Spontaneous inhomogeneous phases in ultracold dipolar Fermi gases

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(Received 18 March 2010; revised manuscript received 13 July 2010; published 5 August 2010)

We study the collapse of ultracold fermionic gases into inhomogeneous states due to strong dipolar interaction in both two-dimensions (2D) and three-dimensions (3D). Depending on the dimensionality, we find that two different types of inhomogeneous states are stabilized once the dipole moment reaches a critical value $d > d_c$: the stripe phase and phase separation between high and low densities. In 2D, we prove that the stripe phase is always favored for $d > d_c$, regardless of the microscopic details of the system. In 3D, the one-loop perturbative calculation suggests that the same type of instability leads to phase separation. Experimental detection and finite-temperature effects are discussed.

DOI: 10.1103/PhysRevB.82.075105 PACS number(s): 03.75.Ss, 05.30.Fk, 71.45.Lr, 71.10.Ay

I. INTRODUCTION

The rapid experimental development of ultracold atomic and molecular physics has opened up new opportunities to study quantum many-body systems with electric and magnetic dipolar interactions. An important feature of dipolar interaction is its explicit spatial anisotropy of the $d_{2s-3p}$-type when dipole moments are aligned by external fields. For the fermionic dipolar systems, $^{40}$K- $^{87}$Rb has been cooled down almost to quantum degeneracy. Anisotropic Fermi liquid theories of the single particle and collective properties have been investigated. Furthermore, unconventional Cooper pairing structures have been studied, including the $p_z$-channel pairing in the single-component systems, and the competition between the $s+d$-wave singlet and the $p_z$-wave triplet channels. In particular, a novel pairing state of the $s+ip$ type broken time-reversal symmetry has been pointed out. Moreover, magnetic dipolar systems of fermions have also been experimentally realized. Exotic states of the ferro-nematic Fermi liquid and unconventional magnetic states have been predicted.

Fermionic systems can spontaneously break translational symmetry in both charge and spin channels. Many years ago, Overhauser pointed out that even in the weak coupling regime of the interacting electron gas, a $2k_F$ spin-density wave state always wins over the uniform paramagnetic state at the Hartree-Fock level. However, correlation effects may suppress this instability and such a state has not been experimentally confirmed. Recently, quantum liquid crystal phases in strongly correlated systems have been intensively studied, particularly in doped Mott insulators. Stripe ordering has been observed in high $T_c$ cuprates, other transition metal oxides, and quantum Hall systems at high Landau levels.

In this paper, we study the instability toward the spontaneous inhomogeneous phase in dipolar fermionic systems. In two-dimensional (2D) systems, the strongest density-channel instability occurs at nonzero momentum, which drives the density wave states under strong dipolar interactions. This effect is based on the peculiar feature of the Fourier transform of the dipolar interaction, which is robust against microscopic details. However in three-dimensions (3D), the instability at the one-loop level occurs at zero momentum, thus it leads to phase separation into high and low density regions.

This paper is organized as follows: in Sec. II, we construct the model Hamiltonian for a single-component dipolar Fermi gas and present the calculation of the static susceptibility of density fluctuations via diagrammatic expansion. Then, we study the instability of the homogeneous ground state in 2D and 3D in Secs. III and IV correspondingly. Here, we present both a nonperturbative conclusion, which is based on the analytic property of the susceptibility and the leading-order perturbative calculation, which is use to testify the nonperturbative conclusion. The experimental detection is then discussed in Sec. V. Finally, we conclude our paper by studying the contributions of thermal fluctuations at finite temperature and the effects of higher-order terms in Sec. VI.

II. MODEL

We consider the single-component dipolar Fermi gas with dipole moment aligned by an external electric field (Fig. 1). The long-distance physics of this system is described by the following Hamiltonian

$$H = \sum_{\mathbf{k}} (\epsilon_k - \mu) c_{\mathbf{k}}^\dagger c_{\mathbf{k}} + \sum_{\mathbf{k},\mathbf{q}} V(\mathbf{q}) c_{\mathbf{k}+\mathbf{q}}^\dagger c_{\mathbf{k}-\mathbf{q}}^\dagger c_{\mathbf{k}-\mathbf{q}} c_{\mathbf{k}} ,$$

with $\epsilon_k$ being the energy dispersion relation and $\mu$ the chemical potential. In 2D, the dipolar interaction in the momentum space $V_{2D}(\mathbf{q})$ takes the form.

