i<j\leq N^\sigma} \sin(G(x_i^\sigma - x_j^\sigma)/2) \]

- 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\(^2\)

\[
\left\langle \rho(x)\rho(0) \right\rangle = A_1 \cos(2k_Fx)\exp(-c_2\sqrt{\ln x})/x + A_2 \cos(4k_Fx)\exp(-4c_2\sqrt{\ln x}) + \cdots
\]

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

\(^1\)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: $2r_s a_0$ mean interparticle distance)
  
  $r_s = \frac{\text{potential energy}}{\text{kinetic energy}}$

  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 $\mu$m$^{-1}$) 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?
Spin-charge separation

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

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


\[ v_o = \frac{\pi}{2} r_s J \]
from Heisenberg spin chain

\[ v_F = \sqrt{\frac{1}{c + \frac{V(k \rightarrow 0)}{\pi k_F}}} \]
from RPA
Our model for the 1D homogeneous electron gas

- Strictly 1D electrons in a **neutralizing homogeneous background**
  \[ \hat{H} = - \sum_i \frac{\nabla_i^2}{2m} + \frac{1}{2} \epsilon \sum_{i \neq j} V(x_i - x_j) + \hat{H}_{e-b} \]

- 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)
July 28 2010, QMC in the Apuan Alps

Model interactions

Unscreened

\[ V(x) = \sqrt{\pi} \frac{x^2}{b} e^{\frac{4b}{x^2}} \text{erfc}\left(\frac{x}{2b}\right) \]

Gate screening

Wire screening

\[ V_g(k, R) = V_g(k) + V_{\text{int}}(k, R) \chi(k)V_{\text{int}}(k, R) \]

Linear response theory for the second wire

Graph showing the relationship between \( V(x) \) and \( x \) for unscreened, screened by wire, and screened by gate cases.
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

![Graph showing screening effects](image)
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:
  \[ m^* = 0.067 \, m_e \]
  \[ \varepsilon = 13.1 \]
  \[ a_0 \approx 10 \, \text{nm} \]
  \[ b = 0.707 \]
  \[ b' = 1.061 \]
  (radial root mean square equal to the lithographic thickness)

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

\[
\chi_{\text{RPA}} = \frac{\chi_0(k)}{1 - V_b'(k) \chi_0(k)}
\]

\[
\chi_0(k) = \frac{1}{\pi k} \ln \left| \frac{k - 2k_F}{k + 2k_F} \right|
\]
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
- Interactions are screened by the second wire
- Vary the number of electrons in the “trap”

\[ W(x) = E_F \left( \frac{2x}{L} \right)^8 \]

Two electrons per peak

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)

Fiete et al. PRB 72, 045315 (2005)
Tserkovnyak et al. PRB 68, 125312 (2003)
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 $\mu$m$^{-1}$

Remarkable agreement with experimental transition at 20 $\mu$m$^{-1}$

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

Spin and Charge Velocities

- 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)

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)
Quasi Wigner Crystal to Impenetrable Particles Crossover

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

• Pair correlation function $g(r)$ exponentially approaches 0 for $r=0$
• In low density limit $g(r)$ becomes independent of spin → like spinless fermions
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 thickness (small $b$)
2. strong coupling (large $r_s$)
3. large screening (small $R$)

$b \ll 1 \quad r_s \gg 8R^2/\pi$
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:
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 $\mu_{\uparrow} = N_{\downarrow}$

Ratio gives effective coupling $\frac{g}{2\sqrt{N}}$
Thomas-Fermi phase diagram

Local density approximation based on the Bethe ansatz solution for the homogeneous system


Phase separation experimentally detectable by imaging the cloud
“Critical” polarization (T=0)


\[ a_z = \sqrt{\frac{\hbar}{m \omega_z}} = 1 \]

\[ a_{1D} = \frac{-2\hbar^2}{mg} = -\frac{2}{g} \]
Trial wave function for VMC and DMC

Slater-Jastrow form \( \Psi = D^\uparrow D^\downarrow J \)

