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To cite this article: Joaquín E. Drut 2018 *J. Phys.: Conf. Ser.* **1041** 012005

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Advances in non-relativistic matter via complex Langevin approaches

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Abstract. The recent progress in understanding the mathematics of complex stochastic quantization, as well as its application to quantum chromodynamics in situations that have a complex phase problem (e.g. finite quark density, real time), has opened up an intriguing possibility for non-relativistic many-body physics which has so far remained largely unexplored. In this brief contribution, I review a few specific examples of advances in the characterization of the thermodynamics of non-relativistic matter in a variety of one-dimensional cases affected by the sign problem: repulsive interactions, finite polarization, finite mass imbalance, and projection to finite systems to obtain virial coefficients.

1. Introduction

This contribution is concerned with computational approaches to the generic quantum many-body problem, as it appears in high-energy, nuclear, condensed matter, and atomic physics; and quantum chemistry. The standard non-perturbative computational methods to this problem can be roughly divided into two large sets: direct methods and stochastic methods [which we will collectively refer to below as quantum Monte Carlo methods (QMC)]. In the former category we find exact diagonalization and configuration interaction approaches. While these are very appealing due to their potential for high precision, their memory requirements (especially in 3 spatial dimensions) can quickly become prohibitive as the system size is increased. Stochastic methods, which are the focus of this work, tend to have much milder memory requirements but suffer from other challenging issues.

Indeed, by far, most interesting problems in quantum many-body physics suffer from the infamous sign problem when one attempts to compute, using stochastic methods, essentially any useful quantity, be it ground-state properties, thermodynamics, or dynamic response (see e.g. [1, 2]). The sign problem is a severe signal-to-noise issue characterized by an exponentially decreasing signal-to-noise ratio as the volume of spacetime is increased (see e.g. [3, 4]). The hallmark of the sign problem can often be detected without doing a single calculation: the probability measure in the path integral may be real but of indefinite sign, or it may be complex, in which case we speak of a ‘phase problem’.

In spite of the general severity of the problem, in some cases it is possible to carry out calculations using a simple re-weighting technique, described next (see also e.g. Ref. [5]). Starting from the path integral formulation of the quantum many-body problem, where the



partition function takes the form (see below for further details on a particular case)

$$\mathcal{Z} = \int \mathcal{D}\sigma e^{-S[\sigma]}, \quad (1)$$

where the action $S[\sigma]$ is generally complex, which complicates the identification of $P[\sigma] = e^{-S[\sigma]}$ as a probability. For example, in the presence of fermionic degrees of freedom (electrons in condensed matter, atoms in ultracold atom experiments, quarks in QCD), one has

$$P[\sigma] = \det M[\sigma], \quad (2)$$

where $M[\sigma]$ contains the dynamics of the system and is generally a complex matrix.

The expectation value of an operator \hat{O} will generally assume the schematic form

$$\langle \hat{O} \rangle = \frac{\int \mathcal{D}\sigma P[\sigma] O[\sigma]}{\int \mathcal{D}\sigma P[\sigma]}, \quad (3)$$

where $P[\sigma]$ is, as mentioned above, what one would normally want to identify as a probability measure (usually a fermion determinant and other pieces of the action), but which will typically be complex. Rearranging the above expression by separating the magnitude $|P[\sigma]|$ and the phase $e^{i\phi[\sigma]}$, and multiplying and dividing by a normalization factor, one obtains

$$\langle \hat{O} \rangle = \frac{\int \mathcal{D}\sigma |P[\sigma]| e^{i\phi[\sigma]} O[\sigma]}{\int \mathcal{D}\sigma |P[\sigma]|} \frac{\int \mathcal{D}\sigma |P[\sigma]|}{\sum_{\sigma} |P[\sigma]| e^{i\phi[\sigma]}} = \frac{\langle \langle e^{i\phi[\sigma]} O[\sigma] \rangle \rangle}{\langle \langle e^{i\phi[\sigma]} \rangle \rangle}. \quad (4)$$

In this expression, the double angle bracket denotes an expectation value with respect to the non-negative measure $|P[\sigma]|$. One may thus use $|P[\sigma]|$ as the probability in conventional Metropolis-based methods. However, the price of such a re-weighting trick can be high: both the numerator and the denominator in the above expression will approach zero exponentially (as a function of the system size, see e.g. Ref. [3]), quickly going beyond the precision of any reasonable calculation (unless astronomical numbers of samples are used), such that obtaining their ratio becomes impractical.

