QMC study of ultracold dipolar fermions in two dimensions

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Outline

1. Introduction: ultracold dipolar gases
2. The model: 2D dipolar fermions
3. Details of QMC calculations
4. Ground state properties: Fermi liquid, Wigner crystal and stripe phases

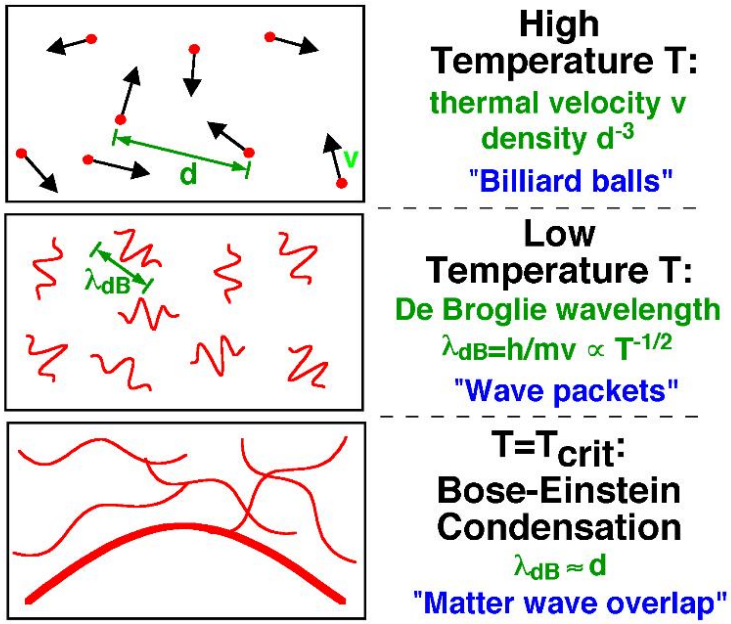
$\Rightarrow$ Conclusion

Introduction:

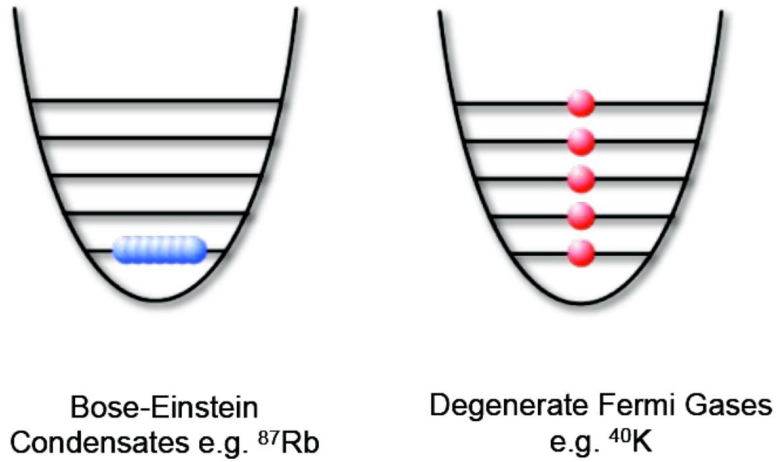
ultracold dipolar gases

What are the ultracold quantum gases?

Cooling down an atomic ensamble



Ground state of bosons and fermions in harmonic potential at $T = 0$



Bose-Einstein Condensates e.g. ^{87}Rb

Degenerate Fermi Gases e.g. ^{40}K

- The first BEC: 1995
- The first degenerate Fermi gas: 1999.

- Densities: $10^{12} - 10^{15} cm^{-3}$
- Temperatures: $10 nK$
- Atom numbers: $10 - 10^6$

Why are the quantum gases interesting?

Ultracold atoms are clean and highly controllable systems:

- tuning of scattering length, density, temperature, number of atoms
- different dimensions: 1D, 2D, 3D
- different spacial arrangments of atoms (square, triangular, honycomb lattices)

$\Rightarrow$ Possibility to study model hamiltonians for different condensed-matter theories:

- Bardeen-Cooper-Schrieffer theory of superconductivity
- Hubbard model
- ferromagnetism
- etc ...

Contact and dipolar interactions

- Atoms without a dipole moment: the s-wave scattering is a dominant process

$$\text{Contact interaction potential: } U_{cont}(\mathbf{r}) = \frac{4\pi\hbar^2 a}{m}\delta(\mathbf{r})$$

Reviews: Rev. Mod. Phys. **74**, 463, 1999 (bosons), Rev. Mod. Phys. **80**, 1215, 2008 (fermions).

- Atoms with a dipole moment: not only the s-wave scattering

$$U_{dd}(\mathbf{r}) = U_{cont} + \frac{d^2}{r^3}(1 - 3\cos^2\theta), \text{ characteristic length: } r_0 = \frac{md^2}{\hbar^2}$$

Reviews: Rep. Prog. Phys. **72**, 126401, 2009 (bosons), Chem. Rev. **112**, 5012, 2012 (fermions).

