Two-dimensional fermionic mixtures with dipolar interactions

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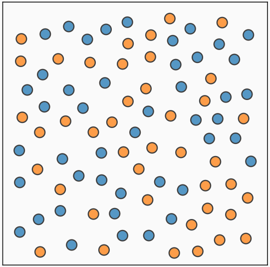
In a nutshell..



- Binary Fermi-Fermi mixture (non-relativistic, 2D, $T = 0$)
- Interatomic dipole-dipole repulsion.
- Fixed-Node Diffusion MC for small/large density regime.

Ultracold dipolar gases

Ultracold atoms

- Low temperature ($< 1\ \mu$K), low density (e.g. $n = 10^{20}\ \text{m}^{-3}$).
- Flexible platform for quantum many-body physics (geometry, interactions, statistics, ..).

Common case: Short-range interatomic interactions

- Interatomic-potential range $\ll$ typical distance.
- Zero-range approximation:

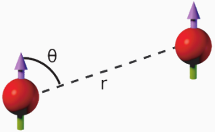
$$V(r) = \frac{4\pi\hbar^2 a_s}{m}\delta_{3\mathrm{D}}(\mathbf{r}).$$

[a_s: s-wave scattering length]

Dipole-dipole interactions

Atoms with permanent magnetic moment (Er, Dy, ..) or molecules with induced dipole moment (^{23}Na^{40}K, ^{40}K^{87}Rb, ..):

$$V(r,\theta) = \frac{\hbar^2 r_0}{m} \frac{1 - 3\cos\theta}{r^3},$$

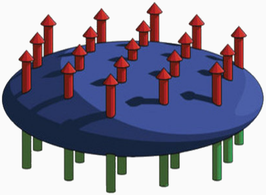


[uibk.ac.at/exphys/ultracold]

[$r_0 = 10 - 20$ nm (atoms), $r_0 \lesssim 600$ nm (molecules)]

2D confinement + z-aligned dipoles $\Rightarrow$ Repulsive interaction.

$$H = -\frac{1}{2}\sum_{i=1}^{N} \nabla_i^2 + r_0 \sum_{i<j} \frac{1}{r_{ij}^3}$$



[Kadau *et al.*, Nature, 2016]

Two-dimensional Fermi dipoles

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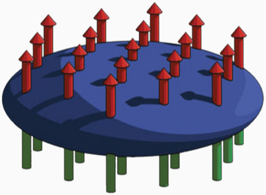

[Kadau *et al.*, Nature, 2016]

Binary mixture:

- Different species or hyperfine states (current study: $m_\uparrow = m_\downarrow$).
- Fixed polarization:

$$P = \frac{N_\uparrow - N_\downarrow}{N_\uparrow + N_\downarrow}.$$

Finding the ground state: Diffusion Monte Carlo

Fixed-Node Diffusion Monte Carlo

- Find ground state of Schrödinger equation through stochastic imaginary-time evolution.
- Systematic errors (under control):
  Finite walker population, finite imaginary-time step
- Fermions: Fixed-node (set nodal structure by hand).
  1. Variational (gives energy upper bound).
  2. Uncontrolled bias due to nodes.
     How large? Check several trial wave functions.

Trial wave functions - 1/2

1. Slater-Jastrow wave function (here for $P = 1$):

$$\Psi\left(\mathbf{r}_1, \ldots, \mathbf{r}_N\right) = e^{-U_{J2}} \times \det\left\{e^{-i\mathbf{k}_n \cdot \mathbf{r}_m}\right\},$$

$$U_{J2}\left(\mathbf{r}_1, \ldots, \mathbf{r}_N\right) = \sum_{m \neq n} f_{J2}\left(r_{nm}\right).$$

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2. Backflow correction:

$$\Psi(\mathbf{r}_1, \ldots, \mathbf{r}_N) = e^{-U_{J2}} \times \det\left\{e^{-i\mathbf{k}_n \cdot \mathbf{q}_m}\right\},$$

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Generalizations [*Holzmann et al., PRB 2006*]:

- Three-body Jastrow: $U_{J2} \to U_{J2} + U_{J3}$.
- Three-body backflow: $\mathbf{q}_m \to \mathbf{q}_m^{3BF}$.

