Imaginary Polarization as a Way to Surmount the Sign Problem in *Ab Initio* Calculations of Spin-Imbalanced Fermi Gases

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From ultracold atoms to quantum chromodynamics, reliable *ab initio* studies of strongly interacting fermions require numerical methods, typically in some form of quantum Monte Carlo calculation. Unfortunately, (non)relativistic systems at finite density (spin polarization) generally have a sign problem, such that those *ab initio* calculations are impractical. It is well-known, however, that in the relativistic case imaginary chemical potentials solve this problem, assuming the data can be analytically continued to the real axis. Is this feasible for nonrelativistic systems? Are the interesting features of the phase diagram accessible in this manner? By introducing complex chemical potentials, for real total particle number and imaginary polarization, the sign problem is avoided in the nonrelativistic case. To give a first answer to the above questions, we perform a mean-field study of the finite-temperature phase diagram of spin-1/2 fermions with imaginary polarization.

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Ultracold Fermi gases provide an accessible and clean environment to study quantum many-body phenomena [1,2], ranging from Bose-Einstein condensation (BEC) to Bardeen-Cooper-Schrieffer (BCS) superfluidity. In the dilute limit, where the range of the interaction is smaller than that of any other scale, a single parameter $(k_F a_s)^{-1}$, where a_s is the s-wave scattering length and k_F is the Fermi momentum, describes the microscopic interactions completely. These are tuned by an external magnetic field in the presence of a Feshbach resonance.

At large a_s values (at the crossover between BEC and BCS), these systems display universal properties. Here, the scale for all physical observables is set solely by k_F (or, equivalently, the density), which is the only scale left in the problem. Thus, no obvious small expansion parameter exists in this limit. This represents a major challenge for theoretical many-body approaches [3]. Recently, experiments in this so-called unitary regime have achieved high precision [4], which potentially facilitates benchmarking of theoretical methods.

Despite rapid experimental and theoretical advances, our understanding of ultracold Fermi gases at unitarity remains incomplete, most notably for the case of spin-imbalanced systems. For a sufficiently large imbalance, one expects a phase transition from a BCS-type superfluid to a polarized normal gas. Such a transition was observed in experiments at MIT and Rice University [5] and is in accordance with various theoretical studies [6–8].

Apart from ultracold gases, a better understanding of imbalanced fermion systems is of great importance also in other research fields. For example, lattice Monte Carlo (MC) calculations of nuclei [9] are confronted with similar problems in isospin asymmetric nuclei, i.e., nuclei with an unequal number of neutrons and protons.

We shall focus on the $a_s \to \infty$ limit for a spin-imbalanced two-component Fermi gas at zero and finite temperature. Unlike previous studies [6–8], however, we consider complex valued chemical potentials of the spin components $\mu_\uparrow$ and $\mu_\downarrow$. In *ab initio* MC calculations, one can thus avoid the sign problem, which impedes studies of spin-polarized systems for real μ.

This approach parallels that of a purely imaginary μ in relativistic quantum field theories, which enables an analysis of the phase structure of QCD [10] at finite but imaginary quark density on the lattice. The physics at real densities is then obtained by analytic continuation to real values of the chemical potential. The applicability of an analytic continuation with polynomials is restricted to small μ values, more precisely $\mu/T \lesssim 1$. So far, this approach has not delivered conclusive evidence for or against the existence of a critical end point of the line of chiral transitions in the T-μ plane [11]. For nonrelativistic fermions in the BEC-BCS crossover, on the other hand, the tricritical end point of the line of (second-order) superfluid transitions is known to exist. Moreover, our present study suggests that this point might be accessible in lattice

calculations using complex-valued chemical potentials. A successful application of such an approach to ultracold Fermi gases may be useful for future lattice QCD studies as well. In fact, it can be very beneficial for present and future studies of the QCD phase diagram to have an experimentally accessible system at hand that allows us to test theoretical approaches and techniques in a clean and controlled environment, especially since the experimental search for the critical point in the QCD phase diagram has proven tremendously difficult and therefore requires reliable guidance from theory.

In this first analysis, we employ a mean-field approach, as discussed elsewhere for the case of real-valued μ (see, e.g., Refs. [6,8]), to study the phase diagram in the complex-valued case. Although this can only be viewed as a lowest-order approximation, it relies only on a single input parameter (e.g., k_F) as is the case for the full evaluation of the associated path integral using, e.g., MC calculations. Thus, our results do not suffer from a parameter ambiguity but only from an uncertainty associated with the underlying approximation. This can be understood on very general grounds from an analysis of the fixed-point structure of fermionic theories [12].

