Stability of a Fully Magnetized Ferromagnetic state in Repulsively Interacting Ultracold Fermi Gases

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We construct a variational wave function to study whether a fully polarized Fermi sea of ultracold atoms is energetically stable against a single spin flip. Our variational wavefunction contains short-range correlations at least to the same level as Gutzwiller’s projected wavefunction. For the Hubbard lattice model and the continuum model with pure repulsive interaction, we show a fully polarized Fermi sea is generally unstable even for infinite repulsive strength. By contrast for a resonance model, the ferromagnetic state is possible if the s-wave scattering length is positive and sufficiently large and the system is prepared to be orthogonal to molecular bound state. However, we can not rule out the possibility that more exotic correlation can destabilize the ferromagnetic state.

Whether a fermion system with repulsive interaction will become ferromagnetic is a long-standing problem in condensed matter physics. Early in 1930’s, Stoner used a simple mean-field theory to predict that ferromagnetism will always take place with sufficient large repulsive interaction \[1\]. However, this conclusion is later challenged by Gutzwiller who took the short-range correlation into account \[2\]. So far, except a few specific cases \[3, 4\], there is no conclusive result on itinerant ferromagnetism. Recently, MIT group reports an experiment on itinerant fermions in an ultracold Fermi gas with large positive scattering length close to a Feshbach resonance \[5\], and they attribute their observations to Stoner ferromagnetism by comparing to theories \[3, 7\]. However, these theories are basically mean-field theory or a second-order perturbation, which neither include the Gutzwiller type short-range correlation nor consider the unitary limited interaction nearby Feshbach resonance. Moreover many of the experimental signatures can be reproduced qualitatively by a non-magnetic correlated state \[8\]. Thus, it calls for a serious study including the effects of both correlation and unitarity in this problem.

In this Rapid Communication we address the question whether a fully magnetized state is stable against a single spin flip. We compare the energy of \(N + 1\) spin-up particles with that of one spin-down particle and \(N\) spin-up particles. A fully magnetized ferromagnetic state is definitely unstable if we can find a variational state of the latter whose energy is lower. Similar idea has been used previously in studying the stability of Nagaoka ferromagnetism in the Hubbard model \[3, 6, 11\], and attractively interacting Fermi gases with large population imbalance \[12, 13\]. In this work, we will explore different realizations of “repulsive interactions” in ultracold Fermi gases:

(I) Single-band Hubbard model in a two-dimensional (2D) square or three-dimensional (3D) cubic lattice. The Hamiltonian \(\hat{H} = \hat{H}_t + \hat{H}_{\text{int}}, \hat{H}_t = -t \sum_{(ij),\sigma} c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.},\) where \((ij)\) are nearest-neighbor sites, and \(\hat{H}_{\text{int}} = U \sum_i n_{i\uparrow} n_{i\downarrow} \quad (U > 0)\).

(II) Continuum model with finite-range interaction potential in three dimension. \(\hat{H} = \sum_{\kappa \sigma} c_{\kappa \sigma}^\dagger c_{\kappa \sigma} + (1/\Omega) \sum_{\mathbf{q}, \mathbf{k}, \mathbf{k}'} V(\mathbf{k} - \mathbf{k}') c_{\mathbf{q} + \mathbf{k}'}^\dagger c_{\mathbf{q} - \mathbf{k}}^\dagger c_{\mathbf{q} + \mathbf{k}}^\uparrow.\) Here \(c_{\mathbf{k}} = k^2/(2m), \Omega\) is system volume, and \(V(\mathbf{k})\) is the Fourier transformation of real space interaction potential \(V(x)\). Let \(r_0\) be the interaction range, and thus \(V(|\mathbf{k}|) \rightarrow 0 \quad |\mathbf{k}| > r_0\). For the convenience of later calculations, we adopt s-wave separable potential \(V(\mathbf{k} - \mathbf{k}') = U w(\mathbf{k}) w(\mathbf{k}')\), and approximate \(w(\mathbf{k}) = 1/\sqrt{1+e^{\alpha(|\mathbf{k}| - k_c)/k_0}}\) with \(\alpha \gg 1\).

