A complex Langevin approach to ultracold fermions

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Motivation

In recent years, tremendous effort was put forward to investigate the physics of ultracold Fermi gases, which has led to the observation of a rich variety of phenomena ranging from BCS superfluidity to Bose-Einstein condensation. Experimentally, this was made possible by the use of Feshbach resonances. Moreover, it became possible to realize experimental setups for low-dimensional quantum gases such that observables for two- and even one-dimensional (1D) configurations are now accessible.

Theoretical progress was achieved by a variety of approaches although mostly by numerical methods, as even in 1D many problems lack analytic solutions. Among the most successful methods, in particular for systems beyond the few-body regime, are *Quantum Monte Carlo (QMC)* approaches. A major drawback, however, is given by the infamous *sign-problem*, for which a general solution is highly unlikely [1]. Nevertheless, stochastic quantization could provide a way out, at least for non-relativistic fermions.

Stochastic Quantization & Complex Langevin

When dealing with ultracold dilute Fermi gases, we can assume a contact interaction between particles of different spin species. To compute observables for such systems we discretize imaginary time and perform a *Hubbard-Stratonovich transformation* in order to arrive at a path-integral expression for the ground-state partition sum $\mathscr{Z}$:

$$\mathscr{Z} = \int \mathscr{D}\sigma \, \det U_\sigma^{(\uparrow)} \det U_\sigma^{(\downarrow)} \equiv \int \mathscr{D}\sigma \, e^{-S_\sigma},$$

where $U_\sigma^{(s)}$ denotes the imaginary time evolution operator or the spin flavour s in single-particle representation. To evaluate the integral, whose dimension is equal to the number of spacetime lattice sites, we may use the *hybrid Monte Carlo (HMC)* algorithm to efficiently produce a *Markov chain* of field configurations σ. Of course, this procedure is only applicable if the integrand in the expression for the path integral is positive semidefinite, or in other words, the effective action S_σ is real.

Alternatively, one may interpret the probability measure in the path integral as the stationary distribution of a stochastic process governed by the *Langevin equation*,

$$\dot{\sigma} = -\frac{\partial S_\sigma}{\partial \sigma} + \eta,$$

an approach that was termed *stochastic quantization* [2]. The dot denotes a derivative in the ficticous phase-space time t. Normally, this procedure is also restricted to real actions S_σ. When the action is complex (sign-problem) we may complexify the auxiliary field σ and obtain a new set of equations of motion:

$$\begin{aligned} \dot{\sigma}_R &= -\mathrm{Re}\left[\frac{\partial S_\sigma}{\partial \sigma}\right] + \eta \\ \dot{\sigma}_I &= -\mathrm{Im}\left[\frac{\partial S_\sigma}{\partial \sigma}\right] \end{aligned}$$

where η is a Gaussian distributed noise with $\langle \eta \rangle = 0$ and $\langle \eta\eta' \rangle = 2\delta^{\eta}_{\eta'}$. To obtain observables, we take the noise average, which becomes formally exact in the limit of an infinite number of samples.

Unfortunately, there is no rigorous mathematical foundation for the *complex Langevin (CL)* approach and despite its elegance there are two caveats with the method. First of all, convergence is not guaranteed due to numerical instabilities and, even if convergence is achieved, it is not certain that the correct result is reproduced [3]. It was shown that the first issue can be cured numerically by adaptive time-step solvers. The latter issue is due to singularities in the imaginary part of the auxiliary field [4]. To prevent the CL algorithm from uncontrolled divergences in the complex plane a regulating term which represents a damping force in the equation of motion was proposed [5]. The discretized equations of motion then read

$$\begin{aligned} \delta\sigma_R &= -\mathrm{Re}\left[\frac{\partial S_\sigma}{\partial \sigma}\right]\delta\tau - 2\xi\sigma_R\delta\tau + \eta\sqrt{\delta\tau}, \\ \delta\sigma_I &= -\mathrm{Im}\left[\frac{\partial S_\sigma}{\partial \sigma}\right]\delta\tau - 2\xi\sigma_I\delta\tau \end{aligned}$$

where the parameter ξ determines the strength of the regulating term. The above expressions now allows us to sample integrals that would be subject to a sign-problem in conventional QMC approaches.

