Tackling the Sign Problem of Ultracold Fermi Gases with Mass-Imbalance

Dietrich Roscher

[D. Roscher, J. Braun, J.-W. Chen, J.E. Drut arXiv:1306.0798]

Advances in quantum Monte Carlo techniques for non-relativistic many-body systems

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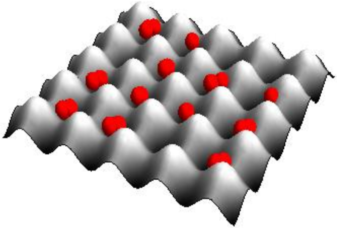
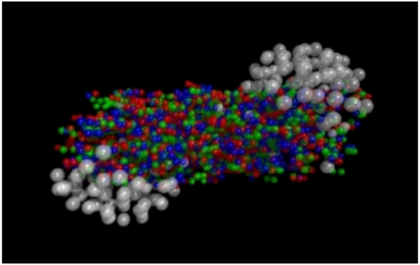
Physics and Versatility of Ultracold Fermi Gases

Why we should care about physics of cold gases:

- “Simple” systems compared to e.g. QCD or nuclear physics, but similar behaviour in certain regimes (e.g. HIC) [e.g. A. Adams *et al.* '12]





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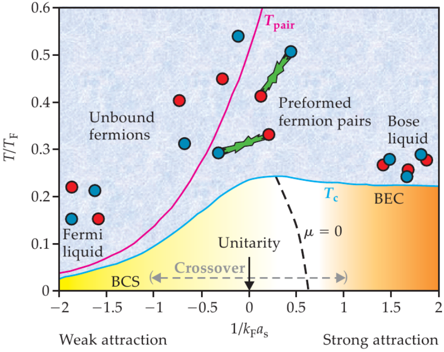

[C.A.R Sa de Melo, '08]

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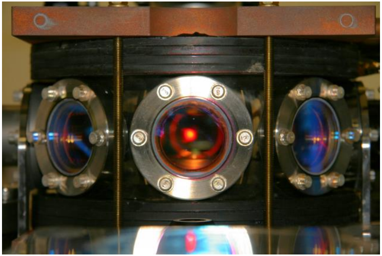
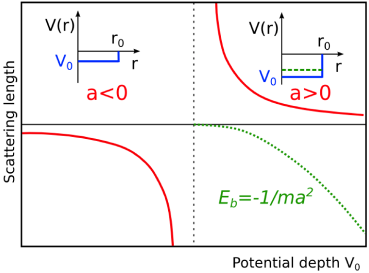


S. Jochim, Uni Heidelberg



[M. Randeria, E. Taylor '08]

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Why "simple" does not mean "easy":

- Lack of small parameter in strongly interacting regimes invalidates naïve perturbation theory
- Monte Carlo calculations often severely hampered by sign problems

Idea of the Talk

How to get rid of (some) sign problems:

- Identify problematic quantity x_s and change into $i \cdot x_s$
- Do an *Auxiliary Field Quantum Monte Carlo* calculation without sign problem
- Analytically continue results from $i \cdot x_s$ to physical value x_s

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This idea has been proposed for lattice QCD at finite chemical potential some time ago. [M. Alford, A.Kapustin, F.Wilczek '98; P. de Forcrand, O. Philipsen '02]
Adapting this approach to imbalanced ultracold Fermi gases will be the main subject of this talk.

Describing the Unitary Fermi Gas

Action of a two component 3D Fermi gas with contact interaction:

$$S[\psi_\uparrow, \psi_\downarrow] = \int_0^\beta \mathrm{d}\tau \int \mathrm{d}^3x \left\{ \sum_{\sigma=\uparrow,\downarrow} \psi_\sigma^* \left(\partial_\tau - \frac{\nabla^2}{2m} - \mu \right) \psi_\sigma + \bar{g} \psi_\uparrow^* \psi_\downarrow^* \psi_\downarrow \psi_\uparrow \right\}$$

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The bare coupling $\bar{g}$ is given by

$$\bar{g}^{-1} = \Lambda g^{-1} = \frac{1}{8\pi} \left(a_s^{-1} - c_{\mathrm{reg}} \Lambda \right)$$

with UV-cutoff Λ and two-body scattering length a_s.

