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Tan's contact and the phase distribution of repulsive Fermi gases: Insights from quantum chromodynamics noise analyses

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Path-integral analyses originally pioneered in the study of the complex-phase problem afflicting lattice calculations of finite-density quantum chromodynamics are generalized to non-relativistic Fermi gases with repulsive interactions. Using arguments similar to those previously applied to relativistic theories, we show that the analogous problem in nonrelativistic systems manifests itself naturally in Tan's contact as a nontrivial cancellation between terms with varied dependence on extensive thermodynamic quantities. We analyze that case under the assumption of gaussian phase distribution, which is supported by our Monte Carlo calculations and perturbative considerations. We further generalize these results to observables other than the contact, as well as to polarized systems and systems with fixed particle number. Our results are quite general in that they apply to repulsive multi-component fermions, are independent of dimensionality or trapping potential, and hold in the ground state as well as at finite temperature.

INTRODUCTION

Cold-atom experimentalists continue to engineer astonishing techniques to probe fundamental properties of quantum mechanics by means of multi-component gases [1–9]. Access to the properties of these remarkable systems has expanded from the simplest thermodynamic quantities to observables characterizing nuanced dynamical and information-theoretic properties (see e.g. [10, 11]). Bridging a broad range of interactions, compositions, and dimensions, this ever-expanding repertoire of techniques is both celebrated and envied by theorists, as attempting to answer similar questions about low-temperature, strongly correlated fermions has historically been a major challenge.

A major aspect of that challenge, one which is particularly formidable and also shared with lattice studies of quantum chromodynamics (QCD), is the complex phase problem associated on the one hand with non-relativistic, repulsive or imbalanced Fermi systems and on the other with QCD at finite quark density [12, 13]. In the QCD case, the problem can be traced back to the breaking of time-reversal invariance at finite chemical potential (which also appears in quasi-relativistic systems like low-energy graphene away from the Dirac point) [14, 15], which bears a strong resemblance to the (mass- or spin-) imbalanced non-relativistic Fermi gas [16]. Repulsive interactions, on the other hand, do not break time-reversal invariance per se, however that symmetry is lost upon decoupling via a Hubbard-Stratonovich transformation [17, 18]. As explained below, the partition function for N_f identical fermion species then takes the path integral form

$$\mathcal{Z}_{N_f} = \int \mathcal{D}\phi \det^{N_f} \mathcal{M}[\phi], \quad (1)$$

where the matrix \mathcal{M} and its determinant are generally complex, such that the latter cannot be used as a proba-

bility measure. In all cases, such complex-valued fermion determinants lead to exponential cancellations creating unmanageable statistical uncertainties in Monte Carlo calculations [19]. Because of its presence in the study of such a diverse class of physical systems, this difficulty has seen considerable attention from numerous perspectives ranging from polarized, low-dimensional systems, to ingenious density-of-states [12], dual variables [20], holomorphic gradient flow [21], and complex Langevin approaches to studying lattice gauge theories [22]. Sadly, as can be expected for such a ubiquitous affliction, no general solution to this problem is believed to exist [23].

Specific though these solutions must be, there is commonality between the remedies that do exist, and the sharing of intuition and techniques between the condensed-matter and high-energy communities has never failed to be a fruitful one. In Ref. [24], in particular, it was shown that by analyzing the distribution of the phase of the fermion determinant in finite-density QCD, it is possible to deduce the form of the associated free energies, and from them it is possible to cast sub-leading volume-dependent corrections to the baryon number in terms of a derivative. This insight allows for a clean demonstration of the origin of the associated signal-to-noise problem and also provides a general non-perturbative analytic tool for obtaining information about the distribution of this phase and in turn the behavior of the theory.

In this work, we generalize that noise analysis to non-relativistic many-flavor fermions with repulsive interactions at finite temperature. We show that in those systems, the phase problem manifests itself naturally in Tan's contact as a nontrivial cancellation between terms with varied dependence on extensive thermodynamic quantities. Tan's contact C has direct relevance to the physics of systems with short-range interactions studied here. Tan showed that short-distance correlations in such systems are governed by C [25]. In particular, the

high-momentum tail of the momentum distribution falls off as $n(k) \sim C/k^4$; C also governs changes in energy under adiabatic changes in the coupling (see also Ref. [26]). It was eventually shown by Braaten and colleagues [27] that the same results can be derived using the operator-product expansion of high energy physics. It was also shown that the contact appears in sum rules involving the shear and bulk viscosities, the superfluid density, and other response functions [28–30] (See also Refs. [31–34]).