1D fermions with unequal masses

We apply our CL method to 1D Fermi mixtures of two spin flavours on a periodic 1D lattice, i.e. a ring [6]:

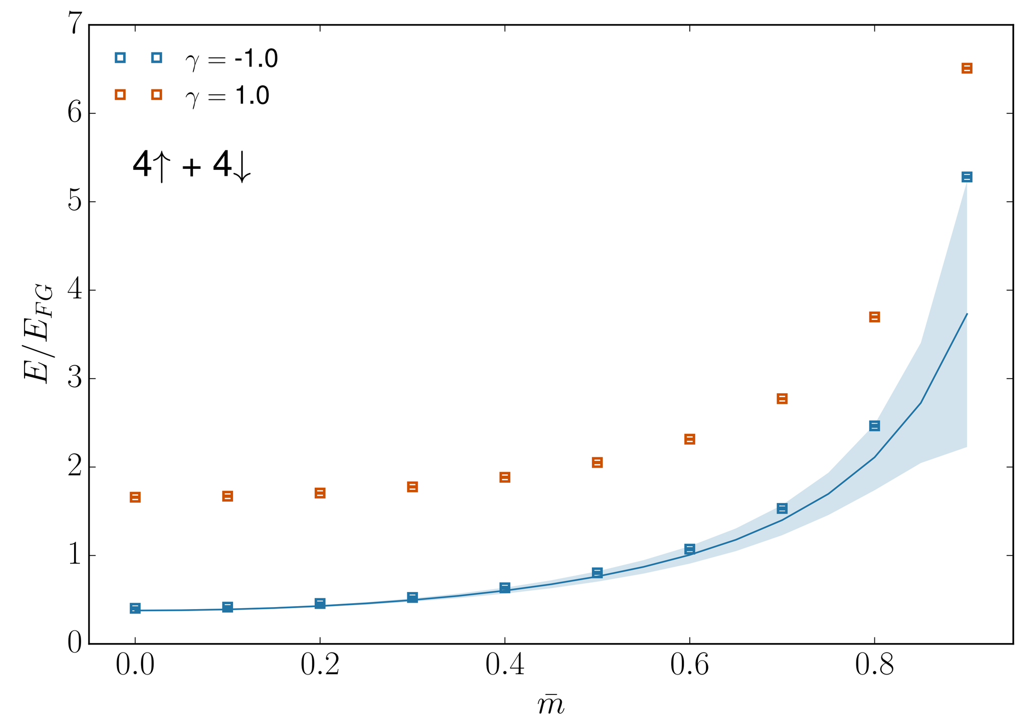
$$\hat{H} = -\sum_{s=\uparrow,\downarrow}\sum_x \hat{\psi}_s^\dagger(x)\frac{\hbar^2\nabla^2}{2m_s}\hat{\psi}_s(x) + g\sum_x \hat{n}_\uparrow(x)\hat{n}_\downarrow(x).$$

- insoluble by analytic means for spin flavours of unequal mass (except for the three- and four-body problem with a few special mass imbalances)
- subject to sign-problem within QMC methods for finite mass imbalance

a) Scales

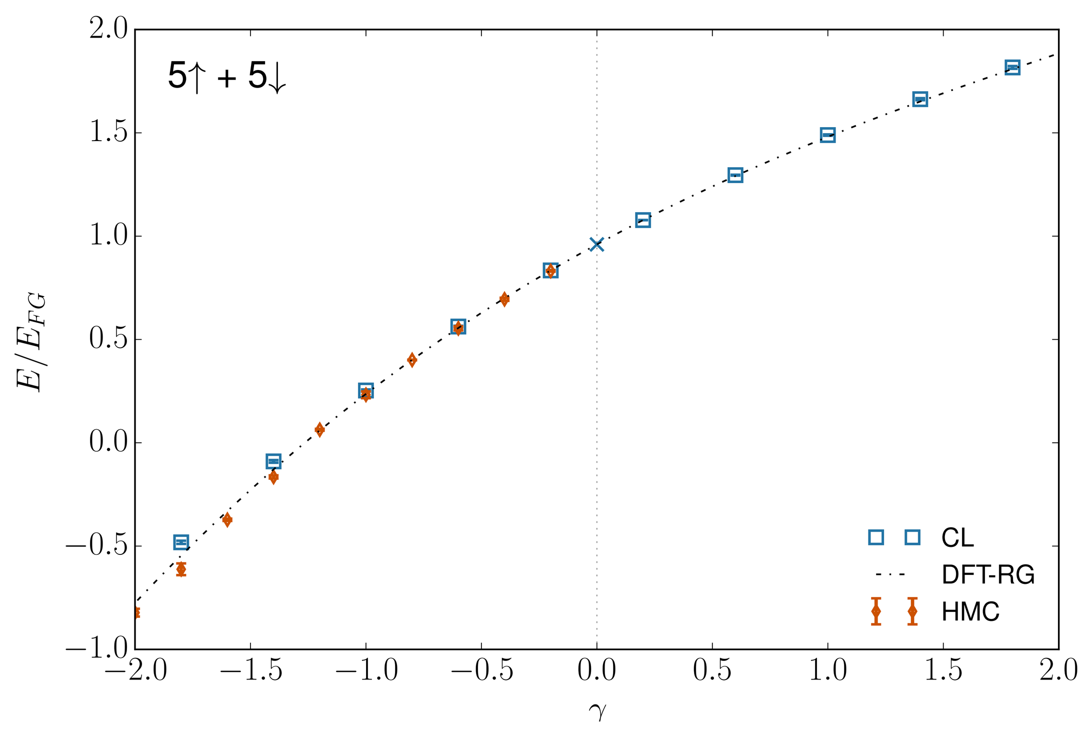
We work in units where $k_B = \hbar = m_0 = 1$. Furthermore, we use the particle density n to define the dimensionless coupling $\gamma = g/n$ and present all results as a function of the dimensionless mass-imbalance parameter $\bar{m} = \frac{m_\uparrow - m_\downarrow}{m_\uparrow + m_\downarrow}$.