Unitary regime: $a_S^{-1} \to 0$

Symmetry and Spontaneous Symmetry Breaking

$$S[\psi_\uparrow, \psi_\downarrow] = \int_0^\beta \mathrm{d}\tau \int \mathrm{d}^3x \left\{ \sum_{\sigma=\uparrow,\downarrow} \psi_\sigma^* \left(\partial_\tau - \frac{\nabla^2}{2m} - \mu \right) \psi_\sigma + \bar{g} \psi_\uparrow^* \psi_\downarrow^* \psi_\downarrow \psi_\uparrow \right\}$$

$U(1)$-Symmetry of the action:

$$\psi_{\uparrow,\downarrow} \longrightarrow e^{i\alpha} \psi_{\uparrow,\downarrow}; \qquad \psi_{\uparrow,\downarrow}^* \longrightarrow \psi_{\uparrow,\downarrow}^* e^{-i\alpha}$$

Spontaneously broken if $\langle \psi_\downarrow \psi_\uparrow \rangle \neq 0$

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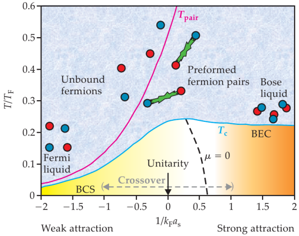
$\Rightarrow$ Condensation of bound states



[C.A.R Sa de Melo, '08]

Partition Function and Observables

Partition function and observables from the path integral:

$$\mathcal{Z} = \int \mathcal{D}\psi_\uparrow \mathcal{D}\psi_\downarrow e^{-S[\psi_\uparrow,\psi_\downarrow]} \quad \Rightarrow \quad \langle \hat{\mathcal{O}} \rangle = \frac{1}{\mathcal{Z}} \int \mathcal{D}\psi_\uparrow \mathcal{D}\psi_\downarrow \mathcal{O} e^{-S[\psi_\uparrow,\psi_\downarrow]}$$

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Hubbard-Stratonovich transformation and integration of fermion fields:

$$1 = \mathcal{N} \int \mathcal{D}\varphi \mathcal{D}\varphi^* e^{-\int d\tau \int d^3x \; m_\varphi^2 \varphi\varphi^*}, \qquad \varphi \longrightarrow \varphi - \frac{g_\varphi}{m_\varphi^2}\psi_\uparrow\psi_\downarrow$$

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$$\mathcal{Z} = \int \mathcal{D}\varphi \mathcal{D}\varphi^* \det\left[\hat{\mathcal{G}}^{-1} + \hat{\Phi}\right] e^{-\int d\tau \int d^3x \; m_\varphi^2 \varphi\varphi^*}$$

$$\hat{\mathcal{G}}^{-1} = \begin{pmatrix} -i\omega_n - \frac{\nabla^2}{2m} - \mu & 0 \\ 0 & i\omega_n - \frac{\nabla^2}{2m} - \mu \end{pmatrix}, \qquad \hat{\Phi} = \begin{pmatrix} 0 & g_\varphi \varphi \\ -g_\varphi \varphi^* & 0 \end{pmatrix}$$

$\Rightarrow$ Starting point for actual computations $\Leftarrow$

Positivity of the Fermion Determinant

$$\mathcal{Z} = \int \mathcal{D}\varphi \mathcal{D}\varphi^* \det\left[\hat{\mathcal{G}}^{-1} + \hat{\Phi}\right] e^{-\int d\tau \int d^3x \; m_\varphi^2 \varphi\varphi^*}$$

If the fermion determinant is positive for all admissible $\varphi(x)$, a positive definite probability measure can be defined for Monte Carlo calculations - there is no sign problem.

$$\det \hat{\mathcal{G}}^{-1} \sim \det \begin{Bmatrix} \hat{A} & 0 \\ 0 & \hat{A}^* \end{Bmatrix} = \det \left[\hat{A}\hat{A}^*\right] \geq 0$$

Since the interaction does not break the symmetry between $\uparrow$ and $\downarrow$ fermions, the symmetry of the eigenvalue distribution is conserved for finite φ.

Thus, the fermion determinant is positive for all $\varphi(x)$.