The s-wave scattering length \(a_s\) is related to \(U/m(4\pi a_s) = 1/(1/\Omega) \sum_{|\mathbf{k}|=0} \mathbf{k} = 1/(2\mathbf{k})\), where \(k_c = k_0 \ln(1 + e^{\alpha})/\alpha\) for a repulsive interaction \(U > 0\). \(a_s\) is positive but upper bounded by \(\pi/(2k_c)\) at \(U \rightarrow +\infty\), and no bound state exists; for an attractive \(U < 0\), \(a_s\) diverges at \(U_c = -2\pi^2/(mk_c)\), and only a sufficient attraction \(U < U_c\) with \(a_s > 0\) can support a two-body bound state.

(III) Continuum model with zero-range interaction potential in three dimension. \(\hat{H} = \sum_{\kappa \sigma} c_{\kappa \sigma}^\dagger c_{\kappa \sigma} + g \sum_{\mathbf{q}, \mathbf{k}, \mathbf{k}'} c_{\mathbf{q} + \mathbf{k}'}^\dagger c_{\mathbf{q} - \mathbf{k}}^\dagger c_{\mathbf{q} + \mathbf{k}}^\uparrow,\) and \(g\) is related to \(a_s\) by \(m/(4\pi a_s) = 1/g + (1/\Omega) \sum_{|\mathbf{k}|=0} \infty \mathbf{k} = 1/(2\mathbf{k})\). There is always a two-body bound state when \(a_s > 0\).

The single-band Hubbard model, as a simplified model for cold atoms in optical lattices (valid when interaction smaller than band gap) and many correlated materials, has been extensively studied before \[3, 9-11\]. The comparison to previous known results justifies the validity of our approach and calibrates the correlation incorporated in our variational wavefunction (w.f.). Then we apply our method to continuum models which are commonly-used for quantum gases and are of our primary interests.

The variational w.f. we used for one down-spin system is similar to that used in the discussion of imbalanced Fermi gases \[12\], which is

\[
\langle \Psi | = \left( \phi_{\mathbf{q}_0 \uparrow} + \sum_{\mathbf{k} > \mathbf{k}_F, \mathbf{q} < \mathbf{k}_F} \phi_{\mathbf{k} \mathbf{q} \uparrow} \phi_{\mathbf{q} - \mathbf{k} \uparrow} \phi_{\mathbf{q} \uparrow} + \ldots \right) | \mathbf{N} \rangle
\]

where \(| \mathbf{N} \rangle\) represents a Fermi sea of \(N\)-spin up particles with Fermi momentum \(k_F\). “...” in (1) represents terms...
contains more than one particle-hole pairs of spin-up particles. We compute the energy $E$ (measured from energy of $|N\rangle$) of $|\Psi\rangle$, and compare it with $E_F = (E_{|N+1\rangle} - E_{|N\rangle})$. Our main results are summarized as follows.

First, for the single-band Hubbard model, we show that under certain conditions, $H_{\text{int}}|\Psi\rangle = 0$ and $E = \langle \Psi | H_I | \Psi \rangle < E_F$ for most range of particle filling, except for nearby half-filling where the ground state is rigorously proved to be ferromagnetic by Nakaoka [3]. (See Fig. 1). This result agrees with previous studies by various other methods [8, 9, 11]; We show that the real space representation of $|\Psi\rangle$ corresponds to Gutzwiller’s w.f. with optimized “backflow” type corrections, which implies $|\Psi\rangle$ includes short-range correlations at least as the Gutzwiller projection. Similarly for the finite-range continuum model, we find $E < E_F$ for all range of $U > 0$. (See Fig. 2). This shows that generally in a purely repulsive interaction model, a fully magnetized fermionic state can not be ground state even for infinite $U$, which is in sharp contrast to Stoner’s mean-field conclusion.