Experimental realization of dipolar quantum gases

- Atoms with large magnetic moment
  - Bosons: ^{52}Cr ($d = 0.054D$), ^{168}Er ($d = 0.065D$), ^{164}Dy ($d = 0.093D$)
  - Fermions: ^{53}Cr, ^{161}Dy

Phys. Rev. Lett. **108**, 210401, 2012; Phys. Rev. Lett. **107**, 190401, 2011; Phys. Rev. Lett. **108**, 215301, 2012

- Heteronuclear polar molecules
  - Bosons: ^{41}K^{87}Rb ($d = 0.56D$), ^{87}Rb^{133}Cs
  - Fermions: ^{40}K^{87}Rb, ^{23}Na^{40}K ($d = 2.7D$), ^{6}Li^{133}Cs ($d = 5.5D$)

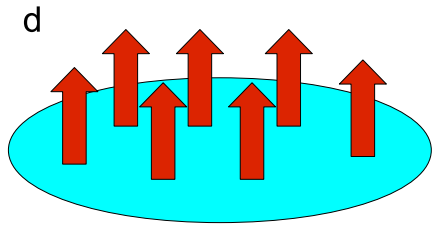
Science **327**, 853, 2010; Nature **464**, 1324, 2010; Phys. Rev. Lett. **109**, 085301, 2012.

Two-dimensional geometry supresses the chemical reaction rate for ^{40}K^{87}Rb

The model:

2D dipolar fermions

The model



$$\hat{H} = \frac{\hbar^2}{2m} \sum_{i=1}^{N} \Delta_i + d^2 \sum_{j<k} \frac{1}{|\mathbf{r_j} - \mathbf{r_k}|^3}$$

- Dipole moments are aligned perpendicular to the plane of motion by an external field.
- Purely repulsive $1/r^3$ interaction.
- Purely two-dimensional system.

The goal is to investigate phase diagram at $T = 0$ by means of FNDMC.

Possible phases

- Fermi liquid phase
  Elementary excitations of interacting fermions are described by almost independent fermionic quasiparticles with the effective mass
- Wigner crystal
  Triangular crystal which appears at large density (contrary to the Coulomb interaction case)
- Stripe phase (stationary density modulations)
  2D dipolar Fermi gas
  Stripe phase is predicted to appear at $k_F r_0 \approx 1.5 - 6$ based on different mean-field approaches.
  2D homogeneous electron gas
  - Microemulsion phases (stripes and bubbles) are predicted to appear between FL and WC (Spivak and Kivelson, PRB **70**, 155114, 2004.)
  - QMC study (Clark and Ceperley, PRL, 2009) did not find a microemulsion phase

Details of FNDMC calculations.

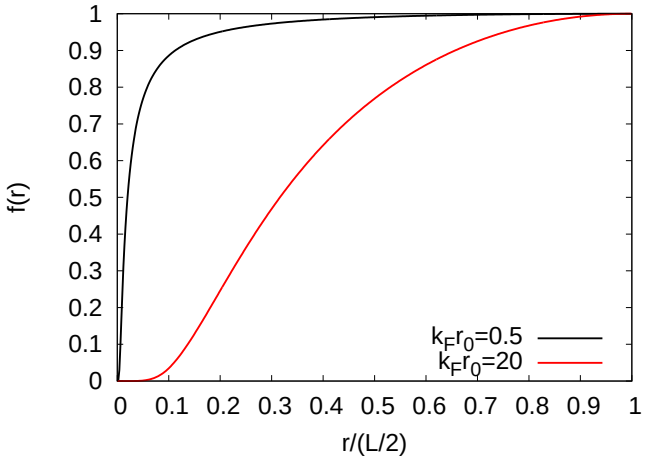
Trial wave function

$$\Psi_T(\mathbf{r_1}, \ldots, \mathbf{r_N}) = \Delta_S \Psi_J$$

Jastrow: $\Psi_J = \prod_{j<k}^{N} f(|\mathbf{r_j} - \mathbf{r_k}|)$,

for $r < \bar{R}$ it is the s-wave solution of a two-body scattering problem,

for $r > \bar{R}$ $f(r) \sim exp(-const/r)$.



Slater determinant:

- Fermi liquid phase $\Delta_S = \det[e^{i\mathbf{q_i}\mathbf{r_j}}]$

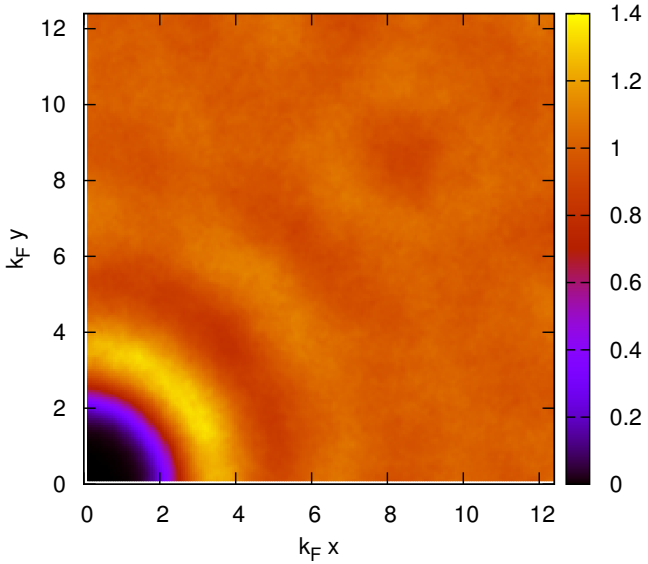
  $\mathbf{q_i} = 2\pi/L(n_x, n_y)$ are PBC wave vectors in a square box
- Wigner crystal phase $\Delta_S = \det[e^{-\alpha(\mathbf{r_i}-\mathbf{R}_m)^2}]$

