Itinerant Ferromagnetism in an Ultracold Atom Fermi Gas

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We address the possible occurrence of ultracold atom ferromagnetism by evaluating the free energy of a spin polarized Fermi gas to second order in its interaction parameter. We find that Hartree-Fock theory underestimates the tendency toward ferromagnetism, predict that the ferromagnetic transition is first order at low temperatures, and point out that the spin coherence time of gases prepared in a ferromagnetic state is strongly enhanced as the transition is approached. We relate our results to recent experiments.

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Introduction.—Itinerant ferromagnetism is common in metals. Nevertheless, because it flows from a strong-coupling Fermi-liquid instability, the microscopic physics that controls its occurrence is less well understood than the physics that controls superconductivity [1]. In the electron gas case, for example, accurate quantum Monte Carlo calculations suggest [2] that the transition to the ferromagnetic state occurs at a critical density nearly 3 orders of magnitude smaller than that predicted by mean-field (Hartree-Fock) theory. Even in the simplest model of interacting electrons, the single-band Hubbard model, solid predictions on the occurrence of ferromagnetism are rare and often restricted to particular band fillings [3,4]. Understanding the nature of the paramagnetic to ferromagnetic phase transition, when it occurs, has also been challenging. Experimental progress has recently been achieved by applying hydrostatic pressure to itinerant ferromagnets with a low Curie temperature, making it possible to study the transition in the zero-temperature limit and to test for theoretically predicted quantum critical [5] behavior. In these experiments, the line of continuous transitions in the temperature-pressure phase diagram appears [6–9] to terminate at a tricritical point with decreasing temperature, connecting with a low-temperature line of first-order transitions. In mean-field theory, first-order magnetic transitions can follow from a nonmonotonic quasiparticle density of states near the paramagnetic state's Fermi energy [10]. Belitz *et al.* [11] have argued, however, that coupling of the order parameter to gapless modes leads to nonanalytic terms in the free energy and generically drives the transition first order. These nonanalytic terms were first predicted by Misawa on the basis of Fermi-liquid theory [12] and are a consequence of gapless particle-hole excitations. Theories of the phase transition are still qualitative, however, and detailed experimental corroboration of this picture is still lacking.

In this Letter, we address the possible complementary realization of ferromagnetism in ultracold fermionic atoms, which are accurately described by a short-range interaction model [13,14]. In Hartree-Fock theory [13,15], the zero-temperature ferromagnetic transition of this model is continuous, and the ground state is ferromagnetic when the gas parameter, i.e., the product of the Fermi wave number k_F of the unpolarized system and the s-wave scattering length a of the short-range potential, satisfies $k_F a \geq \pi/2$. The phase separation predicted by Houbiers *et al.* [16] at the same gas parameter is one plausible manifestation of ferromagnetism but, as we discuss below, not the most likely one. Trapped-atom motivated inhomogeneous generalizations of these Hartree-Fock theories have recently been analyzed by Salasnich *et al.* [17] and Sogo and Yabu [18].

The issue of ferromagnetism in a two-component atomic Fermi gas is of particular interest because of the ongoing experimental study of strongly interacting, degenerate, fermionic alkali atoms [19–25]. The focus so far has been on observing the formation of a fermion pair condensate [26–35] in the BCS-BEC crossover [36–38] regime close to a Feshbach resonance [39,40]. Our interest is in the repulsive interaction side of the resonance, where we believe it will be possible to achieve unprecedented experimental control over ferromagnetism. In making this assertion, we are assuming that the formation time of the molecular Bose-Einstein condensate (BEC) state (which occurs under the same conditions when the state is prepared by crossing from the attractive interaction side of the resonance) can exceed experimental time scales when the state is prepared by approaching the resonance from the repulsive interaction side. Moreover, the ferromagnetic transition temperatures turn out to be high compared to, for example, typical BCS transition temperatures. This implies that, in equilibrium at these temperatures, there will be a significant fraction of atoms that is not bound into Cooper pairs or molecules. On the BEC side of the resonance, these atoms will have strongly repulsive interactions and may, therefore, undergo a transition to the ferromagnetic state.