![FIG. 1. (Color online) The stripe phase in 2D dipolar gases. The three dotted arrows mark the x, y and z axes. The lighter (darker) regions in the 2D plane represent higher (lower) density. The solid line with an arrow represents the direction of the external field, which aligns the direction of the dipoles.](Image)
\[ V_{2D}(\vec{q}) = 2\pi d^2 P_2(\cos \theta) \left[ \frac{1}{e} - q \right] + \pi q d^2 \sin^2 \theta \cos 2\phi_q, \]

where \( d \) is the dipole moment; \( \phi_q \) is the azimuthal angle of the momentum \( \vec{q} \) and \( \theta \) is the angle between the direction of the dipoles and the \( z \) axis. \( e \) is a short-range cutoff roughly equal to the thickness of the system along the \( z \) direction.

Equation (2) is valid for \( qe \ll 1 \). However, as shown below, the main conclusion of this paper only relies on the value of \( V(\vec{q}) \) at small \( q \), and hence all the qualitative results remain invariant even if more accurate and more complicated interactions were taken into account. We shall also emphasize here that for \( \theta = 0 \), \( V_{2D}(\vec{q}) \) is invariant under \( \text{SO}(2) \) rotations. However, for any \( \theta \neq 0 \), the rotational symmetry is reduced to twofold (\( C_2 \)). This symmetry property is crucial as a system undergoes the transition to a charge-density-wave (CDW) phase. As will be discussed below, in a system with \( \text{SO}(2) \) symmetry, the CDW instability usually leads to the formation of a unidirectional \( \text{CDW} \). Using the technique of the diagrammatic expansion, we prove that this system leading to the condensation of density waves. Obviously, \( \Delta_{2D}(\vec{q}) \) is positive definite for any \( \vec{q} \) in the noninteracting Fermi gas. This stability remains for a weakly interacting Fermi liquid. On the other hand, if the interaction has an attractive channel [e.g., the dipolar interaction in Eq. (4)], an inhomogeneous state could take advantage of the attractive interaction. Under strong enough attractive interactions, i.e., \( V_{2D} \to \infty \), the homogeneous ground state is unstable.

III. STRIPE PHASES IN 2D

We begin from the weak coupling side, by tuning up the interaction strength. In general, there is a critical dipole moment \( d_c \) such that \( \Delta_{2D}(\vec{q}) > 0 \) at any \( \vec{q} \) for \( d < d_c \), but \( \Delta_{2D}(\vec{q}) < 0 \) at some \( \vec{q} \) for \( d > d_c \). At \( d = d_c \), \( \Delta_{2D}(\vec{q} = \vec{Q}) = 0 \) for the momenta \( \vec{Q} \) and remain positive at other momenta. If we increase \( d \) further above \( d_c \), the density waves fluctuate with momentum \( \vec{q} \sim \vec{Q} \) undergo an instability and condense. Depending on whether \( \vec{Q} = 0 \) or not, this instability has two different fates. If \( \vec{Q} > 0 \), the condensation carries a nonzero momentum, which leads to a stripe state: a unidirectional charge-density-wave state with wave vector \( \vec{Q} \). On the other hand, if \( \vec{Q} = 0 \), the condensation takes place at an infinite wavelength and results in phase separation between high and low density regions. Here, the typical size of these high (low) density regions and their spatial arrangements are determined by the microscopic details of the system. In the particular case of a dipolar gas, the phase separation is sensitive to the details of the short-range behaviors of the interaction.