We begin by discussing a few general aspects of nonrelativistic theories with complex-valued chemical potentials. In general, the grand canonical partition function $\mathcal{Z}$ of nonrelativistic fermions reads

$$\mathcal{Z}(T, \bar{\mu}, h) = \mathrm{Tr}[e^{-\beta(\hat{H}-\bar{\mu}(\hat{N}_\uparrow+\hat{N}_\downarrow)-h(\hat{N}_\uparrow-\hat{N}_\downarrow))}], \quad (1)$$

where T is the temperature and $\beta = 1/T$. We shall assume that the Hamiltonian $\hat{H}$ describes the dynamics of a theory with two fermion species, denoted by $\uparrow$ and $\downarrow$, interacting via a two-body interaction. Here, $\hat{N}_{\uparrow,\downarrow}$ are the particle number operators associated with each species and $\mu_{\uparrow,\downarrow}$ are the corresponding chemical potentials. For convenience, we introduce the average chemical potential $\bar{\mu} = (\mu_\uparrow + \mu_\downarrow)/2$ and the asymmetry parameter $h = (\mu_\uparrow - \mu_\downarrow)/2$.

As is well-known, MC calculations for unitary fermions can be performed without a sign problem for $h = 0$ (see, e.g., Refs. [13,14]). This is not true in general, however, as polarization leads to a sign problem, regardless of the form of the interaction. To proceed, we consider an imaginary-valued asymmetry parameter h, corresponding to a theory with complex-valued $\mu_{\uparrow,\downarrow}$ and therefore define $h = ih_I$, where h_I is a real quantity. It is easy to verify that MC calculations with imaginary-valued asymmetry can be studied with standard methods without a sign problem: the fermion determinants appearing in the probability measure are complex conjugates of one another. By analytically continuing $\mathcal{Z}(T, \bar{\mu}, h_I)$, one then obtains $\mathcal{Z}(T, \bar{\mu}, h)$, which is the central quantity in studies of imbalanced Fermi gases.

To understand whether the tricritical end point is accessible with such an approach, we study the mean-field phase diagram with complex-valued chemical potentials. We compute the mean-field potential for the $U(1)$ order parameter, starting from the path-integral representation for $\mathcal{Z}$,

$$\mathcal{Z} = \int \mathcal{D}\psi^\dagger \mathcal{D}\psi e^{-S[\psi^\dagger,\psi]},$$

where

$$S[\psi^\dagger, \psi] = \int d\tau \int d^3x \{\psi^\dagger(\partial_\tau - \vec{\nabla}^2 - \bar{\mu})\psi - h(\psi_\uparrow^*\psi_\uparrow - \psi_\downarrow^*\psi_\downarrow) + \bar{g}(\psi^\dagger\psi)(\psi^\dagger\psi)\}, \quad (2)$$

and $\psi^T = (\psi_\uparrow, \psi_\downarrow)$ and $\bar{g}$ denotes the bare four-fermion coupling. The dimensionless renormalized four-fermion coupling $g \sim \bar{g}\Lambda$ is related to the scattering length a_s by

$$4\pi\Lambda g^{-1} = (a_s^{-1} - c_{\mathrm{reg.}}\Lambda). \quad (3)$$

Here, Λ denotes the ultraviolet cutoff and the constant $c_{\mathrm{reg}} > 0$ depends on the regularization scheme. We use units such that $2m = 1$, where m is the fermion mass. The interaction is represented by an auxiliary scalar field $\varphi \sim g_\varphi \psi_\uparrow \psi_\downarrow$, where the parameter g_φ is chosen to reproduce the four-fermion term in the action. Since the resulting action is quadratic in the fermion fields, they can be integrated out. Thus, one obtains the order-parameter potential

$$\beta U(\varphi) = -2\beta\bar{\mu}|\varphi|^2 - \int \frac{d^3q}{(2\pi)^3} \ln\left[\frac{1}{2}(\cosh(\beta h) + \cosh(\beta\sqrt{(\vec{q}^2 - \bar{\mu})^2 + g_\varphi^2|\varphi|^2})\right]. \quad (4)$$