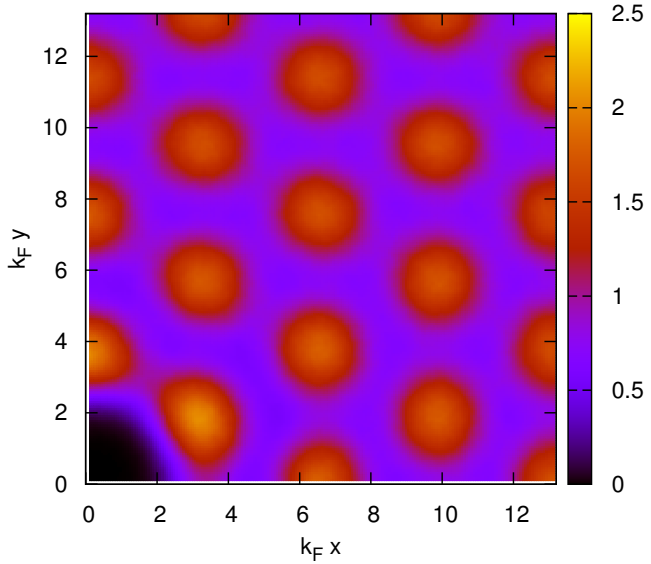
  $\mathbf{R}_m$ are the lattice points of the triangular lattice, α is the variational parameter.
- Stripe phase (pattern of equaly spaced 1D stripes along y-direction)

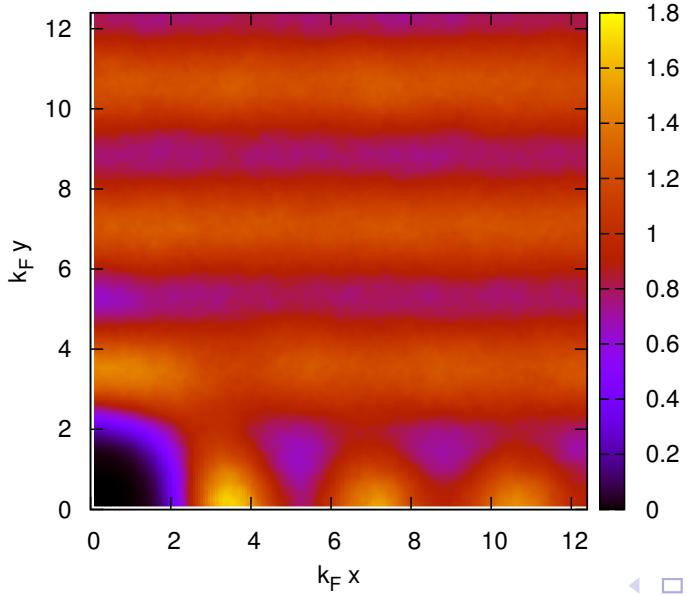
$$\Delta_S = \det[e^{ik_{\alpha x}x_i - \xi(y_i - y_m)^2}]$$

  y_m denotes the y coordinate of the m-th stripe,
  $k_{\alpha x} = 2\pi n_{\alpha x}/L_x$ are the PBC wave vectors in the x-direction,
  ξ is a variational parameter.

Two-dimensional pair-distribution function







Finite size errors

Potential energy

- Summation in real space over all replicas of the simulation box:

$$V_{dd} = \frac{1}{2} \sum_{n_x, n_y} \left(\sum_{i=1}^{N} \sum_{j=1}^{N} \frac{d^2}{|\mathbf{r_i} - (\mathbf{r_j} + \mathbf{n}L)|^3} \right).$$

- Simpler formula:

$$\langle V \rangle = \Sigma + E_{\text{tail}},$$

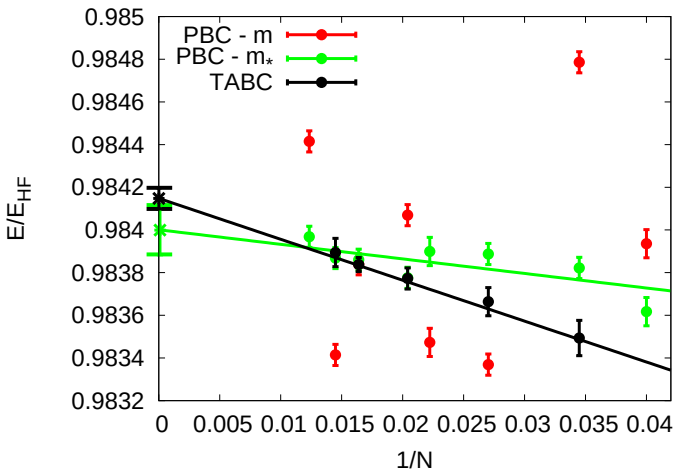
Σ denotes V_{dd} calculated with the constarin $|\mathbf{r}_i - \mathbf{r}_j - \mathbf{R}| \leq L_{cut}$,
$\frac{E_{tail}(m)}{N} = \frac{1}{2} \int_{mL_x}^{\infty} \frac{d^2}{r^3} g(r) 2\pi r \, dr.$