We further generalize these results to observables other than the contact, as well as to polarized systems and systems with fixed particle number.

Our results hold for a much broader class of systems than discussed here, including all electronic systems. However, the simple example we provide is sufficient to demonstrate the techniques. For clarity, we maintain similar notation to Ref. [24], but we stress several points throughout our derivation as they differ significantly in our generalization of these techniques to polarized systems, which we present afterward. Finally, after briefly describing lattice Monte Carlo calculations performed to justify some key assumptions, we detail the extension of these derivations to systems at fixed particle number.

THE PHASE DISTRIBUTION OF REPULSIVE FERMION GASES

In order to make contact with previous numerical work as well as that included in this manuscript, we perform our analysis in the Hamiltonian formulation beginning with a grand canonical Hamiltonian $\hat{H} - \mu\hat{N}$ with a zero-range interaction given by

$$\hat{H} - \mu\hat{N} = \int d^d r \left[\sum_s \hat{\psi}_s^\dagger(\mathbf{r}) K \hat{\psi}_s(\mathbf{r}) + \frac{g}{2} \sum_{s \neq s'} \hat{n}_s(\mathbf{r}) \hat{n}_{s'}(\mathbf{r}) \right], \quad (2)$$

in terms of the differential operator $K = -\nabla^2/(2m) - \mu$, which incorporates the chemical potential μ and the flavor- s fermion number density $\hat{n}_s = \hat{\psi}_s^\dagger \hat{\psi}_s$ which enters quadratically paired to the bare coupling g .

We place the theory on a discrete temporal lattice of dimensionless extent $N_\tau = \lfloor \beta/\tau \rfloor \gg 1$, and after implementing a Trotter-Suzuki decomposition and an auxiliary field transformation (coupled to the density channel), we cast the partition function as

$$\mathcal{Z}_{N_f} = \text{tr} \left[e^{-\beta(\hat{H} - \mu\hat{N})} \right] = \int \mathcal{D}\phi \det^{N_f} \mathcal{M}[\phi], \quad (3)$$

The matrix $\mathcal{M}[\phi]$ encodes the dynamics of the system and separates into free and interacting components (see e.g. Ref. [39] for further details):

$$\mathcal{M}[\phi] = \mathcal{M}_0 + A\delta\mathcal{M}[\phi] \quad (4)$$

for sparse, block matrices \mathcal{M}_0 and $\delta\mathcal{M}[\phi]$ and where $A^2 = 2(e^{-\tau g} - 1)$. While the coupling enters the integrand through the parameter A , the dependence of

the full partition function on g must necessarily be only through even powers of A , because we only have two-body interactions. This distinction is essential for our generalization. For a repulsive interaction, $g > 0$ implies that A is purely imaginary so that under conjugation $A \mapsto -A$. This sign reversal is analogous to the reversal of the sign of the chemical potential in this formalism's QCD application.

In the unpolarized case, we define the phase functional $\theta[\phi]$ for a given auxiliary field configuration ϕ through

$$\det \mathcal{M}[\phi] = |\det \mathcal{M}[\phi]| e^{i\theta[\phi]}. \quad (5)$$

For the following analysis, we define the unquenched expectation value $\langle \cdot \rangle_{N_f}$ for a functional $X[\phi]$ as

$$\langle X \rangle_{N_f} = \frac{1}{\mathcal{Z}_{N_f}} \int \mathcal{D}\phi X[\phi] \det^{N_f} \mathcal{M}[\phi] \quad (6)$$

and the quenched expectation value for the same functional is

$$\langle X \rangle_{|N_f|} = \frac{1}{\mathcal{Z}_{|N_f|}} \int \mathcal{D}\phi X[\phi] |\det^{N_f} \mathcal{M}[\phi]| \quad (7)$$

with

$$\mathcal{Z}_{|N_f|} = \int \mathcal{D}\phi |\det^{N_f} \mathcal{M}[\phi]| \quad (8)$$

With these definitions, we express the probability density function for the phase in terms of the phase-quenched measure via

$$\langle \delta(\theta - \theta_0) \rangle_{N_f} = e^{iN_f\theta_0} \frac{\mathcal{Z}_{|N_f|}}{\mathcal{Z}_{N_f}} \langle \delta(\theta - \theta_0) \rangle_{|N_f|}, \quad (9)$$