Introducing Imbalance

$$S[\psi_\uparrow, \psi_\downarrow] = \int_0^\beta \mathrm{d}\tau \int \mathrm{d}^3x \left\{ \sum_{\sigma=\uparrow,\downarrow} \psi_\sigma^* \left(\partial_\tau - \frac{\nabla^2}{2m_\sigma} - \mu_\sigma \right) \psi_\sigma + \bar{g} \psi_\uparrow^* \psi_\downarrow^* \psi_\downarrow \psi_\uparrow \right\}$$

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Experimental relevance:

- Population imbalance (μ_σ): Tuning of the species relative population via a magnetic field h [e.g. Zwierlein *et al.* '06, Partidge *et al.* '06]
- Mass imbalance (m_σ): Mixtures of different elements, e.g. ^6Li and ^{40}K [e.g. A. Gezerlis, S. Gandolfi, K.E. Schmidt, J. Carlson '09 ;K.B. Gubbels, J.E. Baarsma, H.T.C. Stoof '09]

BUT

Introducing Imbalance

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Population- and/or mass-imbalance destroy the symmetry between $\uparrow$ and $\downarrow$ particles and thus also the positivity of the fermion determinant:

$$\hat{\mathcal{G}}^{-1} = \begin{pmatrix} -i\omega_n - \frac{\nabla^2}{m_+} - \frac{\nabla^2}{m_-} - \bar{\mu} - h & 0 \\ 0 & i\omega_n - \frac{\nabla^2}{m_+} + \frac{\nabla^2}{m_-} - \bar{\mu} + h \end{pmatrix}$$

with

$$\bar{\mu} = \frac{\mu_\uparrow + \mu_\downarrow}{2}, \qquad h = \frac{\mu_\uparrow - \mu_\downarrow}{2}$$

$$m_+ = \frac{4 m_\uparrow m_\downarrow}{m_\downarrow + m_\uparrow}, \qquad m_- = \frac{4 m_\uparrow m_\downarrow}{m_\downarrow - m_\uparrow}$$

Sign Problem!

The Sign Problem and Imaginary Imbalance

The sign problem could be resolved, if the $\uparrow - \downarrow$ symmetry was reinstated. Define complex-valued particle masses $m_\sigma^{\mathbb{C}}$ and chemical potentials $\mu_\sigma^{\mathbb{C}}$ such that:

$$h = ih_I, \quad h_I \in \mathbb{R}, \qquad \bar{m} \equiv \frac{m_+^{\mathbb{C}}}{m_-^{\mathbb{C}}} = i\bar{m}_I, \quad \bar{m}_I \in \mathbb{R}$$

The blocks of $\hat{\mathcal{G}}_{\mathbb{C}}^{-1}$ are again complex conjugates of each other:

$$\hat{\mathcal{G}}_{\mathbb{C}}^{-1} = \begin{pmatrix} -i\omega_n - \frac{\nabla^2}{m_+} - i\bar{m}_I\nabla^2 - \bar{\mu} - ih_I & 0 \\ 0 & i\omega_n - \frac{\nabla^2}{m_+} + i\bar{m}_I\nabla^2 - \bar{\mu} + ih_I \end{pmatrix}$$

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Population- and mass-imbalance behave quiet differently. For population imbalance, see

[J. Braun, J.-W. Chen, J. Deng, J. Drut, B. Friman, C.-T. Ma, Y.-D. Tsai '12]

For a large part of the talk: purely mass imbalanced case ($h = 0$)

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Sign Problem Circumvented!!

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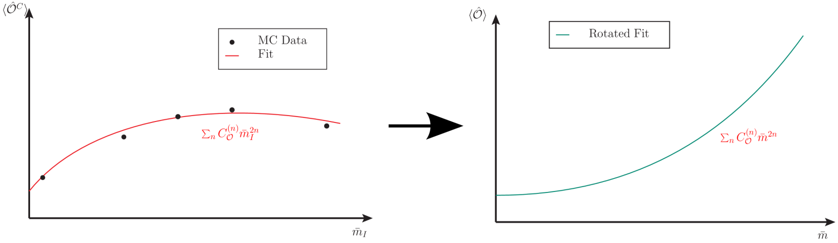
Sign Problem Circumvented!! But...