Kinetic energy

- Shell errors for a noninteracting Fermi gas: $\Delta T_N = T_{TH} - T_N$
- Shell errors for a Fermi liquid: $\frac{m}{m_*} \Delta T_N$
- No shell errors for a Wigner crystal
- Negligible shell errors for 1D stripes

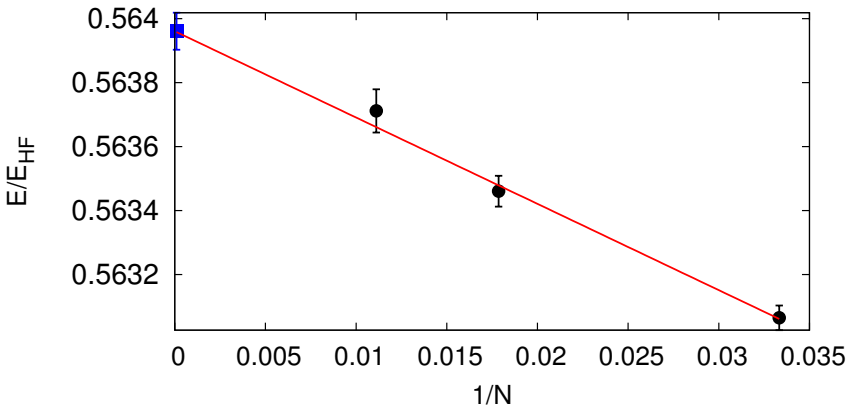
Finite size scaling: Fermi liquid and Wigner crystal phases

Fermi liquid phase



- $N = 25, 29, 37, 49, 61, 81, 89$
- Periodic boundary conditions(PBC)
  $E_N = E + \frac{m}{m_*}\Delta T_N^{PBC} + \frac{a}{N}$
  $\rightarrow$ we can extract the effective mass of a quasiparticle
- Twist-averaged boundary conditions (TABC) give the same E as PBC

Wigner crystal phase



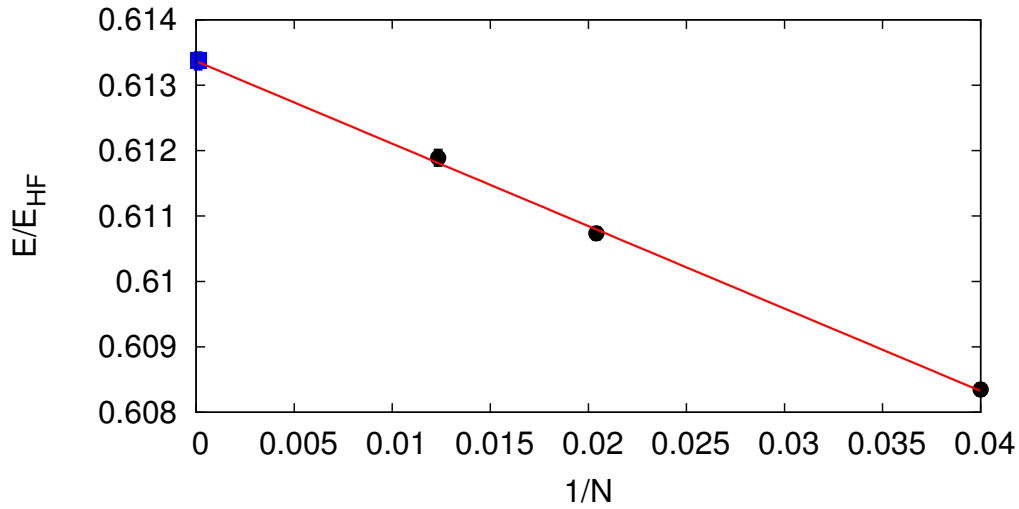
- $N = 30, 56, 90$ (almoust square simulation box)
- $E_N = E + \frac{b}{N}$

Finite size scaling: stripe phase

- The overall density is fixed
- The square simulation box
- The simulations are performed for 25 (5×5), 49 (7×7) and 81 (9×9) particles (we need an odd number of particles per stripe in order to have filled 1D shells)