Second, for the zero-range continuum model, apart from the polaron state with negative energy discussed before in Ref. [10, 12, 13], we find the w.f. orthogonal to the polaron state has a positive $E$ for $a_0 > 0$. At small $k_F a_0$, $E$ as a function of $k_F a_0$ follows the prediction of perturbation expansion very well. At large $k_F a_0$, $E$ saturates (due to unitarity) to $1.82 E_F$. Below $k_F a_0^c = 2.35$, we can find variational state with which $E < E_F$, but fail to find such cases otherwise. (See Fig. 3). This result contradicts to the previous prediction $k_F a_0^c = 1.40$ based on perturbation theory [8, 12]. Thus the necessary condition for ferromagnetism is a large enough $a_0 \gtrsim 2.35/k_F$, which requires a sufficiently attractive interaction potential to support a bound state and cause resonant scattering, and more importantly the system has to be prepared in the metastable scattering state that is orthogonal to molecule state. Nevertheless, our method can not prove this is a sufficient condition. Similar result is found for the finite-range model with $U < 0$ and nearby scattering resonance. The details of our calculation are explained below.

**Single-band Hubbard model:** Here we can first prove

Theorem 1: Under two conditions that (i) $\phi_{kq} \equiv \phi_k$ independent of $q$, and (ii) $\phi_0 = -\sum_{k>k_F} \phi_k$, the w.f.

$$|\psi\rangle_1 = \left( \phi_0 c_{q_0 \uparrow}^\dagger + \sum_{k>k_F, q<k_F} \phi_k c_{q_0 \uparrow + q - k \uparrow}^\dagger u_{q k}^\dagger \right) |N\rangle,$$

(2)

is an exact eigenstate of $\hat{H}_{\text{int}}$, and $\hat{H}_{\text{int}}|\psi\rangle_1 = 0$.

This theorem can be verified straightforwardly. The subscript 1 of $|\psi\rangle_1$ means it contains one particle-hole pairs of up-spins, and the best variational energy for this state is denoted by $E^{(1)}$. Condition (i) ensures that $\hat{H}_{\text{int}}$ acting onto $|\psi\rangle_1$ will not generate two particle-hole term, and condition (ii) ensures zero interaction energy. For an intuitive understanding of this zero interaction energy, we can Fourier transfer it to real space. Using condition (ii),

one can show the w.f. 2 is equivalent to

$$\left( \phi_0 \sqrt{N_s} \sum_m c_{m \uparrow}^\dagger \mathcal{P}_m + \sum_{n \neq m} \phi_{mn} c_{mn \uparrow}^\dagger c_{m \uparrow}^\dagger \right) e^{i q_0 n m} |N\rangle.$$

Here $\mathcal{P}_m = 1 - c_{m \uparrow} c_{m \uparrow}^\dagger$ presents standard Gutzwiller projection operator, $N_s$ is the number of lattice sites, $\phi_{mn} = \sum_{k>q} \phi_k e^{i k (m-n)}$, and the second term presents “backflow” type corrections. It becomes obvious that there will be no double occupancy and no interaction energy. Hence, we have established a momentum space w.f. representation of short-range correlation, which can be generalized to free space straightforwardly.

Next we try to find the minimum total(=kinetic) energy by introducing a Lagrange multiplier that can be proved as just the total energy $E^{(1)}$ (counted from the band bottom), $\mathcal{F} = \langle \psi | H_I | \psi \rangle - E^{(1)} (\psi|\psi\rangle$. Minimization of $\mathcal{F}$ gives $q_0 = 0$ and the self-consistent equation

$$\sum_{k>k_F} \frac{\mathcal{F}}{E^{(1)} - \mathcal{F}(1)} (ek_{kq} - E^{(1)}(1)) = 1,$$

(3)

in which $\epsilon_{kq} = \epsilon_{k-q} + \epsilon_k - \epsilon_q$. Its solution gives $E^{(1)}$.