A. \( \theta = \theta_0 \)

Due to the 2D space-inversion symmetry \( \hat{r} \to -\hat{r} \), \( [\Pi_{2D}^{IR}(\vec{q}, \omega)]^{-1} \) is an even function of \( \vec{q} \). As a result, the Taylor expansion of \( \Delta_{2D}(\vec{q}) \) at small momentum must take the following form:

\[ \Delta_{2D}(\vec{q}) = [\Pi_{2D}^{IR}(\vec{q}, \omega)]^{-1} + \frac{2\pi d^2}{3} q \cos 2\phi_q + \frac{1}{2} \sum_{i,j} \partial_i \partial_j [\Pi_{2D}^{IR}(\vec{q}, \omega)]^{-1} \big|_{\vec{q}=0} \partial_i \vec{q} \partial_j \vec{q} + \cdots. \]  

At small momentum, \( q \to 0 \), Eq. (8) was dominated by the first two terms. And hence the point \( \vec{q} = 0 \) is a local saddle point of \( \Delta_{2D}(\vec{q}) \) (i.e., a local minimum along the line of \( \phi_q = \pi/2 \)). Since \( q = 0 \) is a saddle point, instead of the minimum point of \( \Delta_{2D}(\vec{q}) \), as \( d \) increases, \( \Delta_{2D}(\vec{q}) \) at some finite momentum will become negative before \( \Delta_{2D}(\vec{q} = 0) \) could reach zero. Thus, \( Q \) must be
a nonzero value, which indicates that the system will collapse into a stripe phase for \(d > d_c\), instead of phase separating. This is the main conclusion of this paper. It is noteworthy that this conclusion only depends on the small-momentum (i.e., long-range) behaviors of the interaction \(V(q)\). Therefore, the stripe instability is a universal property of the 2D dipolar Fermi gas at \(d > d_c\), insensitive to the microscopic details of the system. In 2D electron gases, a similar conclusion has been found in the classical limit at high temperature when the quantum fluctuations are negligible.\(^3\)

We emphasize that the conclusion that \(Q > 0\) is a nonperturbative result which remains valid to any order in the loop expansion of Fig. 2. The only assumption required here is the analyticity of \(\Pi^{1\text{IR}}_{2D}(\q, \omega = 0)\) as a function of \(\q\) near \(\q = 0\). In a Fermi liquid, it is well known that \(\Pi^{1\text{IR}}_{2D}(\q, \omega = 0)\) is nonanalytic at \(\q = 2k_F\) where \(k_F\) is the Fermi wave vector. However, there is no reason of a nonanalytic behavior at small momentum in any Fermi liquid to our knowledge. The higher-order diagrams in Fig. 2 contain interaction lines which are nonanalytic at small momenta. However, due to the fact that dipolar interactions are short ranged in 2D, we do not expect any singularity for \(\Pi^{1\text{IR}}_{2D}(\q, \omega = 0)\) around \(\q = 0\).

We check this conclusion using the loop expansion in Fig. 2 to the one-loop level for a 2D system at \(T = 0\) in continuum (\(\epsilon_k = k^2/2m\) with \(m\) being the mass of the particles) and find

\[
\Delta_{2D}(\q) = \frac{2\pi}{m} \left[ \frac{1}{1 - \sqrt{1 - \frac{1}{x} \sin(1 - x)}} + \frac{d^2}{d^2_c} x \cos 2\phi_q \right],
\]

where \(x = q/2k_F\) and \(d_c\) is the critical dipole momentum \(d_c = (3/(2k_Fm))^{1/3}\). \(\phi_q\) is the azimuthal angle of the momentum \(\q\) and \(\eta(x)\) is a step function with \(\eta(x) = 1\) for \(x > 0\) and \(\eta(x) = 0\) for \(x < 0\). As shown in Fig. 3(a), the order wave vector \(Q = 2k_F\). In experiments, it is often more convenient to vary the density for a constant \(d\). There, the density needs to be higher than a critical value to reach the stripe phase. For KRB (\(d = 0.057\) D) the stripe phase requires the interparticle spacing to be smaller than \(\sim 10^{-4}\) cm, and for LiCs (\(d = 5.5\) D), the critical spacing is \(\sim 10^{-2}\) cm. We emphasize that \(Q\) and \(d_c\), we found here are based on the leading order approximation, and can be renormalized by higher-order corrections. However, the fact that \(Q > 0\) remains valid, which is one of the key conclusion of this work.