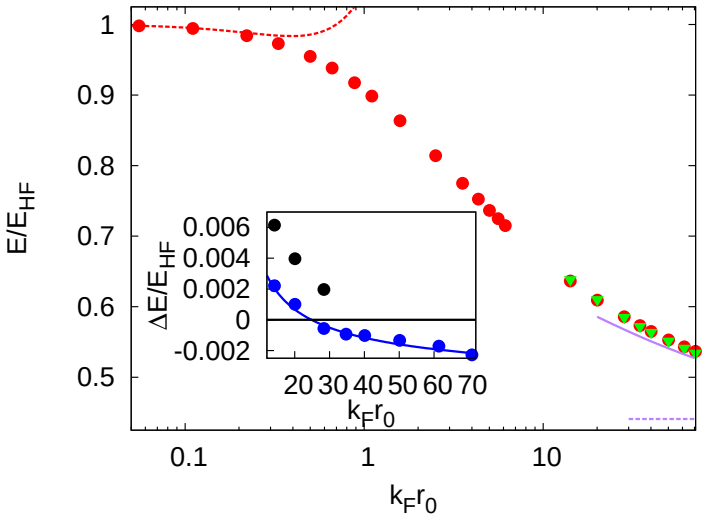
$\rightarrow$ The linear dependence of the energy on the number of particles:

$$E_N = E + \frac{c}{N}$$



Main results.

The equation of state and quantum phase transition

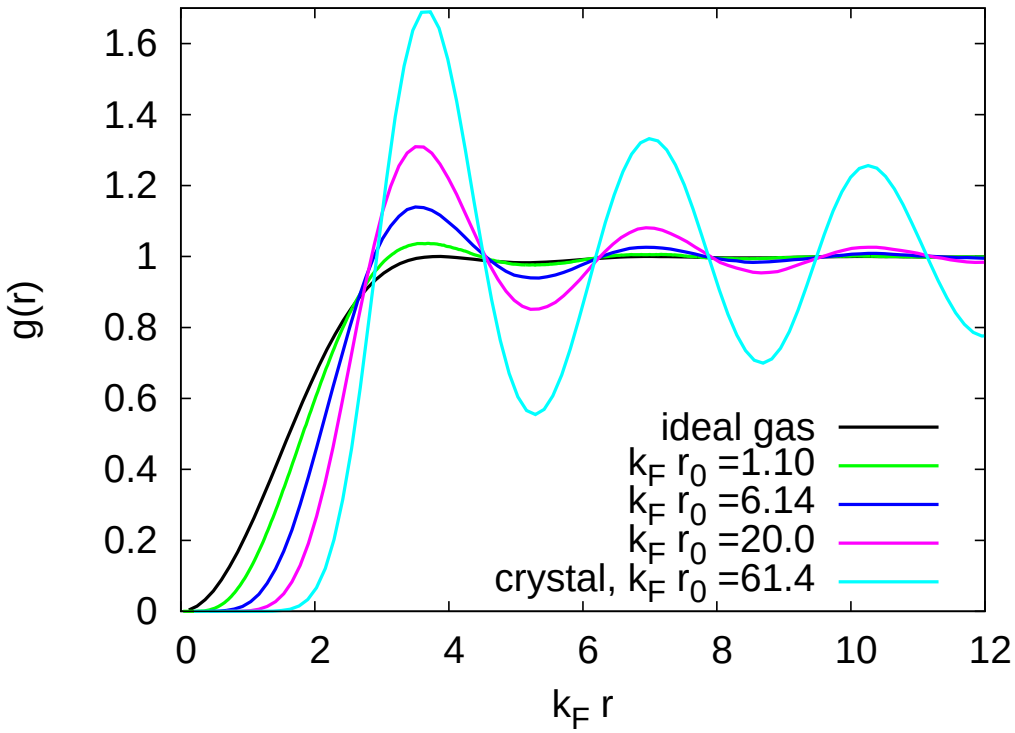


- $E_{HF} = \frac{\epsilon_F}{2}(1 + \frac{128}{45\pi} k_F r_0)$
- Red circles: E_{FL}
- Green triangles: E_{WC}
- Inset, blue circles: $E_{WC} - E_{FL}$
- Inset, black circles: $E_{ST} - E_{FL}$
- Red line: E_{pe}
- Purple solid line: E_{cl}

- At weak interaction we find good agreement with $E_{pe} = E_{HF} + (N\epsilon_F/8)(k_F r_0)^2 \log(1.43 k_F r_0)$ from Lu and Shlyapnikov (2012)
- At strong interaction the WC energy approaches the energy of a purely classical crystal (purple dashed line) corrected by the zero-point motion of phonons from C. Mora *et al* (2007): $E_{cl} = N\frac{\epsilon_F}{2}\frac{k_F r_0}{4}\left(1.597 + \frac{2.871}{\sqrt{k_F r_0}}\right)$.
- Quantum phase transition between FL and WC happens at $k_F r_0 = 25(3)$.
- The region of phase coexistence is very small $\delta k_F r_0 \approx 0.01$.
- The stripe phase is never energetically favorable.