$\delta E = E^{(1)} - E_F$ as a function of particle density $\rho$ in a cubic and a square lattice is plotted in Fig. 4. We find for $\rho < \rho_c$, $\delta E < 0$ means the ferromagnetic state is always unstable even for infinite $U$. In fact, for a cubic lattice, when $\rho \to 0$, $E^{(1)}$ goes like $\rho$ while $E_F$ goes like $\rho^{2/3}$, hence $\delta E$ is negative and shows a much rapid decrease compared with the square lattice. While for $\rho > \rho_c$, $\delta E > 0$, this is consistent with Nagaoka theorem, which forces $\delta E$ to be positive when $\rho \to 1$. $\rho_c$ obtained as 0.59 (0.76) for the square (cubic) lattice agree with previous studies by a finite-size real space evaluation [10] or by using Green functions [11]. By contrast, our variational w.f. (Eq. 2) greatly simplifies the calculation, and also enable calculations in the thermodynamic limit simply by employing density of state in a one-dimensional integral equation. Moreover, this w.f. can be systematically improved by including multiple particle-hole contributions.

**Theorem 2:** Consider the wave function $|\psi\rangle_n$ that con-
tains up to \( n \) particle-hole pairs

\[
\sum_{m=0}^{n} \frac{1}{(m!)^2} \sum_{\{k\}^m_1;\{q\}^m_1} \phi^{(m)}_{\{k\}^m_1;\{q\}^m_1} \mathcal{C}_{\{q\}^m_1} \prod_{i=1}^{m} \epsilon_{k_i} \prod_{j=1}^{m} \epsilon_{q_i} |N\rangle
\]

with \( \mathcal{C}_{\{q\}^m_1} = q_0 + \sum_{i=1}^{m} (q_i - k_i) \), where \( \{k\}^m_1 \) denotes a set \( \{k_1, \ldots, k_m\} \) and \( \{q\}^m_1 \) denotes \( \{q_1, \ldots, q_m\} \). It satisfies \( H_{\text{int}} |\psi\rangle_n = 0 \) under the condition (i) \( \phi^{(m)}_{\{k\}^m_1;\{q\}^m_1} \) can be expressed as \( B^{(m)}_{\{k\}^m_1;\{q\}^m_1} = B^{(n)}_{\{k\}^m_1;\{q\}^m_1} + \ldots + (-1)^{m-1} B^{(m)}_{\{k\}^m_1;\{q\}^m_1} + C^{(m)}_{\{k\}^m_1;\{q\}^m_1} \), with \( B^{(0)} = 0 \), \( C^{(0)} = \phi^{(0)}; \) \( C^{(n)}_{\{k\}^m_1;\{q\}^m_1} = 0 \); and (ii) \( C^{(m-1)}_{\{k\}^m_1;\{q\}^m_1} + \sum_{\{m\}} B^{(m)}_{\{k\}^m_1;\{q\}^m_1} = 0 \) for any \( \{k\}^m_1 \) and \( \{q\}^m_1 \).

Similar to Theorem 1, this theorem can be verified straightforwardly, and condition (i) ensures \( H_{\text{int}} \) acting on \( |\psi\rangle_n \) will not generate \( n + 1 \) particle-hole terms, and condition (ii) ensures zero-energy. Obviously, \( |\psi\rangle_n \) is a special case of \( |\psi\rangle_n \), and hence \( E^{(n)} \leq E^{(n-1)} \), where \( E^{(n)} \) is the best variational energy for \( |\psi\rangle_n \). By including more particle-hole terms, one can always further lower \( E \), and make \( \rho_e \) more close to unity. On the other hand, one can also prove limit \( \rho_e \to 0 \), where \( \{k\}^m_1 \) is given by the integral

\[
\frac{E}{E_F} = 2 \int_0^1 dq \int_0^\infty d\tilde{k} \tilde{k}^2 \sin \theta \left( \frac{1}{2k_F a} - 1 + g \left( \frac{E}{E_F}, \tilde{q} \right) \right)^{-1}
\]

where \( \tilde{q} = q/k_F \) and \( \tilde{k} = k/k_F \). For this model there is always a bound state in a two-body problem for \( a_n > 0 \), and correspondingly, there is always a polaron solution with negative \( E \) when \( a_n > 0 \), which has been extensively discussed in Ref. [12]. In addition, there is always a positive energy solution orthogonal to the polaron solution. For small \( k_F a_n \), applying the second-order perturbation theory [16] to this case, one will obtain

\[
E / E_F = 4 k_F a_n / (3 \pi) + 2 (k_F a_n)^2 / 2.5
\]