Representing the delta functions of Eq. (9) in terms of their Fourier transforms, we are naturally led to consider

$$\langle e^{ip\theta} \rangle_{N_f} \propto \frac{1}{\mathcal{Z}_{N_f}} \left\langle \frac{\det^{p/2+N_f} \mathcal{M}[\phi]}{\det^{p/2} \mathcal{M}[\phi]^*} \right\rangle \quad (10)$$

in the unquenched case and

$$\langle e^{ip\theta} \rangle_{|N_f|} \propto \frac{1}{\mathcal{Z}_{|N_f|}} \left\langle \frac{\det^{p/2+N_f/2} \mathcal{M}[\phi]}{\det^{p/2-N_f/2} \mathcal{M}[\phi]^*} \right\rangle \quad (11)$$

in the quenched case for integer p , both of which can be verified using the polar form of Eq. (5). In both instances the proportionality constant is the normalization for the flat measure $\mathcal{D}\phi$ with the absence of a subscript indicating that the expectation is taken with respect to this measure.

As a result of: a) the peculiar combination of powers appearing inside the expectations present in Eqs. (10) and (11); b) the properties of the matrix $\mathcal{M}[\phi]$ under conjugation; and c) the evenness of these expressions in the

variable A ; there exist transformations under which these expressions are invariant. This is in contrast to the analogous expressions in QCD, where conditions a) and b) provide the same invariance but when instead considered in combination with the nonzero quark chemical potential. In particular, mapping $p \mapsto -2N_f - p$ is equivalent to inverting the ratio in Eq. (10). This reversal combined with evenness in A establishes the aforementioned invariance.

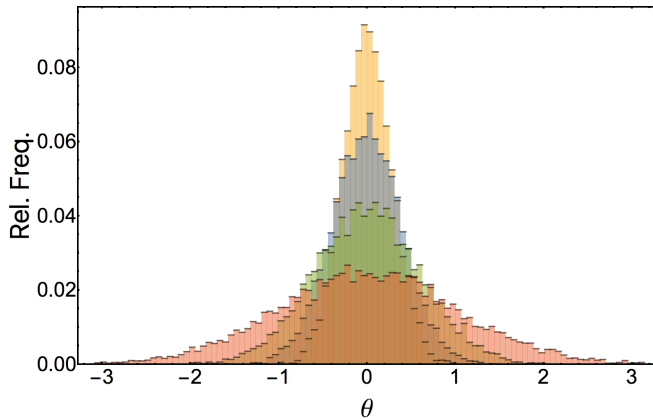


FIG. 1: (color online) Distribution of the phase for an unpolarized system of nonrelativistic repulsive fermions in 1D at finite temperature for physical dimensionless coupling $\lambda = g\sqrt{\beta}$ of $\lambda = 0.25, 0.5, 1.0$, and 2.0 (yellow, blue, green, and red, resp.); for chemical potential $\beta\mu \simeq -0.25$; and for lattice size $N_x = 41$.

Although straightforward physical interpretation requires at least the restriction of p to integer values, the functions of Eqs. (10) and (11) are defined for arbitrary p . The associated free energies $\ln\langle e^{ip\theta} \rangle_{N_f}$ and $\ln\langle e^{ip\theta} \rangle_{|N_f|}$ take the form of power series in p with necessarily extensive coefficients encoding the remaining physics, as can be easily shown via the cumulant expansion. Seeking a simple and convenient form for this power series, we note that for any δp , the transformation $p \mapsto \delta p - p$ is self-inversive so that for any function $f(p)$, the product $f(p)f(\delta p - p)$ is an invariant. Taking $f(p) = p$ provides a parameterization of this series in terms of constants X_j for $0 \leq j < \infty$ and powers of the monic quadratic polynomial $p(p + 2N_f)$. Requiring the measure be normalized eliminates the $j = 0$ contribution, and we write

$$\ln\langle e^{ip\theta} \rangle_{N_f} = - \sum_{j=1}^{\infty} X_j \left[\frac{p}{2} \left(\frac{p}{2} + N_f \right) \right]^j. \quad (12)$$

GAUSSIAN NOISE AND TAN'S CONTACT

It is desirable to truncate the series of Eq. (12) beyond the leading order in p both for the sake of convenience and because such gaussian approximations are in many

cases justified. Support for this truncation in the context of QCD is provided by studies of the phase of the fermion determinant in lattice calculations [35]. Although providing a characterization of the phase for each such system to which our generalizations are applicable is beyond the scope of this work, we do provide this inquiry for our prototype system.