How to get back to real (physical) imbalance?

Physical Results from Imaginary Calculations

Suppose, some observable has been computed for imaginary mass-imbalance. Then fit the data points with, e.g., some polynomial $\langle \hat{\mathcal{O}}^{\mathbb{C}} \rangle \sim \sum_{n=0}^{N_{\max}} C_{\mathcal{O}}^{(n)} \bar{m}_I^{2n}$ and analytically continue $\bar{m}_I \to -i\bar{m}$.

Schematically:



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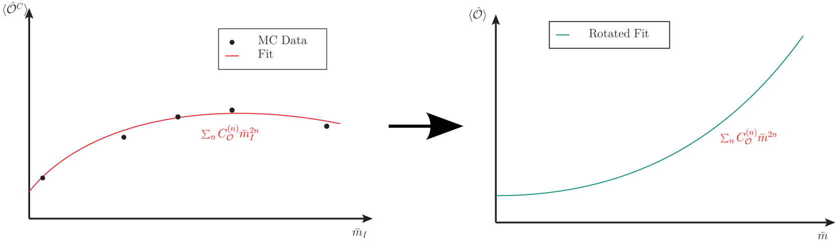


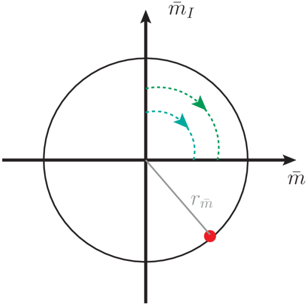
Are there any limits to the method, once Monte Carlo data is available?

Analytic Limits for the Method

Meaningful results can only be expected, if the series representation for $\langle \hat{\mathcal{O}}^{\mathbb{C}} \rangle$ converges in the complex $\bar{m}$-plane:

$$\langle \hat{\mathcal{O}}^{\mathbb{C}} \rangle(-i\bar{m}_I) = \langle \hat{\mathcal{O}} \rangle(\bar{m}) \Leftrightarrow \bar{m}_I \leq r_{\bar{m}}$$

The radius of convergence is determined by the closest singularity.



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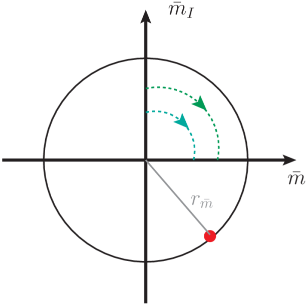

Knowledge of $r_{\bar{m}}$ (the singularity structure) is crucial to ascertain reliability of the results, see also examples below.

$\Rightarrow$ Analytical pre-treatment is required

How can $r_{\bar{m}}$ be obtained?

Plan:

- Perform fully analytical calculation $\varphi =$const mean-field case
- Investigate convergence properties
- Get an idea of the analytic structure of the theory and see what can be used for actual MC data

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Mean-field theory:

Reduce $\mathcal{Z} = \int \mathcal{D}\varphi\mathcal{D}\varphi^* e^{-\Gamma[\varphi,\varphi^*]}$ to $\mathcal{Z}_{\mathrm{MF}} = e^{-\Gamma[\varphi_0,\varphi_0^*]}$ and $\Gamma[\varphi_0,\varphi_0^*] \stackrel{!}{=} \min$

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The grand canonical potential is then just given by

$$\Omega_{\mathrm{MF}} = -\frac{1}{\beta}\ln\mathcal{Z}_{\mathrm{MF}} = \frac{1}{\beta}\Gamma[\varphi_0,\varphi_0^*]$$

Ω_{MF} and the Gap Equation

For φ =const, det $\left[\hat{\mathcal{G}}^{-1} + \hat{\Phi}\right]$ can be computed analytically by performing a Bogoliubov transformation and the Matsubara sum.