This potential is directly related to the grand canonical potential $\Omega = VU(\varphi_0)$, where V is the volume of the system and φ_0 denotes the value of φ that minimizes the potential. In that state, $g_\varphi^2|\varphi_0|^2$ can be identified with the fermion gap Δ, the order parameter of the spontaneously broken $U(1)$ symmetry, associated with a superfluid state. From the (regularized) grand canonical potential we can obtain all thermodynamic observables. In the unitary limit, the dimensionless (universal) quantities, such as the critical temperature for the superfluid transition $T_c/\bar{\mu}$, the corresponding gap $\Delta/\bar{\mu}^2$, and the ground-state energy $E/\bar{\mu}$, are, as expected, independent of $\bar{\mu}$ and g_φ. To compute the critical temperature T_c, it is convenient to employ the gap equation $(\partial U/\partial\varphi)|_{\varphi_0} = 0$ and exploit the fact that the fermion gap $\Delta \sim \varphi_0^2$ vanishes identically at $T = T_c$.

From Eq. (4), it is apparent that mean-field potential U is 2π periodic in βh_I. This is a property not only of the mean-field approximation but of the full theory, as can be seen by inspecting Eq. (2); the imaginary part of h effectively shifts the Matsubara modes of the fermions $\nu_n = (2n + 1)\pi T$ by $h_I T$. [Loosely speaking, ∂_τ is replaced by $i\nu_n$ when the action S is formulated in momentum space.] It follows that it is not possible to study arbitrary asymmetries with this technique: h_I is bounded to values $\beta h_I < \pi$. Nevertheless, a large part of the phase diagram in the physical (T, h) plane can be explored within this approach. As we show

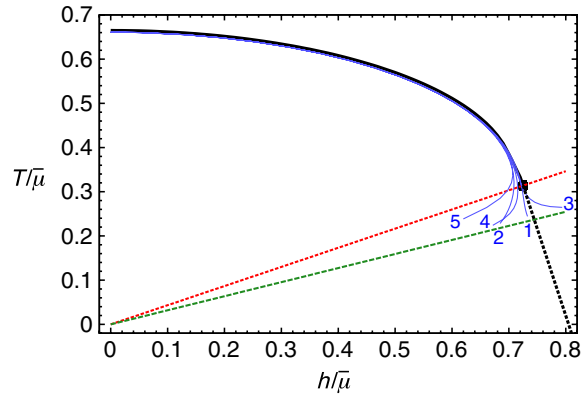

FIG. 1 (color online). Phase diagram of an ultracold Fermi gas at unitarity in the (T, h) plane. The solid (black) curve is a line of second-order phase transitions, which ends at a tricritical point $(h_{\rm cp}/\bar{\mu}, T_{\rm cp}/\bar{\mu})$ and is followed by a line of first-order transitions (see, e.g., Ref. [8]). The (red) dashed line is $T/\bar{\mu} = (T_{\rm cp}/h_{\rm cp})h/\bar{\mu}$, and the (green) dash-dotted line is $\pi T/\bar{\mu} = h/\bar{\mu}$. The (light-blue) thin curves are analytic continuations from imaginary h using Padé approximants of order $N_{\rm max} = 1, 2, \ldots, 5$ [see Eq. (5)].

next, the mean-field calculation presented here suggests that a (tri)critical point in the phase diagram may indeed be accessible in lattice MC calculations with imaginary h.

In Fig. 1, we show the well-known mean-field phase diagram in the (T, h) plane (see, e.g., Refs. [6,8]). We refrain from discussing the appearance of inhomogeneous phases (Sarma and/or FFLO) and focus on the phase boundaries of the homogeneous ones. In Fig. 2, we show the corresponding phase diagram in the plane spanned by the temperature and the imaginary-valued asymmetry parameter. As noted above, the phase diagram is 2π periodic

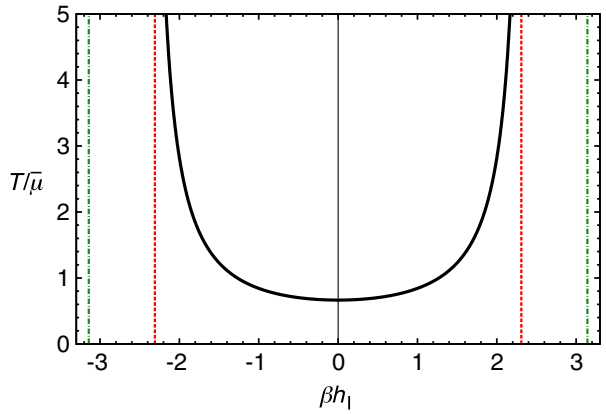

FIG. 2 (color online). Phase diagram in the (T, h_I) plane. The solid line is a line of second-order phase transitions below which the fermion gap is finite. The (red) dashed and (green) dash-dotted lines are the analogues of those in Fig. 1, with h_I replacing h. Between the (red) dashed lines and the (green) dash-dotted lines $T_c \to \infty$ for $\bar{\mu} > 0$. For $\bar{\mu} < 0$, however, T_c remains finite.

in βh_I. We therefore show only the domain $\beta h_I \in [-\pi, \pi]$, bounded by the green dashed-dotted lines.