Trial wave functions - 2/2

Iterative-backflow wave function:

$$\Psi^{(\alpha)} \to \Psi^{(\alpha+1)} = \det\left\{\exp\left(\mathbf{k}_i \cdot \mathbf{q}_j^{(\alpha+1)}\right)\right\}_{ij} \times e^{-U^{(\alpha+1)}}$$

$$\mathbf{q}_i^{(\alpha)} = \mathbf{r}_i + \sum_{\beta\leq\alpha}\left[\sum_{j\neq i}\left(\mathbf{q}_i^{(\beta-1)} - \mathbf{q}_j^{(\beta-1)}\right)\eta^{(\beta)}\left(q_{ij}^{(\beta-1)}\right)\right]$$

[*Taddei et al. PRB 2015*, *Ruggeri et al. PRL 2018*]

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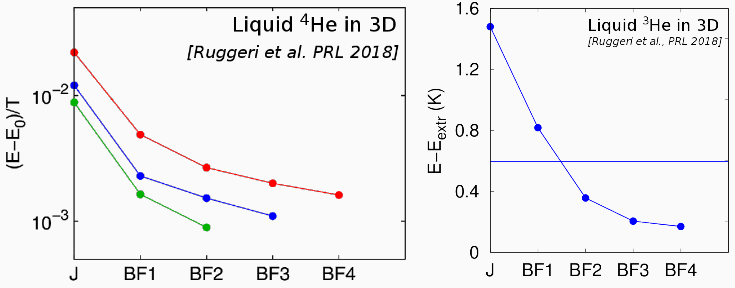

Dipolar fermions - Small density

Dilute dipolar fermions – Analytics

Analytic description of dilute regime ($nr_0^2 \ll 1$)?

- $P = 1$: Hartree-Fock theory (plane-wave orbitals).
- $P \neq 1$: Replace $V(r)$ with contact interaction + Mean Field.

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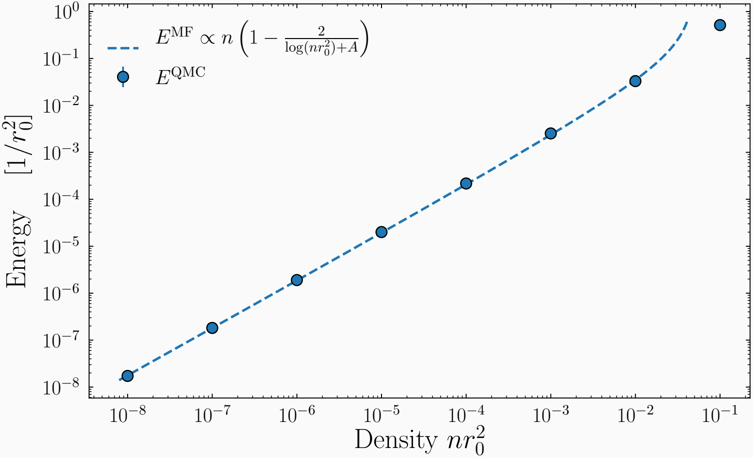
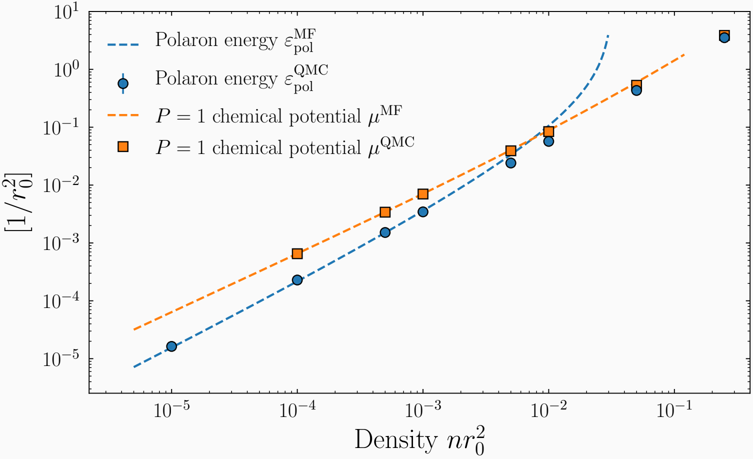
Examples of accessible observables:

- $E\left(N_\uparrow, N_\downarrow\right)$
- $\mu \equiv E(N+1, 0) - E(N, 0)$
- $\varepsilon_{\mathrm{pol}} \equiv E(N, 1) - E(N, 0)$

Equation of state for unpolarized state ($P = 0$)



μ vs $\varepsilon_{\rm pol}$



Small-density Fermi dipoles – Summary

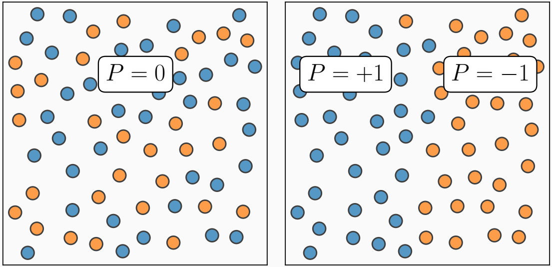
- Predictions for $P = 0$ equation of state
  (in progress: Beyond-mean-field corrections).
- Predictions for impurity observables (polaron energy, ...).
- Assumptions to relax for one-to-one comparison with experiments: $a_{\uparrow\downarrow} = 0$, pure 2D, $T = 0$.
- Small fixed-node bias, Slater-Jastrow is accurate enough.

Dipolar fermions - Large density

Itinerant ferromagnetism

Ground state with $P \neq 0$?

- Kinetic energy favors $P = 0$.
- Interactions favor $|P| = 1$ (less repulsion for aligned spins).



Homogeneous electron gas

- Old question (Bloch, 1929), recent solutions ($\geq$ 2002).
- Hartree-Fock: Stable ferromagnetic phase exists.
- QMC: Ferromagnetic phase exists only in 3D, not in 2D.

Itinerant ferromagnetism in other systems

Homogeneous electron gas

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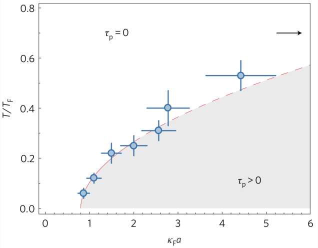
Short-ranged ultracold fermions



- Stoner model (zero range, 3D).
- Ground-state QMC at $k_F a \gtrsim 1$.
- Florence ^{6}Li experiment: Signature of $P = 1$ state.

[Valtolina *et al.*, Nat. Phys. 2017]

Itinerant ferromagnetism for dipoles? Part 1/3

Method #1: Compute $\Delta E \equiv E(P=0) - E(P=1)$.

Itinerant ferromagnetism for dipoles? Part 1/3

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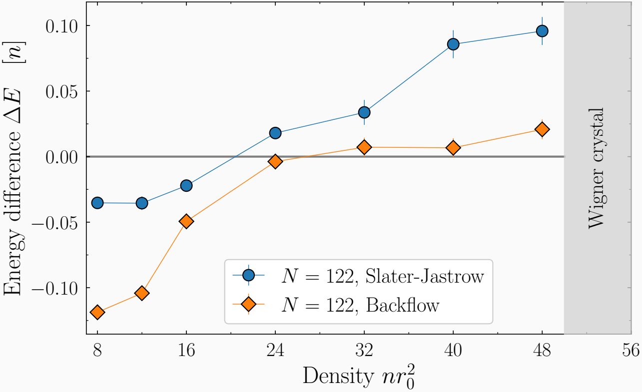
- Polarized ground state at large density (note: $\Delta E/E \lesssim 10^{-3}$).
- Clear dependence on nodal structure.