Result ($m_+ = 1$,regularizing terms dropped):

$$\Omega_{\mathrm{MF}}\left[|\varphi|^2\right] = \int \frac{d^3q}{(2\pi)^3}\left\{\frac{g_\varphi^2|\varphi|^2}{2q^2} - \frac{1}{\beta}\ln\left[\cosh\left(\beta\bar{m}q^2\right) + \cosh\left(\beta\sqrt{(q^2-\bar{\mu}^2)^2 + g_\varphi^2|\varphi|^2}\right)\right]\right\}$$

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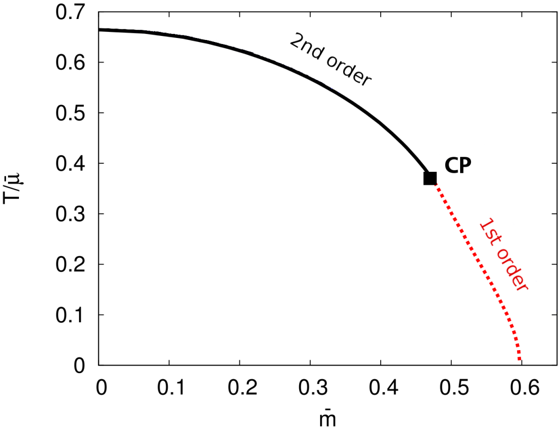
Gap equation with $\frac{g_\varphi^2|\varphi_0|^2}{\bar{\mu}^2}\equiv\bar{\Delta}$:

$$0\stackrel{!}{=}\int dq\left\{\frac{1}{2}+\frac{q^2}{2\sqrt{(q^2-1)^2+\bar{\Delta}}}\left(\frac{1}{1+e^{\beta\bar{\mu}\left(q^2\bar{m}+\sqrt{(q^2-1)^2+\bar{\Delta}}\right)}}-\frac{1}{1+e^{\beta\bar{\mu}\left(q^2\bar{m}-\sqrt{(q^2-1)^2+\bar{\Delta}}\right)}}\right)\right\}$$

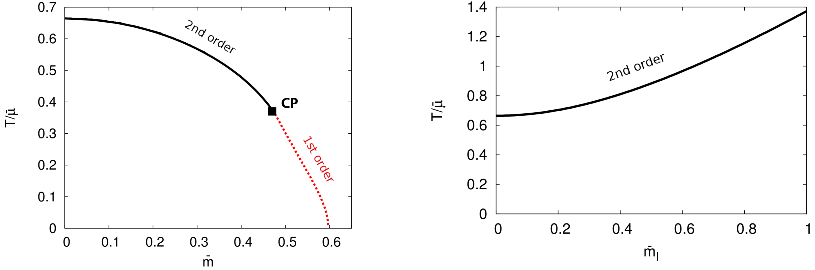
Mean-Field Phase Diagram for the Mass-Imbalanced Unitary Fermi Gas



Position of the critical point: $\left(\frac{T_{CP}}{\bar{\mu}}, \bar{m}_{CP}\right) \approx (0.47, 0.37)$

Comparing Phase Diagrams for $\bar{m}$ and $\bar{m}_I$

Since the functional form of Ω_{MF} is known analytically, both phase diagrams can be determined directly:



- No critical point/1st order transition for $\bar{m}_I$
- Analytic continuation of phase boundary will not reproduce result for all $\bar{m}$ $\Rightarrow$ radius of convergence $r_{\bar{m}}$?

Quantitative bounds on $r_{\bar{m}}$

Functional form of $\Omega_{\mathrm{MF}}(\bar{m})$ not explicitly known due to integration:

$$\Omega_{\mathrm{MF}}\left(\bar{m}\right) = \int \frac{\mathrm{d}^3 q}{(2\pi)^3} \left\{ \frac{g_\varphi^2 |\varphi|^2}{2q^2} - \frac{1}{\beta} \ln\left[\cosh\left(\beta \bar{m} q^2\right) + \cosh\left(\beta \sqrt{(q^2 - \bar{\mu}^2)^2 + g_\varphi^2 |\varphi|^2}\right)\right] \right\}$$

Complex analysis: $r_{\bar{m}}$ bounded from below by singularity structure of the *integrand*, i.e. the log term.