Given a phase diagram for imaginary h, obtained, e.g., using lattice MC calculations, one can access only the temperature regime $T > h/\pi$ in the physical (T, h) plane of Fig. 1. Nevertheless, this represents a fairly large part of the phase diagram, which is at the heart of theoretical and experimental studies. Most remarkably, our analysis suggests that the (tri)critical point may be located within the accessible part of the phase diagram, implying that this point may be within the reach of lattice MC calculations with an imaginary asymmetry parameter. The phase transition line can then be obtained from an analytic continuation of the results for $T_c(h_I)$, as shown below.

The phase structure of the theory in the (T, h_I) plane (Fig. 2) is intriguing. It can be shown analytically that $T_c \to \infty$ for $\beta h_I = (2N + 1)\pi$ with $N \in \mathbb{Z}$ and $\bar{\mu} > 0$. A similar result is found in relativistic fermion models, such as the Gross-Neveu model in $(1 + 1)d$ [15]. Again, we expect this result to remain valid also beyond the mean-field approximation. In fact, for $\beta h_I = (2N + 1)\pi$ the fermionic Matsubara modes $\nu_n = (2n + 1)\pi T$ in Eq. (2) effectively assume the form $\nu_n = 2n\pi T$ associated with bosonic degrees of freedom. Thus, in this case the fermions acquire a (thermal) zero mode, which tends to condense, independently of the actual value of the temperature. However, contrary to relativistic fermion models, we find numerically that $T_c \to \infty$ already for $|\beta h_I| > |(\beta h_I)_\infty| \simeq 2.397$. In other words, for $|(\beta h_I)_\infty| \leq |\beta h_I| < \pi$ there is always a fermion condensate and the $U(1)$ symmetry is not restored by increasing the temperature. For $|\beta h_I| < |(\beta h_I)_\infty|$, the phase transition is second order. The upper limit $|(\beta h_I)_\infty|$ will take a different value when one goes beyond the mean-field approximation.

In our numerical studies we find that the value $|\beta_{\rm cp} h_{\rm cp}|$ associated with the (tri)critical point is slightly lower than $|(\beta h_I)_\infty|$. This close agreement appears to be a mere coincidence. In fact, in the weak-coupling limit the difference between $|\beta_{\rm cp} h_{\rm cp}|$ and $|(\beta h_I)_\infty|$ is larger than in the unitary regime, at least in mean field approximation [16]. In this context, we note that the absence of a (tri)critical point in the (T, h_I) plane as well as the absence of $U(1)$ restoration in the domain $|(\beta h_I)_\infty| \lesssim |\beta h_I| < \pi$ does not imply their absence for real-valued asymmetries.

In analogy to relativistic fermion models [15], the analytic continuation of the phase boundary reproduces the phase boundary only up to the (tri)critical point. However, by means of an analytic continuation of the (full) order-parameter potential, the phase diagram can be mapped out in the complete region where $\beta h < \pi$ of the physical (T, h) plane, including the line of first-order transitions.

We stress that, using imaginary polarizations, the detection of a (tri)critical point appears to be feasible with lattice MC calculations, even though this might require techniques for the computation of the effective potential.

The latter might be borrowed from, e.g., lattice MC studies of supersymmetric models [17]. Also, one may employ Padé approximants to scan the phase diagram and detect the approximate location of the (tri)critical point by determining the point at which the Padé approximants do not converge (see, e.g., Refs. [16,18,19] and also our discussion below). In any case, the analytic continuation of numerical data is difficult since one has to deal with (systematic and statistical) uncertainties of the data from the MC calculation (see, e.g., Ref. [20]).