Pair-distribution function

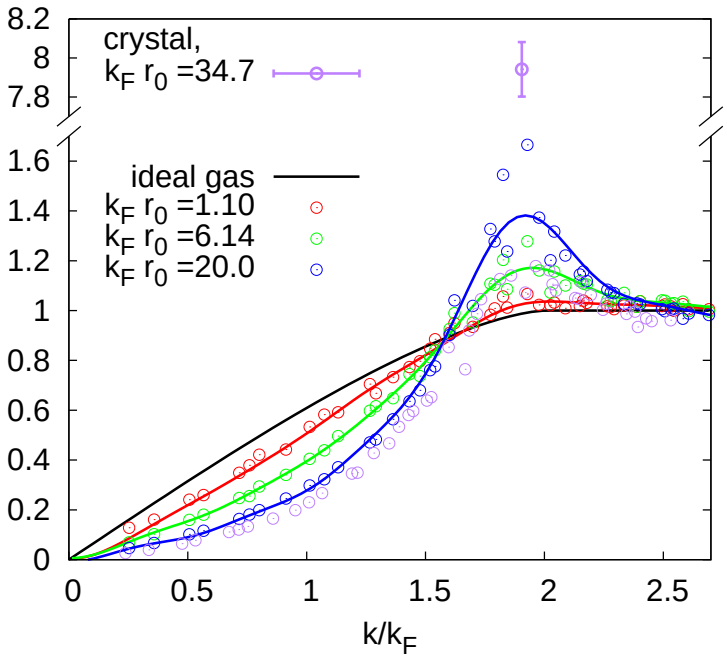
$$g(r) = \frac{1}{n^2}\langle \hat{\Psi}^+(\vec{s})\hat{\Psi}^+(\vec{s}+\vec{r})\hat{\Psi}(\vec{s}+\vec{r})\hat{\Psi}(\vec{s})\rangle$$



- The short-range repulsion increases by increasing the interaction strength.
- The shell structure starts to appear on approaching the freezing density.
- The existence of long-range ordering can be seen from the oscillating behaviour of $g(r)$ at large r.

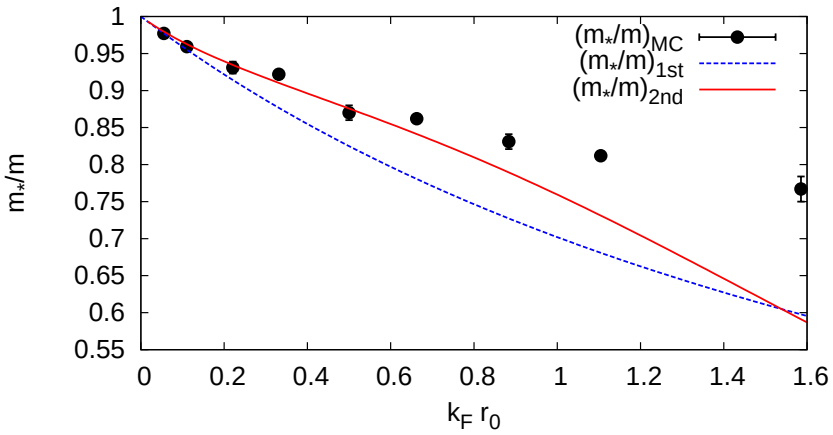
Static structure factor

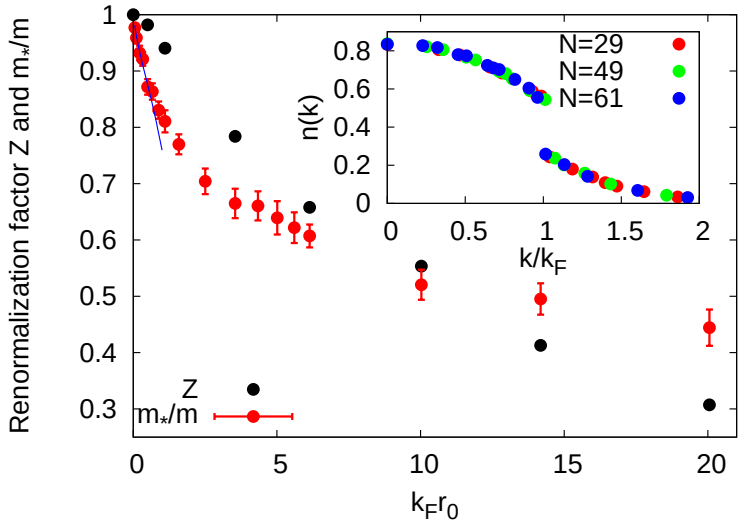
- $S(\mathbf{k}) = 1 + n \int d\mathbf{r} e^{i\mathbf{k}\cdot\mathbf{r}}[g(r) - 1]$
- $NS(\mathbf{k}) = \langle \rho_{\mathbf{k}} \rho_{-\mathbf{k}} \rangle = \langle \sum_{i,j} e^{i\mathbf{k}\cdot(\mathbf{r}_i - \mathbf{r}_j)} \rangle$



- The direct estimator exhibits a more pronounced peak compared to the smoother Fourier transform.
- This peak appears at the wave vector corresponding to the lowest non-zero reciprocal lattice vector of the triangular lattice.

Effective mass and renormalization factor





- Perturbatively calculated effective mass:
  Lu and Shlyapnikov, (2012)

$$(\frac{m_*}{m})_{pe} = 1/(1 + \frac{4}{3\pi} k_F r_0 + 0.25(k_F r_0)^2 \ln(0.65 k_F r_0)).$$

- Effective mass extracted from the fit of FNDMC energy:

$$E_N = E_{TL} + \frac{m}{m_*} \Delta T_N^{PBC} + \frac{a}{N}$$

- There is no dependence of momentum distribution on number of particles.

