Studying finite-size effects in spin-polarized Fermi gases

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M. Ku, JB, A. Schwenk, arXiv:0812.3430 JB, J. Polonyi, A. Schwenk, work in progress

Strongly-Interacting Fermions in Nature



Problem: Microscopic and macroscopic DoFs



How to tackle such strongly-interacting systems?



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Outline



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Unitary Regime

s-wave scattering length is tunable by Feshbach resonance (ext. magnetic field)
interaction strength is proportional to swave scattering length a



Unitary Regime

- •s-wave scattering length is tunable by Feshbach resonance
- interaction strength is proportional to swave scattering length a
- •limit of infinite scattering length a defines a universal regime:

$$0 \approx \frac{1}{|a|} \ll k_F \sim \frac{1}{r} \ll \frac{1}{R} \approx \infty$$

density (~Fermi momentum) is the only scale (unitarity limit)

•Universal properties:

 $E/N, T_c, \dots \propto \text{universal const}(s). \times E_F$

•Example: dilute neutron matter

 $|a_{\rm nn}| \sim 18.5 {\rm fm} \gg R \sim 1.4 {\rm fm}$



Symmetric Fermi Gases

•Experiment: Fermions in different hyperfine states

 provides an experimentally accessible environment for a study of quantum phenomena:

(a) BEC regime: tightly bound molecule $(a_s > 0)$

(b) Unitary regime: crossover delocalized molecule with $E_B = 0$ (c) BCS regime: delocalized Cooper pairs ($a_s < 0$)

•symmetric regime at T=0: smooth crossover, superfluidity persists



Symmetric Fermi Gases at finite T

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symmetric regime at finite T: phase

transition, "melting condensate"





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Asymmetric Fermi Gases

•Spin-polarized Fermi gases, e. g. $N_{\uparrow} > N_{\downarrow}$

Majority fermions N_{\uparrow} , minority fermions N_{\downarrow}

▶ Polarization $P = (N_{\uparrow} - N_{\downarrow})/(N_{\uparrow} + N_{\downarrow})$



•What happens when we have a population imbalance?

•Relevance for various research fields, e. g.: Clogston limit in superconductivity, nuclear physics, astrophysics, QCD at finite T(?), ...

•Experiments with spin-polarized Fermi gases are very useful to explore asymmetric strongly-interacting Fermi systems





Beyond one's own nose: Asymmetric systems in nature



•Nuclear physics:



Most nuclei N > Z (neutron skin)



•Astrophysics:

Neutron star (95% n, 5% p)



(SN 1987A from NASA image server)

Asymmetric spin-polarized systems: **MIT Experiment**

•Experimental setup: harmonic trap with cylindrical symmetry

- $\omega_x = \omega_y = \alpha \omega, \omega_z = \omega; \alpha \sim 5$ $N_{\text{tot}} = N_{\uparrow} + N_{\perp} \sim 10^6 \dots 10^7$
- •Phase separation:
 - ▶Equal density core
 - Partially-polarized shell: diff. densities
 - Outer region of *normal* majority atoms
- •Critical polarization above which equal density core ceases to exist:

$$P_c = 0.70(3)$$









Asymmetric spin-polarized systems: **Rice Experiment**

- •Experimental setup: harmonic trap with cylindrical symmetry
 - $\omega_x = \omega_y = \alpha \omega, \omega_z = \omega; \alpha \sim 35 45$ $N_{\text{tot}} = N_{\uparrow} + N_{\downarrow} \lesssim 10^5$

• Phase separation:

▶ superfluid core

very narrow (almost no) partially polarized region

► Outer region of *normal* majority atoms

•Critical polarization: $P_c > 0.9$



Summary of experimental differences

	MIT	Rice university
$N_{ m tot}$	$10^{6} \dots 10^{7}$	$\lesssim 10^5$
asymmetry $lpha$	~5	3545
partially-polarized shell	clearly visible	extremely thin
critical polarization P_c	0.70(3)	> 0.9

Equation of state (uniform system)

- •single particle energy E_{\downarrow} : energy gain of one single minority fermion interacting resonantly with a majority Fermi sea
- •systems with **large asymmetry**: leading contribution to EoS due to interactions, $E=E_{\uparrow}^{\rm FS}+E_{\downarrow}$



Single particle energy (uniform system)