Toward that end, we implement techniques similar to those in Ref. [36–39], placing the system on a Euclidean spacetime of extent $N_x \times N_\tau$ periodic in the space and anti-periodic in (imaginary) time. As shown in Fig. 1, the phase assumes a roughly gaussian distribution over a broad range of couplings with a width that grows with increasing interaction strength as expected. Approximate gaussian distributions were also found in Ref. [40] for the logarithm of the fermion determinant in a sign-problem free case of two-species fermions in the unitary limit, a property which was then used to predict the ground-state energy of the case of N_f species [41]. It is remarkable that, in the complex-phase case, the phase angle (i.e. the imaginary part of the logarithm of the determinant) also displays a gaussian shape; neither of these properties were expected, yet they are observed fairly universally (see e.g. Refs. [35, 42, 43] for evidence of their appearance, and more recently Ref. [44] where such properties were shown to be useful).

It is also worth noting that a perturbative expansion of Eqs. (10) and (11) in powers of A^2 (odd terms do not contribute for pairwise interactions like the one considered here) reveals that calculating X_j in Eq. (12) requires proceeding to order j in A^2 . In other words: at next-to-leading order, i.e. A^2 , there are no contributions beyond $j = 1$. This suggests that the main qualitative features of the sign distribution can be captured perturbatively. Specific quantitative features can be expected to be non-universal, however.

Hereafter, we truncate the expression in Eq. (12) beyond the first term, and following a Poisson resummation, the distribution of the phase takes the compactified gaussian form

$$\langle \delta(\theta - \theta_0) \rangle_{N_f} = e^{iN_f\theta_0 + X_1 N_f^2/4} \frac{1}{\sqrt{\pi X_1}} \sum_{k=-\infty}^{\infty} e^{-(\theta_0 + 2\pi k)^2 / X_1}. \quad (13)$$

With this parameterization, we turn our attention to Tan's contact, which is governed by the on-site density-density correlation

$$\hat{C} = \frac{1}{2} \int d^d r \sum_{s \neq s'} \hat{n}_s(\mathbf{r}) \hat{n}_{s'}(\mathbf{r}), \quad (14)$$

such that $\langle \hat{C} \rangle_{N_f} = \partial \ln \mathcal{Z}_{N_f} / \partial g$.

Analyzing the phase-fixed quantity $\langle \delta(\theta - \theta_0) \hat{C} \rangle_{N_f}$ by introducing a Fourier representation of the delta function

(as above), we note that

$$\langle e^{ip\hat{C}} \rangle_{N_f} = \frac{\partial}{\partial \bar{g}} \left\{ \frac{1}{\mathcal{Z}_{N_f}} \left\langle \frac{\det^{p/2} \mathcal{M}[\phi] \det^{N_f} \mathcal{M}[\phi, g = \bar{g}]}{\det^{p/2} \mathcal{M}[\phi]^*} \right\rangle_{\bar{g}=g} \right\} \quad (15)$$

As above, we expect that the free energies of the expression in braces above take the form of polynomials in the variable p with coefficients c_k that must depend on the coupling \bar{g} and therefore will be affected by the \bar{g} derivative. Using this form and identifying factors of p with the application instead of derivatives $i\partial/\partial\theta_0$, we obtain

$$\langle \delta(\theta - \theta_0) \hat{C} \rangle_{N_f} = \left(c_0 + ic_1 \frac{\partial}{\partial \theta_0} - c_2 \frac{\partial^2}{\partial \theta_0^2} \dots \right) \langle \delta(\theta - \theta_0) \rangle_{N_f}, \quad (16)$$

which, after integration over θ_0 , provides the zero mode of the distribution, namely

$$\langle \hat{C} \rangle_{N_f} = c_0, \quad (17)$$

which can also be seen easily from Eq. (15) by setting $p = 0$.

This result, as shown in Ref. [24] for the baryon number in QCD, elucidates the nature of the sign problem in these systems: The answer is entirely in the leading term; the subleading terms manifest the delicate cancellations that produce a reliable estimate of the observable. This is in contrast to the result of applying the above derivative directly to our Gaussian form for the distribution of the phase and dropping terms that grow inversely in the moment X_1 . Our generalization extends to statements made in the context of QCD regarding the orthogonality of the signal to the noise.