The grand canonical partition function $\mathcal{Z}$ is, just like the order-parameter potential U, invariant under $h \to -h$. This allows us to expand $\mathcal{Z}$ (and other physical quantities) in powers of $(\beta h)^2$. In the mean-field approximation, we find that the radius of convergence for the grand canonical potential is $r \equiv |\beta h|_{\max} = \pi$ for $\Delta \equiv 0$ and $\bar{\mu} > 0$, but $r > \pi$ in the case of a finite gap Δ. These observations facilitate the analytic continuation from imaginary- to real-valued asymmetry parameter. When performing MC calculations of ultracold Fermi gases, one now has several options for the analytic continuation. For example, one may fit the data for an observable $\mathcal{O}$ at a given temperature $T_0 = 1/\beta_0$ to the ansatz $\mathcal{O} = \sum_{n=0}^{N_{\max}} C_{\mathcal{O}}^{(n)} (\beta_0 h_I)^{2n}$. Here, $C_{\mathcal{O}}^{(n)}$ are constants determined by the fit to the data and $N_{\max}$ represents the truncation order (whose value depends on the amount of data available). Moreover, it is assumed that $\mathcal{O}$ has been made dimensionless with, e.g., a suitably chosen power of $\bar{\mu}$. By means of a simple analytic continuation of the polynomial, one then obtains the dependence of $\mathcal{O}$ on h.

Within the mean-field approximation, we find that the pressure for $0 \leq \beta_0 h \lesssim 1$ (at a temperature $T_0 = 1/\beta_0 \approx \bar{\mu}/2$) can, to a good approximation, be recovered from a fit to the imaginary-h data with $N_{\max} = 2$. Given an approximation for the pressure, one can in principle compute the energy as a function of h. At zero temperature, this would be equivalent to knowing the h-dependence of the so-called *Bertsch* parameter. However, zero-temperature values of physical observables for finite $h/\bar{\mu}$ are obviously not directly accessible within such an approach. Nonetheless, it is known from lattice MC calculations that below the superfluid transition the *Bertsch* parameter at $h = 0$ rapidly approaches its zero-temperature value [14]. In mean-field approximation we find a similar behavior, also at finite $h/\bar{\mu}$. It is therefore conceivable that a reliable estimate of the *Bertsch* parameter at $T = 0$ and finite polarization can be extracted from lattice calculations at finite temperatures and imaginary h by means of an analytic continuation.

One may perform the analytic continuation using more elaborate fit functions such as Padé approximants, also used in lattice QCD studies [10]. In Fig. 1, for example, we have reconstructed the phase boundary at real-valued asymmetry by fitting the phase transition line in the $(\beta h_I, \beta\bar{\mu})$ plane with the function

$$C \frac{1 + \sum_{i=1}^{N_{\max}} a_i [1 - \cos(\beta h_I)]^i}{1 + \sum_{j=1}^{N_{\max}} b_j [1 - \cos(\beta h_I)]^j}, \tag{5}$$

where $N_{\max}$ again defines the truncation order. The coefficients a_i, b_i, and the constant C are determined by the fit. This ansatz respects the 2π periodicity in βh_I and can be generalized to observables other than T_c. In Fig. 1 we show the results for the critical temperature T_c obtained using such a fit for $N_{\max} = 1, 2, \ldots, 5$; see Ref. [16] for details. Finally, we note that the fits may be even further optimized by choosing even more elaborate sets of basis functions [21].

We have completely disregarded any discussion of inhomogeneous phases and, in particular, the possible existence of such phases in the (T, h_I) plane. While such a discussion is left to future work, we do not expect an inhomogeneous condensate $\varphi_0(\vec{x}) \sim e^{i\vec{q}_0 \cdot \vec{x}}$ to show up for imaginary h. In its well-known form, the (center-of-mass) momentum $\vec{q}_0$ is determined by the difference in the chemical potentials of the spin-up and spin-down fermions. From a naive point of view, one expects that the solutions $\varphi_0(\vec{x})$ of the quantum equation of motion turn into $\varphi_0(\vec{x}) \sim e^{-\vec{q}_0 \cdot \vec{x}}$ for complex-valued chemical potentials and hence no longer define the ground state.

We have discussed the possibility of studying polarized Fermi gases with the aid of complex-valued chemical potentials. While the latter are not required in analytic studies, they are in MC calculations, which otherwise would suffer from the sign problem. We have argued that the (tri)critical point is in principle within reach in this framework and that the zero-temperature limit of observables might be indirectly accessible as well. This work therefore suggests that, together with the experimental data at hand, future *ab initio* MC calculations with complex-valued chemical potentials have the capacity to push our understanding of collective many-body phenomena to a new level. Our present study marks the starting point and can already be used to guide these calculations.

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