In spite of remarkable advances toward taming this issue (i.e. find ways to make the phase average stay as close to 1 as possible), the search for a more generic or practical solution beyond the above re-weighting idea continues. Remarkably, some lines of research have shown that in specific cases the sign problem can be completely avoided (see e.g. [1, 2]); however, we will here focus on methods that attempt to overcome the problem by implementing some form of complex stochastic quantization, also known as complex Langevin (CL), which was brought up in Refs. [6, 7]. The idea of complex stochastic quantization is, in fact, a line of research that has flourished in recent years after multiple abandoned attempts in the area of lattice QCD [8, 9]. As it appears that the understanding of CL is now far better than ever before, it is an appealing candidate for addressing the sign problem in areas outside QCD.

In this contribution we show some of the recent attempts to use CL to overcome the sign problem in a class of non-relativistic many-body problems, keeping in mind their realization in ultracold atom experiments. We begin by describing some of the operational aspects of the method, leaving the formal aspects to the excellent extant literature (see e.g. [10, 11, 12, 13, 14]). We then review recent results for spin-1/2 fermions in one spatial dimension (1D) focusing on repulsive interactions at finite temperature, spin polarized systems, and mass-imbalanced systems. Finally, we show progress towards implementing particle projection algorithms via CL, which enables the stochastic calculation of high-order virial coefficients. Note that, in the 1D cases described here, we implement contact interactions, as befits dilute gases. In some cases the sign problem can be avoided entirely by using other algorithms [15]; however, those algorithms do not generalize to higher dimensions, which makes them less interesting for our objectives.

2. Outline of formalism and methods

For reference, it is useful to recall here the basic operations involved in the hybrid Monte Carlo (HMC) algorithm [16, 17, 18, 19]. We begin by writing the grand-canonical partition function

$$\mathcal{Z} = \text{tr} e^{-\beta(\hat{H} - \mu\hat{N})}, \quad (5)$$

as a path integral, where \hat{H} is the Hamiltonian, \hat{N} is the total particle number operator, β is the inverse temperature, and μ the chemical potential. Following conventional steps (see e.g. [18]), we begin by discretizing the imaginary time direction as $\beta = N_\tau\tau$ for a given time step τ and using a Suzuki-Trotter decomposition of the transfer-matrix operator, e.g.

$$e^{-\tau\hat{H}} = e^{-\tau\hat{T}}e^{-\tau\hat{V}} + O(\tau^2), \quad (6)$$

where \hat{T} is the kinetic energy operator and \hat{V} is the potential energy operator containing the interaction (we assume that an external potential, if present, is included in \hat{T}). A Hubbard-Stratonovich (HS) transformation (of which there are many choices, see e.g. [18]) then allows us to write the interaction factor as a path integral over the auxiliary field σ (which would typically be the photon field in electrodynamics and the gluon field in QCD):

$$e^{-\tau\hat{V}} = \int \mathcal{D}\sigma e^{-\tau W[\sigma]}, \quad (7)$$

where $W[\sigma]$ is simply a one-body operator containing the external auxiliary field σ . Inserting the factorization and HS-transformed expressions into the partition function, we arrive at the the path integral form mentioned above, namely

$$\mathcal{Z} = \int \mathcal{D}\sigma e^{-S[\sigma]}, \quad (8)$$

where the effective action $S[\sigma]$ is typically the logarithm of a fermion determinant and potentially includes pure σ terms, as in QCD (though not necessarily so in non-relativistic physics).