b) Comparison of CL & iHMC



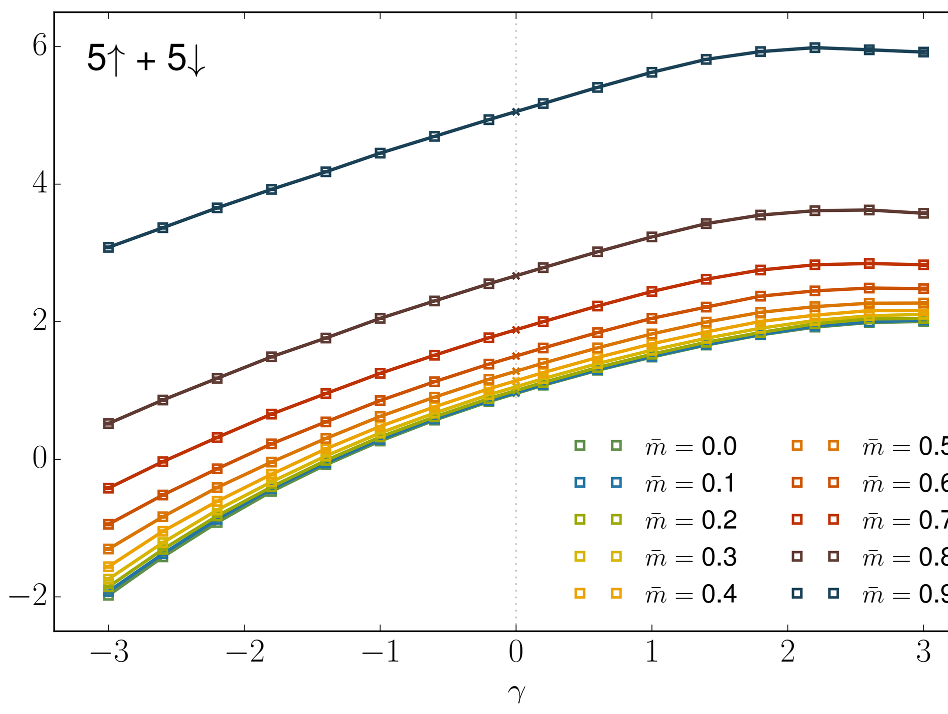
- attractive systems with small to medium mass-imbalance accessible via *MC simulation with imaginary mass imbalance (iHMC)* [6, 7]
- perfect agreement up to mass imbalances of $\bar{m} \sim 0.6 - 0.7$

c) Comparison of CL, HMC & DFT-RG



- perfect agreement of CL with few-body results from DFT-RG calculations [8] for weak to medium attractive and repulsive interactions

d) Equation of state



- possible experimental mass-imbalances within reach: $\bar{m} \sim 0.74$ for ^{6}Li and ^{40}Ka mixtures, $\bar{m} \sim 0.6$ for ^{40}Ka and ^{161}Dy mixtures
- perfect agreement with exact non-interacting values at $\gamma = 0$ (computed analytically)

Conclusion & Outlook

The complex Langevin method allows to study the ground state of 1D Fermi mixtures with a finite mass imbalance between the spin species. In areas of parameter space that are accessible to other methods, such as iHMC and DFT-RG, we find excellent agreement between the methods which validates the presented approach. Therefore, we have a method to address the sign-problem in ultracold Fermi gases.

Most notably, the complex Langevin method presented here can also be applied to higher dimensional Fermi gases with finite spin polarization and mass imbalance in a straightforward way. Our future work will aim at calculating inhomogeneous phases in Fermi gases such as the *Fulde-Ferrell-Larkin-Ovchinnikov (FFLO)* phase. Further steps towards this goal will include:

- spin-imbalanced Fermi gases
- extension to the 3D unitary Fermi gas
- long-term goal: fully nonperturbative phase diagrams of spin- and mass-imbalanced Fermi gases

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