The character of the ferromagnetic state that can be realized experimentally in these systems requires some comment [41]. Since s-wave scattering does not occur between identical fermions, interaction effects require the presence of two hyperfine (pseudospin) species. Using

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standard techniques, the atomic system can be prepared in a pseudospin coherent (ferromagnetic) state, in which all atoms share the same spinor:

$$|\Psi_{\mathrm{FM}}(t)\rangle = \frac{1}{\sqrt{2}} \prod_{|\mathbf{k}|<2^{1/3}k_{\mathrm{F}}} (c^{\dagger}_{\mathbf{k},\uparrow} + e^{i(\varphi - \Delta E t/\hbar)} c^{\dagger}_{\mathbf{k},\downarrow})|\mathrm{vac}\rangle. \quad (1)$$

($c^{\dagger}_{\mathbf{k},\alpha}$ creates an atom with momentum $\mathbf{k}$ and hyperfine spin α.) In Eq. (1), φ specifies the orientation of the magnetic order parameter in the $x-y$ plane and ΔE is the Zeeman energy difference between the hyperfine states. (Since the number of atoms in each is conserved, we can transform to a rotating wave picture and let $\Delta E \to 0$.) Overall spin polarizations in the $\hat{z}$ direction are not accessible. This fully spin coherent state always has a lower energy than the phase-separated state discussed in Refs. [16–18] since, in the magnetic language, the latter has a domain wall which costs finite energy. Ferromagnetism in these systems will be manifested by persistent coherence between hyperfine states.

In this Letter, we argue that ferromagnetism occurs on the repulsive interaction side of a Feshbach resonance. Our principle results are summarized in Figs. 1 and 3. We find that (i) Hartree-Fock theory underestimates the tendency towards ferromagnetism [42], (ii) the transition between ferromagnetic and paramagnetic states is first-order at low temperatures, and (iii) the coherence decay rate decreases rapidly as the thermodynamic stability region of the ferromagnetic state is approached from the repulsive side of the resonance.

Second-order perturbation theory.—It is convenient to view the gas as a mixture of two independent noninteracting gases of spinless fermions. The grand-canonical Hamiltonian of the system is then

$$H = \int d\mathbf{x} \sum_{\alpha=\{+,-\}} \psi^{\dagger}_{\alpha}(\mathbf{x}) \left(-\frac{\hbar^2 \nabla^2}{2m} - \mu_{\alpha} \right) \psi_{\alpha}(\mathbf{x}) + g \int d\mathbf{x} \psi^{\dagger}_{+}(\mathbf{x}) \psi^{\dagger}_{-}(\mathbf{x}) \psi_{-}(\mathbf{x}) \psi_{+}(\mathbf{x}), \quad (2)$$

with $g = 4\pi a \hbar^2/m$. The chemical potentials are determined by $n_{\alpha} = \partial p_{0\alpha}/\partial \mu_{\alpha}$, where n_{α} is the density of atoms in hyperfine state $|\alpha\rangle$, and the pressure of the noninteracting gas is given by

$$p_{0\alpha} = \frac{k_{\mathrm{B}} T}{V} \sum_{\mathbf{k}} \ln[1 + e^{-\beta(\epsilon_{\mathbf{k}} - \mu_{\alpha})}], \quad (3)$$

with $k_{\mathrm{B}}T$ the thermal energy, V the volume, and $\epsilon_{\mathbf{k}} = \hbar^2 \mathbf{k}^2/2m$ the single-particle dispersion. The entropy density is determined by $s = \partial(p_{0+} + p_{0-})/\partial T$, and the total free energy density is given by $f(n_+, n_-) = e - Ts$, with the total energy density expressed as the sum of three contributions, $e = e^{(0)} + e^{(1)} + e^{(2)}$. The first two contributions correspond to Hartree-Fock theory and are given by

$$e^{(0)} + e^{(1)} = \frac{1}{V} \sum_{\mathbf{k}} \left[\sum_{\alpha=\{+,-\}} N_{\mathbf{k},\alpha} \epsilon_{\mathbf{k}} \right] + g n_+ n_-, \quad (4)$$