When $S[\sigma]$ is real, the usual methods sample the field σ according to $P[\sigma] = e^{-S[\sigma]}$. The HMC algorithm carries out that sampling in a global fashion (i.e. modifying the whole σ field at the same time) by enlarging the phase space with the introduction of an auxiliary momentum field π conjugate to σ whose dynamics factorizes in the partition function and therefore does not alter the physics of the problem. Explicitly,

$$\mathcal{Z} = \int \mathcal{D}\sigma \mathcal{D}\pi e^{-\mathcal{H}[\sigma, \pi]}, \quad (9)$$

where $\mathcal{H}[\sigma, \pi] = \frac{1}{2} \sum_x \pi(x)^2 + S[\sigma]$. The classical equations of motion for $\mathcal{H}[\sigma, \pi]$, in a fictitious phase-space time t , are then used to update the fields:

$$\dot{\sigma} = \pi, \quad (10)$$

$$\dot{\pi} = -\frac{\delta S[\sigma]}{\delta \sigma}. \quad (11)$$

In the above phase-space evolution, a trajectory of length $t \sim O(1)$ is considered a full update of the field (although several such trajectories are usually required to ensure decorrelation). In between trajectories, a Metropolis step is implemented to ensure that the correct distribution is being sampled, and the momentum π is refreshed using a Gaussian distribution. Note that, in such a classical evolution, the fictitious energy given by the value of \mathcal{H} is conserved (as long as

the integrator is accurate enough), which ensures a very high acceptance rate in the Metropolis step. The HMC algorithm thus succeeds at implementing global updates with high acceptance rate. From this brief operational description, it can be inferred that the most costly part of the algorithm is the calculation of the force $\delta S[\sigma]/\delta\sigma$.

The stochastic quantization sister of the HMC method is what one may call real Langevin (RL) [20, 21], which enables global updates as well. In RL, however, there is no Metropolis step and the equations of motion take the form

$$\dot{\sigma} = -\frac{\delta S[\sigma]}{\delta\sigma} + \eta, \quad (12)$$

where we note that there is no auxiliary momentum field π but a t -dependent noise field η appears instead. The latter satisfies $\langle\eta(x, \tau)\rangle = 0$ and $\langle\eta(x, \tau)\eta(x', \tau')\rangle = 2\delta_{x,x'}\delta_{\tau,\tau'}$ for spacetime points (x, τ) and (x', τ') , and may be chosen to be Gaussian. The similarities between RL and HMC are clear; most notably, the calculation of the ‘drift’ (as is often called in the context of stochastic quantization) given by $\delta S[\sigma]/\delta\sigma$, is the most computationally intensive part of the method.

The conventional mathematical underpinnings of HMC and RL depend on $P[\sigma]$ being positive semidefinite (i.e. $S[\sigma]$ being real), a property which fails to hold in non-relativistic physics for repulsive interactions (away from the half-filling point), polarized systems, mass-imbalanced systems, and so on, and the calculation is then said to have a sign problem (or more generally a complex-phase problem). In the case of HMC, this means that the Metropolis step is simply no longer well-defined and thus the algorithm is no longer available. For RL, on the other hand, a generalization is possible into what we referred to above as CL.

Operationally, in CL one complexifies the HS field σ via

$$\sigma = \sigma_R + i\sigma_I, \quad (13)$$

where σ_R and σ_I are both real fields and defines equations of motion by

$$\delta\sigma_R = -\text{Re}\left[\frac{\delta S[\sigma]}{\delta\sigma}\right]\delta t + \eta\sqrt{\delta t}, \quad (14)$$

$$\delta\sigma_I = -\text{Im}\left[\frac{\delta S[\sigma]}{\delta\sigma}\right]\delta t, \quad (15)$$

where now $S[\sigma]$ is to be understood as a complex function of the complex variable σ . Clearly, when the action is real, the imaginary part of the force vanishes and CL reduces to RL. We also note that we chose real noise, but complex noise is also a possibility (see e.g. Ref. [10]).

3. Results

As anticipated, this section reviews some of the recent applications of the complex Langevin method to non-relativistic systems. Four different situations are briefly described (all corresponding to fermions in 1D with a zero-range interaction): repulsive interactions, finite polarization, finite mass imbalance, and particle number projection. It should be pointed out that, while 1D systems can be tackled with the Bethe ansatz (see e.g. Ref. [22]), although the latter runs into difficulties at finite temperature and in the grand-canonical ensemble, and at finite mass imbalance. All of the results presented here correspond to nonrelativistic fermions with an interaction of the form

$$\hat{V} = \int dx g \hat{n}_\uparrow(x) \hat{n}_\downarrow(x), \quad (16)$$

where g is the coupling and \hat{n}_s is the density operator for particles of spin s .