We have specialized the discussion to Tan's contact as thermodynamically conjugate to the coupling g , which is the natural generalization of the baryon number as conjugate to the quark chemical potential as considered in Ref. [24]. However, the result is in fact more general than advertised there: other one-body operators \hat{O} can be considered, with the corresponding modification of Eq. (15) when including such source terms $j\hat{O}$. The differentiation with respect to j would then be followed by the limit $j \rightarrow 0$, and the coefficients c_k are modified accordingly:

$$\langle \delta(\theta - \theta_0) \hat{O} \rangle_{N_f} = \left(c_{O,0} + ic_{O,1} \frac{\partial}{\partial \theta_0} - c_{O,2} \frac{\partial^2}{\partial \theta_0^2} \dots \right) \langle \delta(\theta - \theta_0) \rangle_{N_f} \quad (18)$$

It is worth noting that the case of the contact is peculiar because, even though it is a two-body operator, the Hubbard-Stratonovich transformation allows one to compute it via a single derivative, as with the one-body operator described above.

POLARIZED SYSTEMS

In order to investigate a polarized two-species gas [45–47], we return to the partition function given in Eq. (3), taking the chemical potentials $\mu_\downarrow \neq \mu_\uparrow$ to be distinct and writing

$$\mathcal{Z}_{\uparrow\downarrow} = \text{tr} \left[e^{-\beta(\hat{H} - \mu_\uparrow \hat{N}_\uparrow - \mu_\downarrow \hat{N}_\downarrow)} \right] \quad (19)$$

$$= \int \mathcal{D}\phi \det \mathcal{M}_\uparrow[\phi] \det \mathcal{M}_\downarrow[\phi], \quad (20)$$

where we have added an additional indication of which chemical potential appears in the fermion matrix $\mathcal{M}_{\uparrow,\downarrow}[\phi]$. We then write

$$\det \mathcal{M}_s[\phi] = |\det \mathcal{M}_s[\phi]| e^{i\theta_s[\phi]} \quad (21)$$

for $s = \uparrow, \downarrow$. In a fashion analogous to that presented previously, considering the joint distribution $\langle \delta(\theta_\uparrow - \theta_{\uparrow,0}) \delta(\theta_\downarrow - \theta_{\downarrow,0}) \rangle_{\uparrow\downarrow}$ immediately yields a relationship between this distribution and its value relative to the phase-quenched measure. As before, this naturally motivates the investigation of joint characteristic functions of the form

$$\langle e^{ip\theta_\uparrow} e^{iq\theta_\downarrow} \rangle_{\uparrow\downarrow} \propto \frac{1}{\mathcal{Z}_{\uparrow\downarrow}} \left\langle \frac{\det^{(p+2)/2} \mathcal{M}_\uparrow[\phi] \det^{(q+2)/2} \mathcal{M}_\downarrow[\phi]}{\det^{p/2} \mathcal{M}_\uparrow[\phi]^* \det^{q/2} \mathcal{M}_\downarrow[\phi]^*} \right\rangle \quad (22)$$

by means of their symmetries. Careful examination precludes a parameterization as simple as the one given in Eq. (12): the characteristic functions must be invariant under the transformations $p \mapsto -p - 2$ and $q \mapsto -q - 2$ taken together, but separately these replacements are not permitted. This condition can be ensured by taking

$$\ln \langle e^{ip\theta_\uparrow} e^{iq\theta_\downarrow} \rangle_{\uparrow\downarrow} = - \sum_{j=1}^{\infty} C_j(p, q). \quad (23)$$

where

$$C_j(p, q) = A_j^\uparrow p^j (p+2)^j + A_j^\downarrow q^j (q+2)^j - B_j (p-q)^{2j}, \quad (24)$$

and where the moments A_j^\uparrow , A_j^\downarrow , and B_j depend on both chemical potentials. This requirement can be seen in the residual dependence of the measure on say μ_\uparrow even in the case where $p = 0$ and similarly for the case where $q = 0$. More information can be gleaned immediately by noting that we may exchange the chemical potentials if we similarly perform the swap $p \leftrightarrow q$. This observation relates the coefficients for the homogeneous terms. Finally, it is straightforward to relate the diagonal of these coefficients to the moments X_j by taking the chemical potentials to be as in the previous section and equating the phases. Truncating this expression again at first order, we may again perform a Poisson resummation, and the result of this calculation provides access to an analysis similar to that previously obtained for the contact. More general systems including copies of each flavor are approachable by essentially the same techniques [56].