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Complex analysis: $r_{\bar{m}}$ bounded from below by singularity structure of the *integrand*, i.e. the log term. With $\Phi = g_\varphi \varphi$

$$\Rightarrow \boxed{r_{\bar{m}} \geq r_{\min} = \sqrt{\frac{\beta^2|\Phi|^2 + \pi^2}{\beta^2|\Phi|^2 + \pi^2 + \beta^2\bar{\mu}^2}}}$$

Properties and Usefulness of $r_{\min}$

$$r_{\min} = \sqrt{\frac{\beta^2|\Phi|^2 + \pi^2}{\beta^2|\Phi|^2 + \pi^2 + \beta^2\bar{\mu}^2}}$$

Limiting cases:

- $r_{min}|_{T\to\infty} = 1$, i.e. access to all possible $\bar{m}$ for high temperatures
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- If $\Omega^{\mathbb{C}}$ itself is computed for certain $(\bar{m}_I, T)$, T fixed, it can be continued to Ω inside the interval $[0, r_{\min}(T)[$
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- If observables $\langle \hat{\mathcal{O}}^{\mathbb{C}} \rangle$ are computed directly, as it is most often the case with Monte Carlo, things get a little more complicated...

Application I: Phase Boundary

Information provided by Ω:

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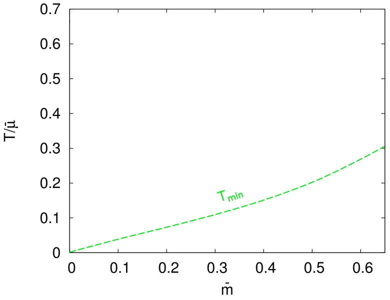

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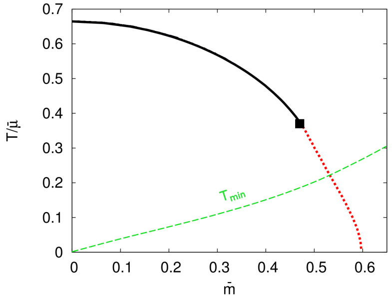
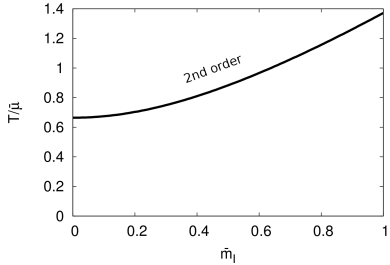
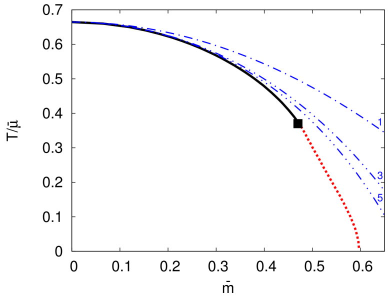


Phase Boundary from $\bar{m}_l$

Continuation of the $\bar{m}_l$ data yields:





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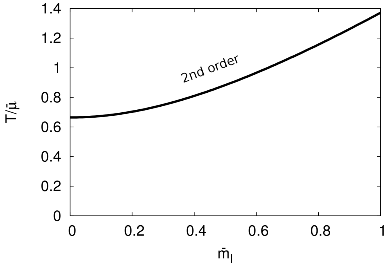

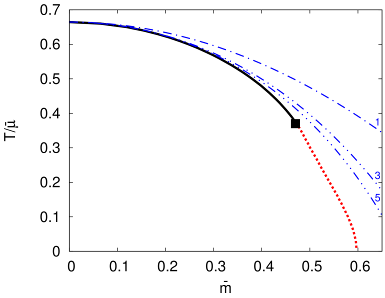

- Fair reproduction of phase boundary up to the critical point
- Non-analytic behaviour of $T_c(\bar{m})$ itself limits applicability
- Way out: computation & continuation of Ω itself, critical point should then be within reach

Application II: Bertsch Parameter $\xi_{T=0}$

Definition:

$$\xi = \frac{\bar{\mu}}{\epsilon_F}, \qquad \xi_{T=0}^{\mathrm{Free}} = 1 \quad \forall \bar{m} \in [0,1)$$