• Hamiltonian: (Chevy '06)

$$H = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} a_{\mathbf{k},\sigma}^{\dagger} a_{\mathbf{k},\sigma} + \frac{g}{V} \sum_{\mathbf{k},\mathbf{k}',q} a_{\mathbf{k}+\mathbf{q},\uparrow}^{\dagger} a_{\mathbf{k}'-\mathbf{q},\downarrow} a_{\mathbf{k}',\downarrow}^{\dagger} a_{\mathbf{k},\uparrow}$$

•variational ansatz (include 1p1h excitations):





Single particle energy (uniform system)

•gap equation: (Chevy '06)

$$E_{\downarrow} = \frac{1}{V} \sum_{|\mathbf{q}| < k_F} \frac{1}{\frac{1}{g} + \frac{1}{V} \sum_{|\mathbf{k}| > k_F} \frac{1}{\epsilon_{\mathbf{k}} + \epsilon_{\mathbf{q}-\mathbf{k}} - \epsilon_{\mathbf{q}} - E_{\downarrow}}}$$
$$= \int_{\Gamma} \int_{$$



•at unitarity:

$$\bullet \eta = E_{\downarrow}/E_F \approx -0.607$$

▶ agrees well with MC studies (see e.g. Lobo et al. '06)

▶ 2p2h contributions shown to be small (Combescot & Giraud '08)

Phase diagram of an imbalanced system of spinpolarized atoms at unitarity (*uniform system*)

- •consider a system of spin-up and spin-down fermion at unitarity with $N_{\uparrow}>N_{\downarrow}$
- •phase diagram at T=0



Trapped system of imbalanced spin-polarized atoms at unitarity (T=0)

•energy density functional $(N_{\uparrow} \gg N_{\downarrow})$ in LDA: (see e.g. Recati et al. '08)

$$\begin{split} \Gamma[n_{S}, n_{\uparrow}, n_{\downarrow}] &= 2 \int_{|\mathbf{r}| < R_{S}} d\mathbf{r} \Big\{ \xi_{S} \frac{3}{5} \frac{(6\pi^{2} n_{S}(\mathbf{r}))^{\frac{2}{3}}}{2m} + V(\mathbf{r}) - \mu_{S} \Big\} n_{S}(\mathbf{r}) \\ &+ \int_{R_{S} < |\mathbf{r}| < R_{\uparrow}} d\mathbf{r} \Big\{ \frac{3}{5} \frac{(6\pi^{2} n_{\uparrow})^{\frac{2}{3}}}{2m} \left(1 - \frac{5}{3} \eta \left(\frac{n_{\downarrow}}{n_{\uparrow}} \right) + \frac{m}{m^{*}} \left(\frac{n_{\downarrow}}{n_{\uparrow}} \right)^{\frac{5}{3}} + B \left(\frac{n_{\downarrow}}{n_{\uparrow}} \right)^{2} \right) n_{\uparrow}(\mathbf{r}) \\ &+ V(\mathbf{r})(n_{\downarrow}(\mathbf{r}) + n_{\uparrow}(\mathbf{r})) - \mu_{\uparrow} n_{\uparrow}(\mathbf{r}) - \mu_{\downarrow} n_{\downarrow}(\mathbf{r}) \Big\} \\ \bullet \text{ground state:} \quad \frac{\delta \Gamma}{\delta n_{S}} = \frac{\delta \Gamma}{\delta n_{\uparrow}} = \frac{\delta \Gamma}{\delta n_{\downarrow}} = 0 \,, \quad \frac{\delta \Gamma}{\delta R_{S}} = 0 \,, \quad (\mu_{\uparrow} + \mu_{\downarrow}) = 2\mu_{S} \end{split}$$

•what we know from the *continuum*:

Superfluid phase: $\epsilon_S = \xi_S \frac{(6\pi^2 n_S)^{\frac{2}{3}}}{2m}$

energy gained when a spin-down fermion is added to a Fermi sea of spin-up fermions: E

$$E_{\downarrow} = \eta \frac{(6\pi^2 n_{\uparrow})^{\frac{2}{3}}}{2m}$$

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Trap effects & single particle energy