3.1. Spin-1/2 fermions in 1D: repulsive interactions at finite-temperature

Our first results with CL focused on the density equation of state n of unpolarized fermions with repulsive interactions at finite temperature, which were first published in Ref. [23]. This equation of state is of interest because it is relatively easy to measure in experiments (see e.g. [24, 25, 26]) and from it one may obtain the pressure by integration and the compressibility by differentiation. In short, it is the simplest observable characterizing the thermodynamics of these quantum systems.

The auxiliary field method gives a sign problem for this system regardless of the dimension, but we focused on 1D as a starting point and compared our CL results with lattice perturbation theory up to next-to-leading (NLO), next-to-next-to-leading (N2LO), and next-to-next-to-next-to-leading order (N3LO), in Fig. 1 (left panel) for several values of the coupling λ . In the region of large fugacity, i.e. $\beta\mu \gg 0$ (where β is the inverse temperature and μ the chemical potential, such that $z = \exp(\beta\mu)$ is the fugacity), we expect perturbative results to be reliable, and we find that CL agrees with them. As the coupling is increased, perturbation theory begins to break down, but CL continues to converge, giving a prediction for the grand canonical equation of state for the density.

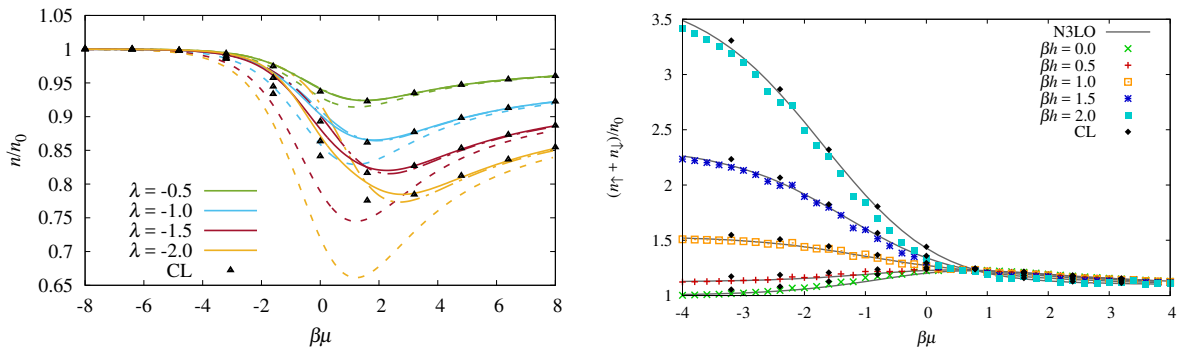


Figure 1. Left panel: Density equation of state n of 1D fermions with repulsive interactions, in units of the noninteracting counterpart n_0 . Black diamonds show the CL results. Dashed, dash-dotted, and solid lines show results of NLO, N2LO, and N3LO lattice perturbation theory, respectively [23]. Right panel: Density equation of state of 1D fermions with attractive interactions at finite chemical potential asymmetry βh , which leads to different densities n_\uparrow and n_\downarrow for each spin species. Black diamonds show the CL results. Solid lines show results of N3LO lattice perturbation theory. Colored data points show the results of imaginary-polarization calculations of Ref. [27].

3.2. Spin-1/2 fermions in 1D: finite polarization at finite-temperature

Following up on the success of our study of repulsive interactions, we move on to polarized systems, which are especially interesting due to the possibility of realizing exotic superfluids such as the Fulde-Ferrell-Larkin-Ovchinnikov phase. As in the previous case, we compared with perturbative results, but also with the imaginary-polarization approach of Ref. [27] (which used an idea first put forward in Ref. [28]), in Fig. 1 (right panel). This case is more remarkable than the previous one because we obtain results that are not only in agreement with N3LO perturbation theory but also with the entirely different non-perturbative approach of imaginary polarization.

3.3. Spin-1/2 fermions in 1D: ground-state of mass-imbalanced systems

The realization of ultracold atomic gases with different atomic species yields another area of research where the sign problem prevents useful calculations. However, by implementing imaginary mass-imbalance and CL approaches [29, 30, 31], we have shown that this field is entirely open for attractive interactions and at least partially open for the repulsive case. Indeed, a signal-to-noise issue reappears due to vanishing weight $P[\sigma]$ in the complex σ plane (i.e. the appearance of singularities in $S[\sigma]$) at large repulsive interactions. This issue is currently open and under investigation. Progress in this direction is shown in the left panel of Fig. 2, where we show the ground-state energy (in units of its non-interacting counterpart) of 10 fermions, as a function of the coupling $\gamma = g/n$. The plot shows results for several mass imbalances $\bar{m} = (m_{\uparrow} - m_{\downarrow})/(m_{\uparrow} + m_{\downarrow})$.