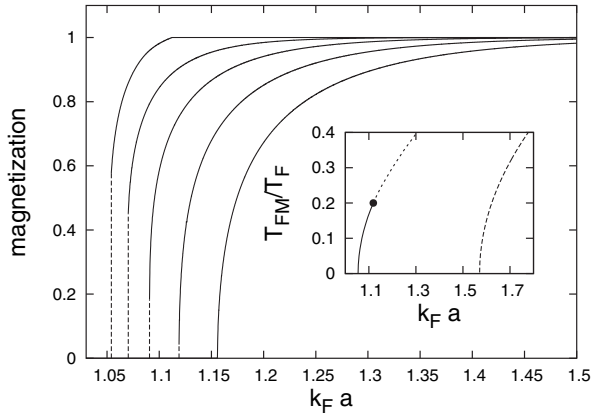

FIG. 1. Magnetization ξ as a function of $k_{\mathrm{F}}a$, for various temperatures. From left to right $T/T_{\mathrm{F}} = 0, 0.1, 0.15, 0.2, 0.25$. The dashed lines indicate magnetization jumps. The inset shows the critical temperature as a function of the gas parameter. The solid line indicates first-order transitions, and the dotted line second-order transitions. The dashed line is the Hartree-Fock theory result.

where $N_{\mathbf{k},\alpha}$ is a Fermi occupation factor. The contribution to the energy density that is second-order in interactions is given by [13]

$$e^{(2)} = -\frac{2g^2}{V^3} \sum{}' \frac{N_{\mathbf{k}_1,+} N_{\mathbf{k}_2,-} (N_{\mathbf{k}_3,+} + N_{\mathbf{k}_4,-})}{\epsilon_{\mathbf{k}_1} + \epsilon_{\mathbf{k}_2} - \epsilon_{\mathbf{k}_3} - \epsilon_{\mathbf{k}_4}}, \quad (5)$$

where the prime indicates that the sum is over wave vectors such that $\mathbf{k}_1 + \mathbf{k}_2 = \mathbf{k}_3 + \mathbf{k}_4$. The above second-order correction takes into account the so-called unitarity limit, i.e., the energy dependence of the vacuum scattering amplitude to all orders in ka, to second order [43]. Note also that, because of the use of the renormalized interaction strength g, this second-order term is not negative definite as in the case of the electron gas.

Results.—The magnetization results, summarized in Fig. 1, were obtained by numerically minimizing the total free energy $f(n_-, n_+)$ vs $\xi \equiv (n_+ - n_-)/(n_+ + n_-)$ for a series of temperatures and total densities $n_+ + n_- = k_{\mathrm{F}}^3/3\pi^2$. At zero temperature, we find that the system becomes partially polarized if $k_{\mathrm{F}}a \geq 1.054$ and reaches the fully polarized state at $k_{\mathrm{F}}a = 1.112$. For higher temperatures, interactions have to be stronger to polarize the system. For temperatures $T < T_{\mathrm{tc}}$, where $T_{\mathrm{tc}} \simeq 0.2 T_{\mathrm{F}}$, with T_{F} the Fermi temperature, the transition is discontinuous, and the magnetization exhibits a jump. The jump becomes smaller with increasing temperature, vanishing at T_{tc}. The inset shows the transition temperature as a function of $k_{\mathrm{F}}a$. A line of first-order transitions, denoted by the solid line, joins a line of continuous transitions, denoted by the dotted line at $T = T_{\mathrm{tc}}$ and $k_{\mathrm{F}}a = 1.119$.