Ku, JB, Schwenk '08

•revisited: energy gain of a (trapped) Fermi sea of spin-up fermions when a spin-down fermion is added; Hamiltonian:

$$H = \sum_{\mathbf{n},\sigma} \varepsilon_{\mathbf{n}} a_{\mathbf{n},\sigma}^{\dagger} a_{\mathbf{n},\sigma} + \sum_{\mathbf{n}_{\uparrow},\mathbf{n}_{\downarrow},\mathbf{n}_{\uparrow}^{\prime},\mathbf{n}_{\downarrow}^{\prime}} \langle \mathbf{n}_{\uparrow}^{\prime}, \mathbf{n}_{\downarrow}^{\prime} | V | \mathbf{n}_{\uparrow}, \mathbf{n}_{\downarrow} \rangle a_{\mathbf{n}_{\uparrow}^{\prime},\uparrow}^{\dagger} a_{\mathbf{n}_{\downarrow}^{\prime},\downarrow}^{\dagger} a_{\mathbf{n}_{\downarrow},\downarrow} a_{\mathbf{n}_{\uparrow},\uparrow}$$

•variational ansatz (include 1p1h excitations):



Ku, JB, Schwenk '08

•self-consistent equation for energy gain:

•choose:
$$E_{\downarrow} - \varepsilon_{\mathbf{0}} = \sum_{\varepsilon_{\mathbf{h}} \leqslant \varepsilon_{F}} \sum_{\mathbf{S}, \mathbf{L}} F(\mathbf{0}, \mathbf{h}, \mathbf{S}) \left[M^{-1}(\varepsilon_{F}, E_{\downarrow} + \varepsilon_{\mathbf{h}}) \right]_{\mathbf{S}, \mathbf{L}} F(\mathbf{0}, \mathbf{h}, \mathbf{L}) ,$$

$$E_{\downarrow} = \eta(\alpha, N) E_{F}(\alpha, N) \quad \text{with} \quad E_{F}(\alpha, N) = \frac{(6\pi^{2}n_{\uparrow}(0))^{\frac{2}{3}}}{2m} \xrightarrow{N \gg 1} \omega (48N)^{\frac{1}{3}}$$

•results for the isotropic trap:

Trap effects & single particle energy

Ku, JB, Schwenk '08

- •Clear finite-size and confinement effects
- •fixed α , we find that the energy ...
 - ... decreases with $N_{\rm tot}$
 - ... stronger dependence on $N_{\rm tot}$ for larger α
 - ... saturates to -0.61 for large N_{tot}
- •fixed $N_{\rm tot}$, we find that the energy ...
 - ... inreases with lpha

Ku, JB, Schwenk '08

•How does the critical polarization P_c depend on the trap configuration? •energy density functional ($N_{\uparrow} \gg N_{\downarrow}$) in LDA:

$$\begin{split} \Gamma[n_{S}, n_{\uparrow}, n_{\downarrow}] &= 2 \int_{|\mathbf{r}| < R_{S}} d\mathbf{r} \Big\{ \xi_{\mathrm{S}} \frac{3}{5} \frac{(6\pi^{2} n_{\mathrm{S}}(\mathbf{r}))^{\frac{2}{3}}}{2m} + V(\mathbf{r}) - \mu_{S} \Big\} n_{\mathrm{S}}(\mathbf{r}) \\ &+ \int_{R_{S} < |\mathbf{r}| < R_{\uparrow}} d\mathbf{r} \Big\{ \frac{3}{5} \frac{(6\pi^{2} n_{\uparrow})^{\frac{2}{3}}}{2m} \left(1 - \frac{5}{3} \eta \left(\frac{n_{\downarrow}}{n_{\uparrow}} \right) + \frac{m}{m^{*}} \left(\frac{n_{\downarrow}}{n_{\uparrow}} \right)^{5/3} + B \left(\frac{n_{\downarrow}}{n_{\uparrow}} \right)^{2} \right) n_{\uparrow}(\mathbf{r}) \\ &+ V(\mathbf{r})(n_{\downarrow}(\mathbf{r}) + n_{\uparrow}(\mathbf{r})) - \mu_{\uparrow} n_{\uparrow}(\mathbf{r}) - \mu_{\downarrow} n_{\downarrow}(\mathbf{r}) \Big\} \\ \bullet \text{ground state:} \quad \frac{\delta\Gamma}{\delta n_{S}} = \frac{\delta\Gamma}{\delta n_{\uparrow}} = \frac{\delta\Gamma}{\delta n_{\downarrow}} = 0 \,, \quad \frac{\delta\Gamma}{\delta R_{S}} = 0 \,, \quad (\mu_{\uparrow} + \mu_{\downarrow}) = 2\mu_{S} \\ \bullet \text{for simplicity, calculations are done for} \end{split}$$

(I) MC values: $\frac{m^*}{m} = 1.09, B = 0.14$ and $\xi_S \approx 0.4$ (see Pilati & Giorgini '08, Carlson '03) (II) $\frac{m^*}{m} = 1, B = 0$

Ku, JB, Schwenk '08

• How does the critical polarization P_c depend on the trap configuration?

clear indications for strong trap dependence which helps to understand the different findings at MIT and Rice U.
 however, our calculations need still to be improved: dependence of effective mass on trap, terms beyond LDA, ...