\[\text{FIG. 3. (Color online) One-loop calculation of } \Delta_q(\q) \text{ in (a) 2D and (b) 3D. In the 2D case, we choose } \phi_q = \frac{\pi}{2} \text{ and for the 3D, } \theta_q = \pi/2. \text{ From top to bottom, the dipole momentum for each of the curves are: } d/d_c = 0, 0.9, 1, \text{ and } 1.1 \text{ respectively. The dashed vertical line marks the momentum } 2k_F.\]

For \(\theta \neq \theta_0\), the same conclusion applies for the single-component case. The \(\epsilon\)-term in Eq. (2) is momentum independent, which corresponds to short-range contact interaction. Thus it has no effect on the single-component fermions, and hence

\[
V(q) = q^2 \pi d^2 \left[ -2P_2(\cos \theta) \sin^2 \theta \cos 2\phi_q \right].
\]

Along \(\phi_q = \frac{\pi}{2}\) which remains the direction of the strongest instability,

\[
V(q) = -2q^2 \pi d^2 \cos^2 \theta,
\]

which is negative and grows linearly with \(q\) for an arbitrary value of \(\theta\). Thus, the above conclusion still holds. We notice that even for \(\theta = 0\), i.e., when the dipoles are perpendicular to the plane, the stripe instability still exists at large values of \(d\) although the interaction is now repulsive. For such an isotropic system (at \(\theta = 0\)), it is often assumed that three charge density waves form a triangular lattice to minimize the breaking of the rotational symmetry.\(^3\) However, if the rotational symmetry is spontaneously broken before the homogeneous state becomes unstable, a stripe phase can be stabilized at zero temperature.\(^3\) In this case, the stripe ordering spontaneously breaks both the rotational symmetry and the translational symmetry in the direction perpendicular to the stripes, while only the latter is spontaneously breaking in the stripe phases at \(\theta \neq 0\). Due to its unique symmetry breaking pattern, the low-energy properties of the stripe phase at \(\theta = 0\) is described by the quantum McMillan-de Gennes theory, which is fundamentally different from other similar phases at \(\theta = 0\).\(^3\) As a result, the stripe phase at \(\theta = 0\) is unstable at any finite temperature due to thermal fluctuations.\(^3\) While the stripe phases at \(\theta \neq 0\) has a power-law quasi-long-range order blow a transition temperature \(T_{KT}\) (See below).

\[\text{IV. FERMIIONS IN 3D AND MULTICOMPONENT FERMIIONS}\]

In this section, we study two more classes of systems with similar dipolar interactions: (a) dipolar gases in 3D and (b) 2D dipolar gases composed by multicomponent fermions.

In 3D, the dipolar interaction is

\[
V_{3D}(\q) = \frac{8 \pi d^2}{3} P_2(\cos \theta_q),
\]

with \(\theta_q\) measuring the angle between \(\q\) and the dipole moment. Due to the structure of \(V_{3D}\), the linear term of \(\q\) in Eq. (8) is now absent in 3D, and hence we could not exclude the possibility of \(\q\) being zero. In fact, the one-loop calculation at \(T = 0\) for a system in continuum shows that

\[
\Delta_{3D}(\q) = \frac{4\pi^2}{m k_F} \left[ \left( 1 + \frac{1 - x^2}{2x} \log \frac{1 + x}{1 - x} \right)^{-1} d^2 \right] + \frac{d^2}{d^2_c} \left( 3 \cos \theta_q^2 - 1 \right),
\]

where \(x = q/2k_F\) and \(d_c = \sqrt{16\pi}/(k_F m)\). As can be seen from
in the one-loop approximation, implying a phenomenon of phase separation for \(d > d_c\). As discussed above, this is sensitive to the short-range details of the interaction and no universal conclusion is available for the case.