The first-order behavior at low temperatures is expected on the basis of the arguments of Belitz *et al.* [11]. In our case, the gapless modes that drive the transition first order are particle-hole excitations. The coupling of these excitations to the magnetization is neglected in Hartree-Fock

theory, which therefore always predicts a continuous transition. Equation (5) takes the coupling between the magnetization and the particle-hole excitations into account to lowest order.

Experimental implications.—The ferromagnetic state can be identified by measuring the interaction energy, either by studying the expansion properties of the gas [44] or by using radio frequency spectroscopy [33–35,45]. The fully polarized state is distinguished by the absence of any interaction energy. In the experiments by Bourdel *et al.* [44] on ^{6}Li gases, the interaction energy appears to vanish when the regime of strong repulsive interactions is approached. In Fig. 2, we plot the interaction energy divided by the kinetic energy for their experimental parameters, as a function of the magnetic field. Given the fact that we have not taken into account the inhomogeneity of the system, the agreement is remarkable, suggesting that a ferromagnetic transition occurs in this system. (For other possible explanations of these experiments, see Refs. [46,47].) If we interpret the experimental data accordingly, the transition is found to occur at $k_F a \simeq 1$ at $T = 0.6T_F$, which is slightly smaller than our calculated value ($k_F a = 1.56$) at this temperature. In the experiments of Gupta *et al.* [34], the value of $k_F a$ at which the mean-field shift appears to vanish is even smaller compared to the value we predict for the onset of ferromagnetism. Since the atom system in these experiments is prepared in a ferromagnetic state, these discrepancies between theory and experiment could be due to the rapid increase in spin coherence time which is expected as stable ferromagnetism is approached, as we now explain.

Pseudospin decoherence in these systems is due to spatial inhomogeneities in the Zeeman energy ΔE. Suppose the potential the $|\uparrow\rangle$ atoms feel is $E^{\uparrow}(\mathbf{x})$, and the potential the $|\downarrow\rangle$ atoms feel is $E^{\downarrow}(\mathbf{x})$. The decay rate of the fully coherent state is suppressed because the quasiparticle energies of the unoccupied pseudospins are shifted by the interactions. Fermi's golden rule implies a coherence decay rate

$$\Gamma = \frac{2\pi}{\hbar} \sum_{\mathbf{k}',\mathbf{k}} |\Delta E_{\mathbf{k}',\mathbf{k}}|^2 \delta(\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}'} - gn)(N_{\mathbf{k},+} - N_{\mathbf{k}',-}), \quad (6)$$

where

$$\Delta E_{\mathbf{k}',\mathbf{k}} = \frac{1}{V} \int d\mathbf{x} \left(\frac{E^{\uparrow}(\mathbf{x}) - E^{\downarrow}(\mathbf{x})}{2} \right) e^{i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{x}}. \quad (7)$$

The consequences of interactions can be illustrated by taking $|\Delta E_{\mathbf{k}',\mathbf{k}}|^2 = \delta E^2 e^{-\Lambda^2(\mathbf{k}-\mathbf{k}')^2}$ where Λ is the length scale of magnetic-field inhomogeneities. In Fig. 3, the $T = 0$ spin coherence time is shown for a series values of Λ. These results were obtained by taking a trapping frequency $\omega/2\pi = 20$ Hz, estimating δE as the difference in Zeeman splitting change between the edge and the center of the cloud, and assuming 7×10^6 atoms at a density $n \sim 4 \times 10^{13}$ cm^{-3}, following Gupta *et al.* [34]. Clearly, the spin coherence time is strongly enhanced for increasing interactions. The difference in experimental results between Bourdel *et al.* [44] and Gupta *et al.* [34] might be related to differences in magnetic field. We note that the magnetic-field inhomogeneities are necessary for the equilibration of the hyperfine spin degrees of freedom. Since molecule formation cannot occur in the fully polarized state, ferromagnetism competes kinetically with Bose-Einstein condensation of molecules [41].