Outline

Ground-state properties of strongly-interacting many-body problems

Trapped Fermions

Nuclear Landscape

ground-state properties for heavy nuclei from microscopic interactions?

How to study ground-state properties from first principles?

•MC simulations?

How to study ground-state properties from first principles?

- MC simulations
 - ▶ "volume" problem:

▶ "construct" nucleus out of quarks: computationally (almost) impossible

restricted to small nuclei (A<8?) (Savage '06)

• Hamiltonian approaches, such as coupled-cluster theory?

How to study ground-state properties from first principles?

- •MC simulations
 - ▶ "volume" problem:

"construct" nucleus out of quarks: computationally (almost) impossible

restricted to small nuclei (A<8?) (Savage '06)

- Hamiltonian approaches, such as coupled-cluster theory:
 - Frewrite ground-state wave-function: $|\psi\rangle = e^{(T_1+T_2+...)}|\phi\rangle$

allows to include systematically n-particle-nhole excitations of a given (reference) state

▶ still computationally expensive

▶ sets benchmarks for closed-shell medium-mass nuclei (Hagen et al. '07)

• Density Functional Theory?

•Density Functional: $\Gamma[\rho] = \ln \int \mathcal{D}\psi^{\dagger} \mathcal{D}\psi e^{-S[\psi^{\dagger},\psi] + \int \frac{\delta\Gamma}{\delta\rho} \cdot (\psi^{\dagger}\psi)}$

with
$$S[\psi^{\dagger},\psi] = \int \psi^{\dagger} \Big[\partial_t - \frac{1}{2m}\Delta\Big]\psi + \frac{1}{2}\int \psi^{\dagger}\psi V_{2b}\psi^{\dagger}\psi + \mathcal{O}(V_{3b})$$

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•Density Functional: $\Gamma_{\lambda}[\rho] = \ln \int \mathcal{D}\psi^{\dagger} \mathcal{D}\psi e^{-S_{\lambda}[\psi^{\dagger},\psi] + \int \frac{\delta\Gamma_{\lambda}}{\delta\rho} \cdot (\psi^{\dagger}\psi)}$

with
$$S_{\lambda}[\psi^{\dagger},\psi] = \int \psi^{\dagger} \Big[\partial_t - \frac{1}{2m}\Delta + (1-\lambda)U_{\lambda}\Big]\psi + \frac{1}{2}\int \psi^{\dagger}\psi\lambda V_{2b}\psi^{\dagger}\psi + \lambda \mathcal{O}(V_{3b})$$

external potential, e.g. trap potential

• DFT-RG flow:

(JB, Schwenk, Polonyi, in prep.)

density basis expansion scales favorably to heavy nuclei

 allows for a calculation of ground-state (g.s.) properties from microscopic interactions

• Currently: application to trapped systems of ultracold fermions in 1+1d, compare to Green's Function MC (Casula, Ceperley, Mueller '08)

•For Nuclei: validate results for medium-mass nuclei against coupled-cluster calculations

Conclusions

- energy gain in N+1 body problem depends on trap geometry and total particle number
- sensible finite-size and confinement effects in experiments with imbalanced systems of trapped spin-polarized ultracold atoms, contributes to understand experimental discrepancies, e.g. critical polarization
- **Density Functional Theory + FRG**: promising tool for first-principle description of many-body systems, e. g. cold atoms in traps or nuclei

Outlook

- go beyond the N+1-body problem: N+M-body problem (Ku, JB, Schwenk)
- **cold atoms**: trap effects on the finite-T phase diagram?
- computation of full energy density functional with MC?! (with M. M. Forbes)
- **DFT-RG**: large(r) 1+1d systems and comparison to GFMC