FINITE SYSTEMS

In order to comment on systems at fixed particle number, we restrict the grand-canonical partition function via Fourier projection writing the canonical partition function for an N -particle system via

$$Q_N = \int \mathcal{D}\phi P_N[\phi] \quad (25)$$

where

$$P_N[\phi] = \frac{1}{2\pi} \int_0^{2\pi} d\alpha e^{-iN\alpha} \det^{N_f}(\mathbb{1} + e^{i\alpha}\mathcal{U}[\phi]), \quad (26)$$

where the matrix \mathcal{U} contains all the physical input for the system (see e.g. [39]). Analysis of this measure leads to characteristic functions of the form

$$\frac{1}{Q_N} \int \mathcal{D}\phi P_N[\phi] e^{ip\theta} \propto \frac{1}{Q_N} \left\langle \frac{P_N^{(p+2)/2}[\phi]}{P_N^{p/2}[\phi]^*} \right\rangle, \quad (27)$$

where now we must require integer N so that by a change of variables, the denominator can be rewritten so as to be accessible by techniques described earlier. After changing variables, we find again that the conjugation amounts to reversing the sign of A , and the above expressions are invariant under the transformation $p \mapsto -p - 2$. The analysis then proceeds as detailed previously.

SUMMARY AND CONCLUSIONS

In this work, we have elucidated the origin of the debilitating fluctuations in lattice Monte Carlo calculations of the Tan contact in repulsive Fermi systems, and we investigated similar issues in polarized nonrelativistic gases as well as in systems projected to fixed particle content. We have, furthermore, generalized the analysis of Tan's contact to arbitrary one-body operators.

We accomplished the above by generalizing techniques used to study the baryon number for finite-density QCD, and by showing that similar arguments provide insight into the complex phase problem encountered in the exploration of the repulsive sector of the parameter space. In these systems, some previous analytic work carries over almost without modification, although key dissimilarities force a different correspondence: the phase problem in finite-density QCD is due to explicit breaking of time-reversal invariance, while in repulsive Fermi gases it is due to the signature of the interaction; furthermore, rather than glean information about particle number from the fluctuations in the action, we are led naturally to relations involving Tan's contact. Specifically, we show the direct relationship between Tan's contact and the zero mode of the phase distribution, which also indicates the delicate cancellations that must take place between

the higher-order terms (i.e. the features) of said phase distribution.

In addition to the concrete insights provided by our analysis, we have demonstrated the applicability of a huge variety of techniques outside of their original domains, as similar partition-function-based analytic methods, with a basis in random matrix theory, have been applied in the context of lattice QCD, successfully providing a wealth of information beyond that which has been generalized above [48, 49].

We perform lattice Monte Carlo calculations to verify that the onset of these phase problems indeed present quasi-Gaussian phase distributions. Studying repulsive, finite-temperature fermions in one spatial dimension, we found results similar to those originally used to justify the application of these techniques in relativistic theories. A perturbative analysis of the problem indicates a direct connection between moments of the phase distribution and orders in perturbation theory: at a given order in the latter, contributions are only present in moments of up to a fixed order and otherwise vanish. Clearly, the accessibility of these insights to perturbation theory suggests they could be further explored combining methods detailed above with recent advances [50].

After providing this analogy and detailing the numerical calculations required to verify key assumptions, we demonstrated that the technique applies further still to the case of a general two-species gas, and we have detailed the modifications made to pivotal algebraic arguments. Polarized systems require that the generally distinct fermion determinants be treated independently, and the two resulting phase angles lead to generalized free energies that are multi-variate polynomials. Finally, we show that our insights apply equally well to systems at fixed particle number. This generality establishes numerous directions for further inquiry, all of which necessarily beyond the scope of the present study.

Although we have considered the case of two-body contact interactions exclusively, we expect our results to generalize to more general interactions and to mixed Bose-Fermi ensembles, a subject of growing relevance [51–55]. We leave such investigation for future study.

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- [56] In that case, Eq. (24) is modified in two ways. First, the homogeneous terms are invariant under different transformations, each depending on the relative abundance of each flavor. Second, the factors comprising the inhomogeneous term also include as a summand the difference

between these two transformations so that it remains invariant under their combination.