Antisymmetric product of Hermite polynomials

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

one-body, two-body, and three-body Jastrow factor \( J \)

**delta function potential** handled with **cusp conditions**

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

30 independent variational parameters

Stochastic reconfiguration method to minimize the energy
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N=200, g=50

Distance from the center of the trap

Polarization

Density

Spin

P=0.04
P=0.10
P=0.15
P=0.20
Spin density profile

total spin density, N=100, g=5

QMC

Thomas-Fermi
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 \( \rho = \rho_{\text{harmonic}} \rho_{\text{Fermi}} \rho_{\text{interaction}} \)

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

with \( \lambda = \hbar^2 / 2m \)

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

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

Dependence on $T$

$g=8 \ N=200 \ P=4\%$

$T = 0.05\ E_F$

Fully polarized wings

$T = 0.10\ E_F$

Polarization is only partial at higher temperatures
Dependence on $T$

$g=20$ $N=200$ $P=4\%$

$T = 0.05 \ E_F$

$T = 0.10 \ E_F$

Fully paired region

$\beta=0.025$  $\beta=0.05$  $\beta=0.10$  $\beta=0.15$  $\beta=0.17$  $\beta=0.20$
Momentum and pair momentum distribution

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

\[ \rho(x,y) = \int dx_2 \cdots dx_N \Psi(x,x_2,\ldots,x_N) \Psi(y,x_2,\ldots,x_N) \]

\[ \rho_{\text{pair}}(x,y) = \int dx_3 \cdots dx_N \Psi(x_3,x_3,\ldots,x_N) \]

\[ \times \Psi(y_3,y_3,\ldots,x_N), \]

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 \(|k^\uparrow - k^\downarrow|\)
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)
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…)
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 (analytic continuation is necessary)
  - Ergodicity problems at strong coupling in QMC simulations
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- 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

Momentum Resolved Excitation Energies

- **Transient Estimate**
  \[ S(k, \tau) = \frac{\langle \psi_T | \rho(k, 0) e^{-\tau H} \rho(-k, 0) | \psi_0 \rangle}{\langle \psi_T | e^{-\tau H} | \psi_0 \rangle} \]

- **Use forward walking to calculate the matrix element**

- **S(k, \tau) can be expanded in terms of energy eigenstates**
  \[ S(k, \tau) = \sum_i c_i e^{-\epsilon_i k \tau} \]

- **At large \( \tau \) 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**
  \[ E(k, \tau) = \frac{1}{S(k, \tau)} \frac{\langle \psi_T | \rho(k, 0) e^{-\tau H} \rho(-k, 0) | \psi_0 \rangle}{\langle \psi_T | e^{-\tau H} | \psi_0 \rangle} \]

- **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
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 susceptibility 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 function helps)
- Need of better moves in PIMC

\[ g=15 \quad N_{\text{up}}=33, \quad N_{\text{down}}=27, \quad T=0.5 \]
Quasi 1D effects on the phase diagram

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
    \[ |\psi(\tau + \delta\tau)\rangle = e^{-\hat{H}\delta\tau} |\psi(\tau)\rangle = \sum_{i=0}^{\infty} c_i e^{-\epsilon_i \delta\tau} |\phi_i\rangle \]
  - Recast projection as an integral
    \[ |\psi(\mathbf{R}', \tau + \delta\tau)\rangle = \int d\mathbf{R} G(\mathbf{R}', \mathbf{R}, \tau) |\psi(\mathbf{R}, \tau)\rangle \]
    where \[ G(\mathbf{R}', \mathbf{R}, \tau) = \langle \mathbf{R}' | e^{-\tau(\hat{H} - E_T)} | \mathbf{R} \rangle \]
  - The two methods principally differ in how they sample the Green’s function
Diffusion Monte Carlo

- Observables are now calculated as:

\[
\langle \psi_T | O | \psi_0 \rangle = \frac{\int \Psi_T(R) \Psi_0(R) O(R) \Psi_T(R) dR}{\int \Psi_T(R) \Psi_0(R) dR}
\]

- 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!