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Appendix I

Strongly-interacting Fermi gas in a harmonic-oscillator trap:

$$H = \sum_{\mathbf{n},\sigma} \varepsilon_{\mathbf{n}} \, a_{\mathbf{n},\sigma}^{\dagger} \, a_{\mathbf{n},\sigma} + \sum_{\mathbf{n}_{\uparrow},\mathbf{n}_{\downarrow},\mathbf{n}_{\uparrow}^{\prime},\mathbf{n}_{\downarrow}^{\prime}} \langle \mathbf{n}_{\uparrow}^{\prime}, \mathbf{n}_{\downarrow}^{\prime} | V | \mathbf{n}_{\uparrow}, \mathbf{n}_{\downarrow} \rangle \, a_{\mathbf{n}_{\uparrow}^{\prime},\uparrow}^{\dagger} \, a_{\mathbf{n}_{\downarrow}^{\prime},\downarrow}^{\dagger} \, a_{\mathbf{n}_{\downarrow},\downarrow}^{\dagger} \, a_{\mathbf{n}_{\uparrow},\uparrow}^{\dagger} \, a_{\mathbf{n}_{\downarrow},\downarrow}^{\dagger} \, a_{\mathbf{n}_{\uparrow},\uparrow}^{\dagger} \, a_{\mathbf{n}_{\downarrow},\downarrow}^{\dagger} \, a_{\mathbf{n}_{\downarrow},\downarrow}^{\dagger} \, a_{\mathbf{n}_{\uparrow},\uparrow}^{\dagger} \, a_{\mathbf{n}_{\downarrow},\downarrow}^{\dagger} \, a_{\mathbf{n}_{\downarrow},\downarrow}^{\dagger} \, a_{\mathbf{n}_{\uparrow},\uparrow}^{\dagger} \, a_{\mathbf{n}_{\downarrow},\downarrow}^{\dagger} \, a_{\mathbf{$$

- Contact interaction with separable cutoff in momentum space: $\langle \mathbf{p}|V|\mathbf{p}'\rangle = C(\Lambda) e^{-(p^2+p'^2)/\Lambda^2}$ where $C(\Lambda) = \frac{4\pi/m}{\frac{1}{a_s} - \frac{\Lambda}{\sqrt{2\pi}}}$
- Interaction matrix elements: can be expressed as a sum over separable functions (S: center of mass quantum numbers.)

$$\langle \mathbf{n}_1, \mathbf{n}_2 | V | \mathbf{n}_3, \mathbf{n}_4 \rangle = C(\Lambda) \sum_{\mathbf{S}} F(\mathbf{n}_1, \mathbf{n}_2, \mathbf{S}) F(\mathbf{n}_3, \mathbf{n}_4, \mathbf{S})$$

Appendix II

• Strongly-interacting Fermi gas in a harmonic-oscillator trap:

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Appendix III

• Self-consistent equation for E in anistropic traps

$$\begin{split} E - \varepsilon_{\mathbf{0}} &= \sum_{\varepsilon_{\mathbf{h}} \leqslant \varepsilon_{\mathbf{F}}} \sum_{\mathbf{S}, \mathbf{L}} F(\mathbf{0}, \mathbf{h}, \mathbf{S}) \left[M^{-1}(\varepsilon_{\mathbf{F}}, E + \varepsilon_{\mathbf{h}}) \right]_{\mathbf{S}, \mathbf{L}} F(\mathbf{0}, \mathbf{h}, \mathbf{L}) \\ \\ \text{Matrix } M: \quad M(\varepsilon_{\mathbf{F}}, E + \varepsilon_{\mathbf{h}})_{\mathbf{S}, \mathbf{L}} = \left[\frac{1}{C(\Lambda)} - D(\alpha, \Delta \widetilde{E}) \right] \delta_{\mathbf{S}, \mathbf{L}} \\ &+ \sum_{\varepsilon_{\mathbf{p}} \leqslant \varepsilon_{\mathbf{F}}} \sum_{\mathbf{m}} \frac{F(\mathbf{m}, \mathbf{p}, \mathbf{S}) F(\mathbf{m}, \mathbf{p}, \mathbf{L})}{E + \varepsilon_{\mathbf{h}} - (\varepsilon_{\mathbf{p}} + \varepsilon_{\mathbf{m}})} \end{split}$$

Where $\Delta \widetilde{E} = \alpha (S_x + S_y + 2) + S_z + 1 - (E + \varepsilon_h)/\omega$

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General α : *D* has series expression

• Divergent part cancels with the cutoff term in $1/C(\Lambda)$