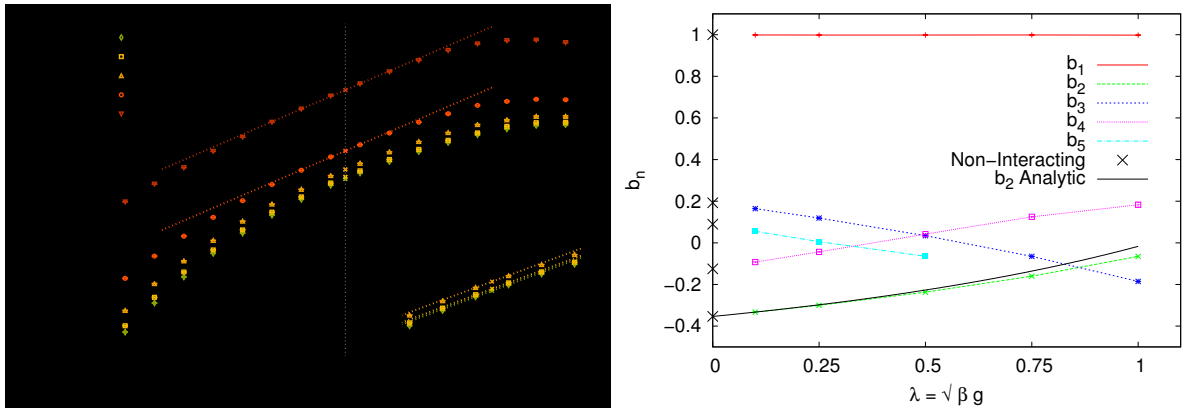


Figure 2. Left panel: Ground-state energy E of 10 mass-imbalanced fermions in 1D, as a function of the coupling $\gamma = g/n$ [31], where n is the density, in units of the noninteracting counterpart E_{FG} . Dashed lines show a first-order perturbative result. Right panel: First few virial coefficients b_n of the attractive 1D Fermi gas, obtained by Fourier-based particle projection.

3.4. Particle-projection approach to clusters and high-order virial coefficients

The idea of implementing a Fourier-transform particle-number projection of a grand-canonical calculation to obtain information about finite systems is not new; it is quite common in the context of nuclear physics (see e.g. [32]). However, to our knowledge it has not been applied by way of the complex Langevin algorithm, nor has it been applied to the stochastic extraction of virial coefficients from grand canonical calculations. Here, we report briefly on progress toward that goal, focusing on 1D systems as test cases, as done in previous subsections. In Fig. 2 we show our first results, which indicate that it may be possible to extract up to fifth order coefficients. In that figure we map out the coupling-constant dependence of those virial coefficients and compare with the analytic result of Ref. [33] for b_2 . The remarkable agreement in the case of b_2 (up to systematic effects as λ increases), along with the relative smoothness of the results for the other coefficients, indicate that the method is robust, although certainly not as precise as other approaches based on the exact solution of the n -body spectrum. Note that the approach also correctly reproduces $b_1 = 1$ for all couplings. It remains an open question whether the method remains viable in higher dimensions, but a priori nothing indicates otherwise.

4. Conclusions

In this contribution we have reviewed the recent exploration of the application of complex stochastic quantization to the non-relativistic quantum many-body problem. Remarkably, a wide range of applicability was found and validated in several ways, e.g. with third-order perturbation theory or imaginary-asymmetry methods. Specifically, we were able to obtain equations of state of polarized and mass-imbalanced matter with attractive and repulsive interactions in 1D. We have also shown that practical calculations of high-order virial coefficients is possible using the idea of particle-number projection along with CL.

Acknowledgments

I would like to thank J. Braun, A. C. Loheac, L. Rammelmüller, and C. R. Shill for discussions and data. This material is based upon work supported by the National Science Foundation under Grants No. PHY1452635 (Computational Physics Program). Numerical calculations have partially been performed at the LOEWE-CSC Frankfurt.

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