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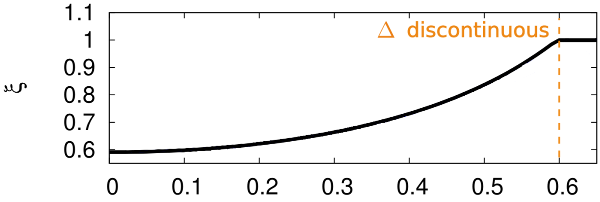
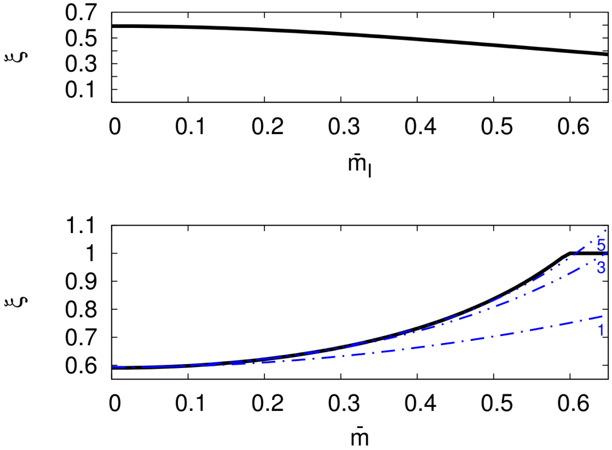


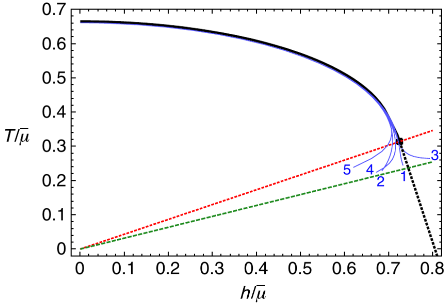
- Smooth observable implicitly depends on $\bar{\Delta}$
- By complex analysis: $r_\xi \leq \min[r_{min}, r_\Delta]$
- First order phase transition is expected to limit continuation of $\xi^{\mathbb{C}}$

Bertsch Parameter from $\bar{m}_l$



- Good reproduction of ξ up to the $\bar{\Delta}$ discontinuity
- Smooth observables indeed limited by $r_{\min}$ or r_{Δ}

Detour: Population-Imbalance



[J. Braun, J.-W. Chen, J. Deng, J. Drut, B. Friman, C.-T. Ma, Y.-D. Tsai '12]

$$\mathcal{G}_{\uparrow}^{-1} = -i\omega_n - \frac{\nabla^2}{m_+} - i\bar{m}_I\nabla^2 - \bar{\mu} - ih_I, \qquad \omega_n = (2n+1)\pi T$$

- Due to interference with Matsubara frequencies: $h_I \overset{!}{<} \pi T$
- Continuation of $\xi_{T=0}$ not possible for population imbalanced case
- Structurally similar to finite μ problem in lattice QCD

Remarks on r_{min} for Monte Carlo

Schematic structure of the grand canonical potential from Monte Carlo:

$$\Omega_{MC} \sim \ln \left\{ \sum_{\{\varphi(x)\}} \det \left[\hat{\mathcal{G}}^{-1} + \hat{\Phi} \right] e^{-\int m_\varphi^2 |\varphi(x)|^2} \right\}$$

Rigorous statements:

- For every fixed configuration $\varphi(x)$, the corresponding analytical calculation would correspond to the above mean-field procedure
- Overall radius of convergence: $r_{\mathrm{MC}} \geq \min_{\{\varphi(x)\}}[r_{\mathrm{min}}]$
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First practical estimate: $r_{\mathrm{MC}} \geq r_{\mathrm{min}}(\varphi = 0)$

Summary

- Imbalanced strongly interacting Fermi gases are tough systems to compute with Monte Carlo methods due to a sign problem
- Imaginary imbalance parameters remove the sign problem
  - Physical observables may be extracted by analytic continuation
  - Large parts of the phase diagram of the 3D unitary Fermi gas are in reach
- Extraction of physical results is limited by convergence issues
  - Radius of convergence of the grand potential Ω
  - Analyticity of the observables and dependencies
  - Type of imbalance
- Analytic structure at mean-field level provides hints for treatment of genuine Monte Carlo data

Outlook

- Extend investigation of convergence properties of observables
- Make connection to Monte Carlo more rigorous, ideally provide rigorous quantitative bounds
- Apply method in an actual Monte Carlo study

$\Rightarrow$ Work in progress by Joaquín Drut $\Leftarrow$