Main results

- The phase diagram of a 2D single-component homogeneous dipolar Fermi gas at $T = 0$ was investigated by means of FNDMC.
- The important characteristics of Fermi liquid such as the effective mass of quasiparticles and the renormalization factor were found.
- Quantum phase transition between Fermi liquid and Wigner crystal phase occurs at $k_F r_0 = 25(3)$.
- Stripe phase is never energetically favorable.

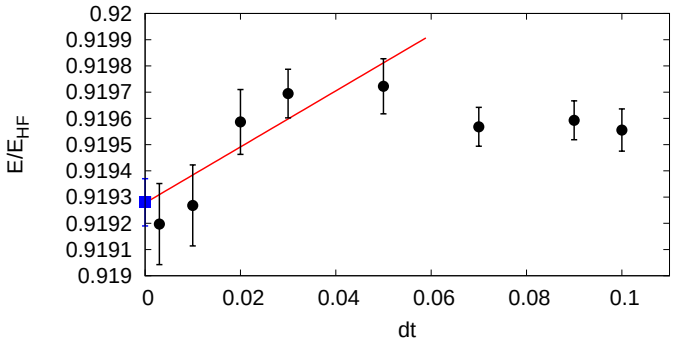
The extention of this work:
"The impurity problem in a bilayer system of dipoles", arXiv:1306.5588v1.

Thank you for your attention!.

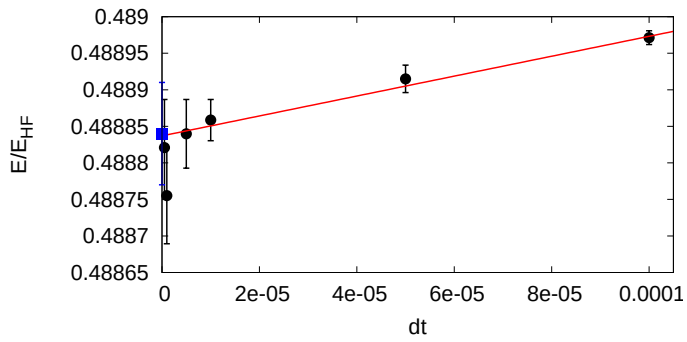
Recent review on QMC study of ultracold gases:
L. Pollet, Rep. Prog. Phys. **75**, 094501, 2012.

Optimization of DMC parameters: time step and number of walkers

Dependence of DMC energy on the time step dt.

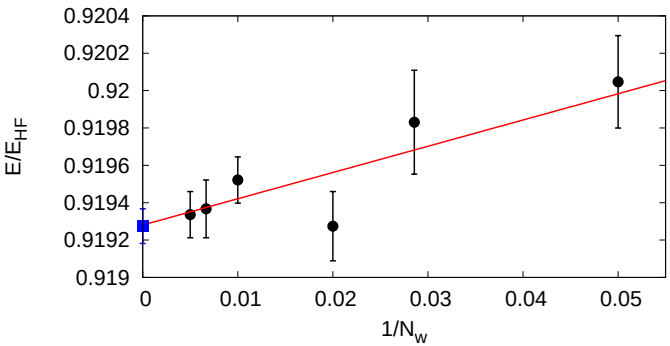


$k_F r_0 = 0.5$

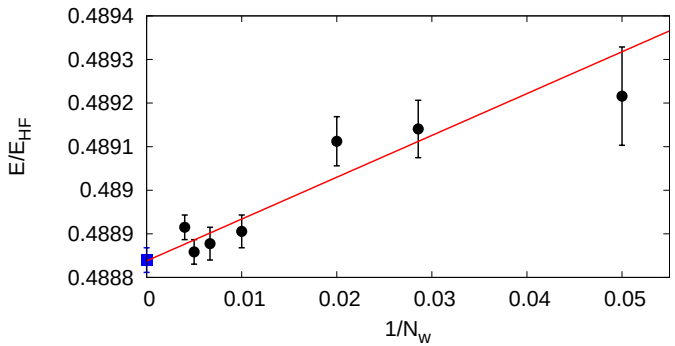


$k_F r_0 = 20$

Dependence of DMC energy on the number of walkers N_w.