Coherence decay and atomic ferromagnetism can also be studied by measuring the size of the cloud. In a local density approximation, valid since the oscillator length exceeds the Fermi wavelength, the size of the cloud is proportional to the square root of the Fermi energy. It follows that the radius of the fully polarized state is a factor $2^{1/3}$ larger than that of the unpolarized state. The first-order character of the phase transition could be detected by performing experiments with a mixture of fermions and bosons. (The interactions between bosons and the fermions

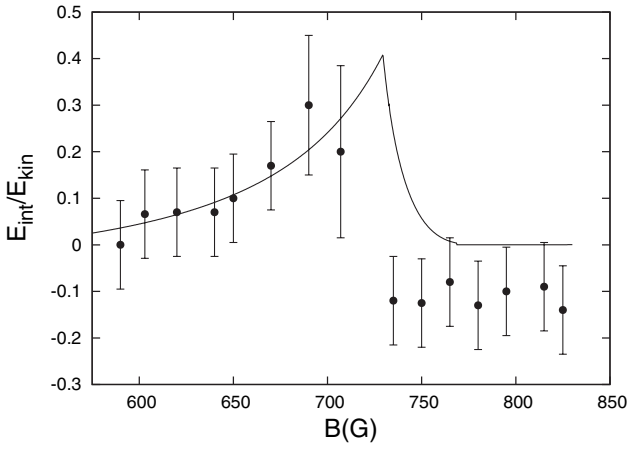

FIG. 2. Interaction energy divided by kinetic energy as a function of magnetic field for the experimental parameters of Bourdel *et al.* [44]. We take a temperature $T = 3.5\ \mu\text{K} = 0.6T_F$. For details on the magnetic-field dependence of the scattering length, see, for example, Ref. [44].

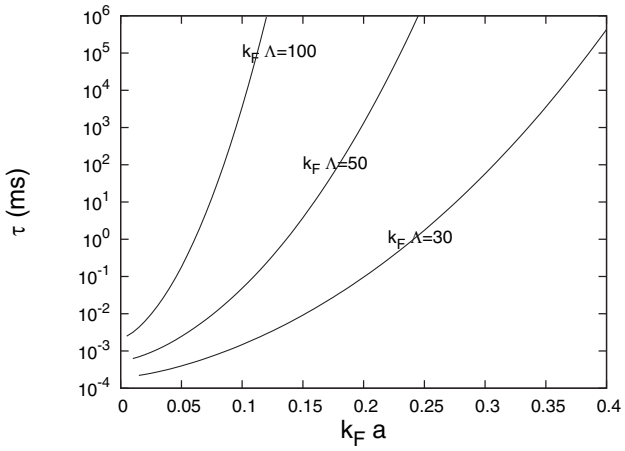

FIG. 3. Magnetic-field inhomogeneity limit on the spin coherence time of the fully polarized state.

should be weak enough to make boson mediated attractive interactions between fermions negligible.) Suppose, for example, that the mixed system is in equilibrium and that the energy and number of atoms are conserved as the bias field is varied. Adiabatically increasing $k_F a$ from the paramagnetic to the ferromagnetic regime will lead to a temperature increase that is tied to the entropy reduction in the ordered state. For $T < T_{tc}$, the temperature variation should be hysteretic. These temperature changes, although typically relatively small ($\sim 10^{-3} T_F$), are larger for a smaller boson to fermion mass ratio and boson concentration and might be observable.

Discussion and conclusion.—Although ferromagnetism is a strong-coupling instability and our theory is perturbative, we nevertheless believe that the phase diagram in the inset in Fig. 1 is reliable. The interaction energy of the fully polarized state, which is an eigenstate of the full Hamiltonian, is exactly zero. Moreover, a calculation to third order in the gas parameter shows that the energy of the paramagnetic state energy is increased in comparison to the second-order result [48]. Hence, we expect that the second-order perturbation theory underestimates the transition gas parameter. However, since consistency requires that the critical point lies in the strong-coupling regime where $k_F a \sim 1$, there appears to be little room for movement. An experimental determination of the phase diagram appears to be within reach and would be interesting.

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