Now we briefly discuss the multicomponent case in 2D (e.g., the degrees of freedom of hyperfine spins) whose Hamiltonian is

\[
H = \sum_{\mathbf{k}, \sigma} (\epsilon_{k} - \mu) c_{\mathbf{k}, \sigma}^\dagger c_{\mathbf{k}, \sigma} + \sum_{\mathbf{k}, \mathbf{q}, \sigma, \sigma'} V(\mathbf{q}) c_{\mathbf{k}+\mathbf{q}, \sigma}^\dagger c_{\mathbf{k}, \sigma}^\dagger c_{\mathbf{k}+\mathbf{q}, \sigma'} c_{\mathbf{k}, \sigma'},
\]

where the spin indices \(\sigma\) and \(\sigma'\) run from \(-N/2\) to \(+N/2\) for some integer \(N\). Here, \(V(\mathbf{q})\) remains the same as the single-component case in Eqs. (2) and (12). For a single-component dipolar gas, due to Pauli exclusion principle, the \(e\)-term in Eq. (2) (short-range interactions) has no contribution to any physical properties of the system. However, for multicomponent fermion gases, this term naturally exists in the intercomponent interactions and suppresses the stripe instability if it is repulsive. For simplicity we only consider the case of \(N = 2\). For \(\theta > \theta_0 (\theta < \theta_0)\), this short-range part is attractive (repulsive), and hence the stripe state become unfavorable for \(\theta < \theta_0\). Furthermore, such an finite momentum instability does not exist in the spin channel because the spin channel interaction arises from the exchange interaction which is regular for small vector of \(\mathbf{q}\).

\section{V. Experimental Detection}

The stripe phase has a density modulation in the direction perpendicular to the stripes, which can be detected directly via the measurement of the local densities. In addition, any scattering experiments would show two interference Bragg peaks at momentum \(\pm \mathbf{Q}\) in a stripe phase due to this density modulation.

There are also other indirect tools to detect a stripe phase. Considering a density wave with density varying along the \(y\) axis, whose density profile (to the leading order) is

\[
\rho(x, y) = \rho_0 + \rho_1 \cos(Qy + \phi),
\]

with \((x, y)\) being the 2D coordinate in the real space, if we place this system in a shallow potential trap and then introduce an extra narrow one-dimensional (1D) potential well along the direction of the stripe, for example,

\[
V(x, y) = -\alpha \delta(y - y_0),
\]

it is energetically favorable to have \(y = y_0\) being a high density region due to the potential well \(V(x, y)\). We emphasize that in reality, this 1D potential well of \(V(x, y)\) shall have a finite width in the \(y\) direction. However, as long as the width is much smaller than the wavelength of the stripe, one can treat it as a \(\delta\) function to the leading order approximation. If we move the potential trap along the \(x\) direction but keep the location of the potential well \(V(x, y)\) unchanged, the stripes will largely remain at their initial positions if the displacement of the trap is less than half the wavelength of the stripes \(\pi/\mathbf{Q}\), and the stripes will jump over a distance of \(2\pi/\mathbf{Q}\) if the displacement becomes larger than \(\pi/\mathbf{Q}\) to same the potential energy. On the other hand, the jump would not happen in a homogeneous state. This jump will lead to a center of mass oscillation for the trapped particles due to the lack of dissipation, which could serve as an indirect signature for the stripe phase.

This technique is in close analogy to the “pinning” effect, which was used to experimentally distinguish the nematic phase from a putative stripe phase in two-dimensional electron gases (2DEG) under high magnetic field.\(^{40–42}\) There, the impurities in the crystal provide similar effects as the local potential in Eq. (16), which will pin down the stripe if the stripe exists. In principle, the presence of stripes will lead to the pinning effect, which shall result in nonlinear signal in the \(I-V\) curve at low bias. However, in the 2DEG under high magnetic field, the absence of such a nonlinear \(I-V\) curve was interpreted as the absence of the stripe ordering. Different from the 2DEG, in the case we studied here, the similar pinning effect would lead to oscillations for a system with stripe ordering, due to the absence of dissipation in ultracold dipolar gases.