Itinerant ferromagnetism for dipoles? Part 2/3

Method #2: Is the fully-polarized state stable?

Compute spin-exchange energy gap.

Itinerant ferromagnetism for dipoles? Part 2/3

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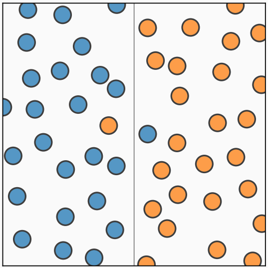
Compute spin-exchange energy gap.

Gap for spin exchange between polarized domains:

$$\Delta E^{\star} = 2\left(\varepsilon_{\mathrm{pol}} - \mu^{P=1}\right)$$

Spin exchange is energetically favorable if $\Delta E^{\star} < 0$.



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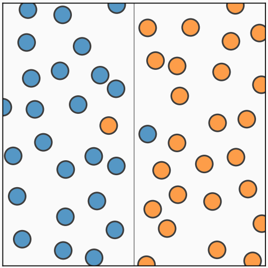


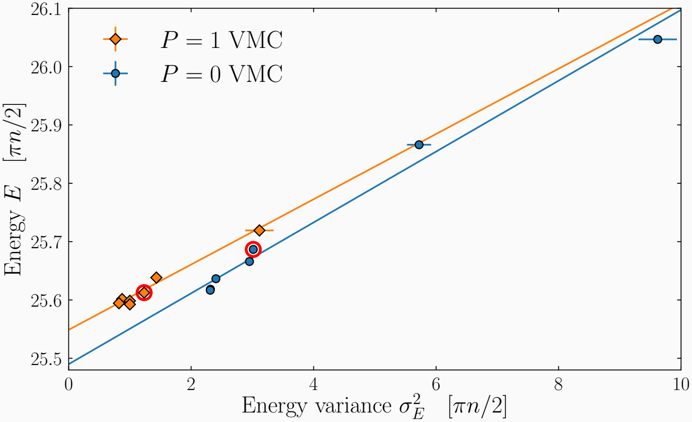
QMC result at large density: $\Delta E^{\star} \approx -n$

$\Rightarrow$ Fully polarized state is unstable.

Contradiction between methods #1 and #2!

Energy-variance extrapolation with better wave functions:

No itinerant ferromagnetism



[data by Markus Holzmann]

Itinerant ferromagnetism for dipoles? Part 3/3

Energy-variance extrapolation with better wave functions:

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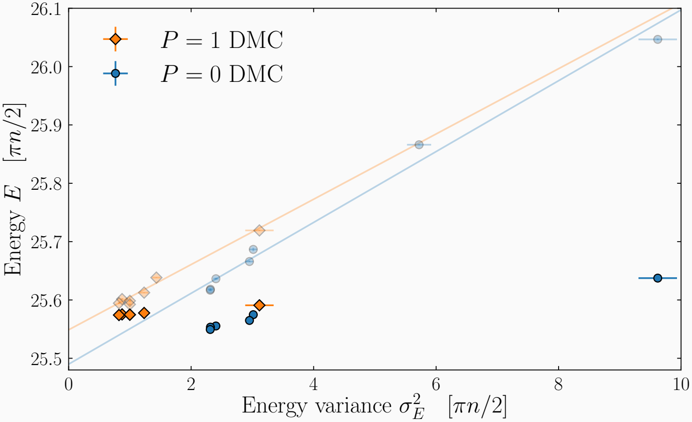

[data by Markus Holzmann]

Small-density Fermi dipoles – Itinerant ferromagnetism?

- No itinerant ferromagnetism in 2D dipoles.
- Fundamental question, far from current experiments.
- Open: Crossing point at larger density? Partial polarizations?

- Small energy differences $\rightarrow$ high-accuracy QMC needed.
- Fixed-node approximation to be treated with care (simple wave functions $\rightarrow$ wrong results).