$k_F r_0 = 0.5$

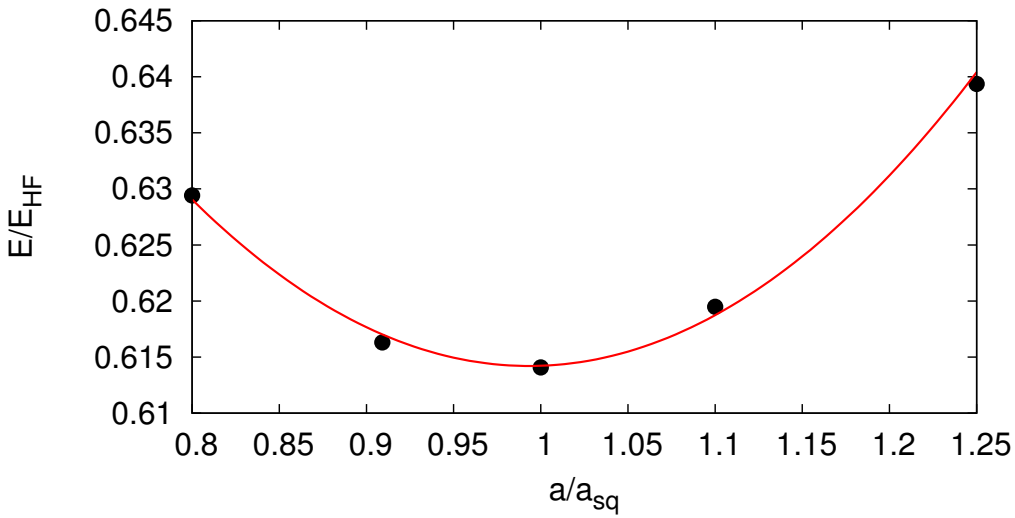


$k_F r_0 = 20$

Stripe phase: optimization of the stripe separation

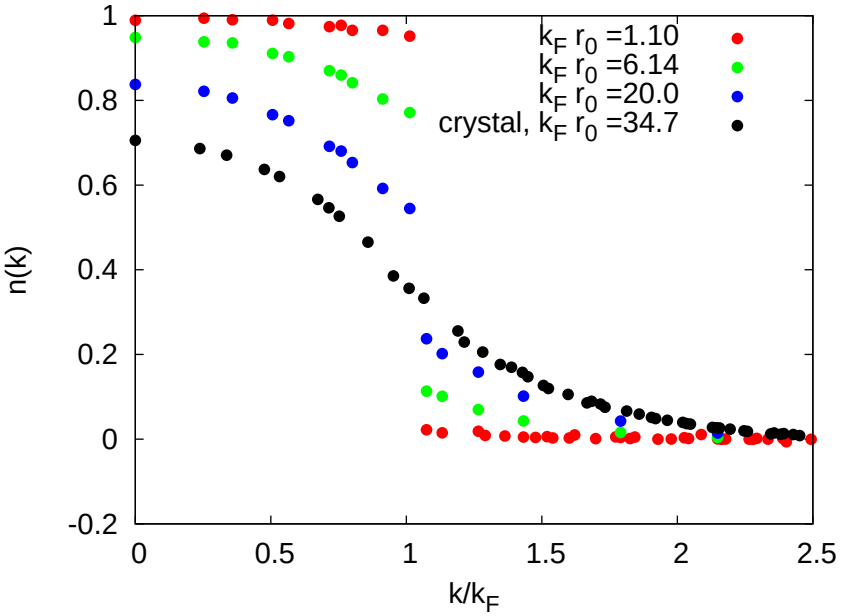
The distance between two stripes $a = |y_{m+1} - y_m|$

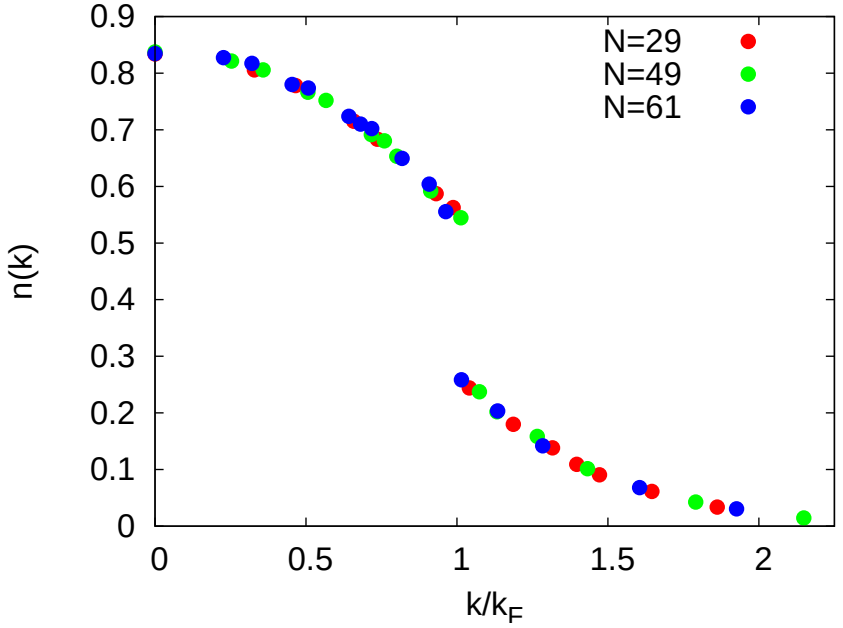
- The overall density in the simulation box with area $S = L_x \times L_y$ is fixed
- The distance a is changed when the ratio $\rho = L_x/L_y$ changes



$\rightarrow$ The optimal value is $a = a_{sq}$, where a_{sq} is the stripe separation for a square box.

Momentum distribution





- FL: the discontinuity of $n(k)$ at $k = k_F$ decreases with the increase of $k_F r_0$, but always stays finite
- WC: $n(k)$ does not have a discontinuity
- Momentum distribution does not depend on the system size