\section{VI. Discussions}

Since a real system has a finite temperature, the contribution of the thermal fluctuations comes into play. Their effects can be studied based on the symmetry-breaking pattern of the ordered phase. For a 2D system in the continuum, the homogeneous phase at \(d < d_c\) has continuous translational and twofold rotational symmetries (rotation by \(\pi\)) at \(\theta \neq 0\). For \(d > d_c\), the stripe phase spontaneously breaks the continuous translational symmetry in one direction and leads to one gapless Goldstone mode as required by symmetry. In a 2D system with \(d > d_c\), if we increase the temperature from \(T=0\), such a Goldstone mode will destroy the long-range order of the stripe phase. However, a quasi-long-range power-law correlation would still remain for temperature below a transition temperature \(T_{KT}\).\(^{39}\) For \(T < T_{KT}\), although the real-space density oscillation of the stripes is hard to observe due to the lack of a true long-range order, the density profile in Fourier space will have two peaks located at \(\pm \mathbf{Q}\) which decays as a power-law function of \(|\mathbf{q}| < \mathbf{Q}|\). Above \(T_{KT}\), the correlation becomes short-ranged and the phase transition at \(T = T_{KT}\) belongs to the usual Kosterlitz-Thouless (KT) universality class.

For dipolar molecules in a 2D optical lattice, if the wave vector of the stripe phase is commensurate with the lattice wave vector, the stripe phase breaks no continuous symmetry and hence no gapless Goldstone mode is present. Therefore, the long-range order of the stripe phase remains at finite \(T\) below a critical temperature \(T_C\). However, if the stripe phase is incommensurate with the underlying lattice, a KT transition is expected.

In the study of Secs. III and IV, we were focusing on the susceptibility shown in Eq. (5). Effectively, this procedure is equivalent and closely related to the linear-response approximation. Thus, the higher-order terms beyond the liner-
response approximation were ignored in our study. These higher-order terms are highly nontrivial and could become nonlocal at certain wave vector. For example, the free energy contains terms proportional to \( \rho(q)^{3/2} \) or \( \rho(q)^{7/2} \) at \( q \sim 2k_F \), as shown in Refs. 43 and 34. Although these terms could be studied perturbatively within certain approximations, there is no available technique to take care of them nonperturbatively in a general way. In general, the contributions of these higher-order terms are nonuniversal. In the case of a second-order phase transition, from the homogeneous phase to the inhomogeneous phase, these higher-order term are unimportant at low energy and hence all the conclusions above remains. However, if the transition is first order, their contributions could become dominant. For a system with short-range interactions only, a first order transition is usually believed to leads to phase separation (as in the liquid/gas-solid transition). However, it was also shown that a stripe phase was favored in the presence of long-range interactions like Coulomb or dipolar interactions. This effect, where a long-range Coulomb interaction stabilizes the stripe ordering, was referred to as the Coulomb frustration.

In summary, we find that the 2D dipolar Fermi gas undergoes a stripe ordering at large dipolar interaction strength, i.e., the density wave instability at finite momentum, instead of phase separation. For the single-component case, this instability occurs regardless of the dipole orientation. This arises from the fact that the Fourier transform of the dipolar interaction increases linearly with wave vector. For the multicomponent case, due to the short-range Hartree interaction, the stripe instability only exists at \( \theta > \theta_0 \).

Note added. After the completion of the first online version of the manuscript, we learned of the work by Yamaguchi et al. in which the charge-density-wave instability of dipolar Fermi gas is studied using mean-field approximation.

ACKNOWLEDGMENTS

K.S. and S.D.S. are supported by JQI-NSF-PFC and AFOSR-MURI. C.W. is supported by NSF under Grant No. DMR-0804775, and Sloan Research Foundation.

37 The degeneracy between \( \bar{Q} \) and \( -\bar{Q} \) is due to the space-inversion symmetry \( \vec{r} \rightarrow -\vec{r} \).