It is found our variational results fit quite well to this expansion in the regime \( |k_F a_n| \leq 0.6 \) (see inset of Fig. 3), and start to deviate substantially when \( k_F a_n \geq 0.6 \). At \( k_F a_n \to +\infty \), we find the energy under this trial w.f. saturates at 1.82\( E_F \) instead of diverging as perturbation theory predicts. This saturation is due to unitary limit of resonance interaction. We find \( E < E_F \) for \( k_F a_n < 2.35 \), which means a fully polarized ferromagnetism is definitely unstable below a critical \( k_F a_n^c = 2.35 \). It contradicts to previous results based on a second-order perturbation [7] which predicts the system becomes fully magnetized at \( k_F a_n = 1.40 \) [17]. The reason for this discrepancy is because the second order perturbation overestimates the interaction effects in the regime \( k_F a_n > 1 \). Similar behavior is found for a resonance scattering with finite interaction range, as shown in the \( U_0 < 0 \) part of Fig. 2(a).
We would like to point out several intrinsic relations between (a) single-band Hubbard model at $U \gg t$, (b) finite-range continuum model at $U_0 = +\infty$ and (c) zero-range continuum model at $a_s = +\infty$. First is the relation between the coefficient of different terms in the w. f. (Eq. 2): for (b) we have $\phi_0 + \sum_{k > k_F} w_k \phi_k = 0$; this is equivalent to (a) with all $w_k = 1$ and a momentum cut-off imposed by $\pi/a_l$ instead of $k_0$ ($a_l$ is the lattice constant); for (c) we can define $\chi_0 = \phi_0 + \sum_{k > k_F} w_k \phi_k$ then we have $\phi_{kq} = \chi_0 / (E - \epsilon_{kq})$ with $\chi_0 = g \chi_q / \Omega_0$, so at unitary limit one can get similar relation as $\phi_0 + \sum_{k > k_F} (\phi_q + \chi_0 / (2c_k)) + \sum_{q < k_F} 1 / (2c_q) = 0$. Second, for (a) at low density limit and (b) with $k_F \ll k_0$ we can show $E / E_F \sim k_F r_{\text{eff}}$, here the effective range $r_{\text{eff}} = a_l$ for (a), and $1/k_0$ for (b), which directly leads to the instability of ferromagnetism in these limits; while (c) does not fall into the class of pure repulsive interactions.

The calculation above uses the w.f. that contains only one particle-hole pairs of up-spins. Including multiple particle-hole pairs can systematically improve the results, lead to further lower $E$ and increased $k_F a_s^c$. However, from the experience in studies of polaron branch, it is found the single particle-hole w.f. can already produce a result very close to Monte Carlo simulation [14] and later experiments [15], and the reason for this perfect agreement is understood as a nearly perfect destructive interference of higher-order particle-hole contributions [13]. Hence it is unlikely $E / E_F$ at resonance can be reduced from 1.82 to below unity. Even though, we only prove ferromagnetic is stable against single spin flip above a critical $k_F a_s^c$, and we can not rule out the possibility that a state with more down-spin can be energetically more favorable due to more exotic correlations.

Our results bring forward two intriguing issues. (i) for $0.6 \lesssim k_F a_s < 2.35$, the system cannot be fully ferromagnetic nor be well described by perturbation theory. It is in a very interesting strongly interacting quantum phase with large ferromagnetic and/or short-range fluctuations; (ii) for $k_F a_s > 2.35$, our approach predicts the system will become ferromagnetic. If it is true, what is the smoking gun experimental evidence? If future experiments find it is not true, then it means the system contains much stronger correlations than discussed here.

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[17] $k_F$ in our paper is the Fermi momentum for a fully polarized state, thus differs by a factor of $2^{1/3}$ from that previously defined for each component in a non-magnetic state [3,8]. Hence the prediction for fully polarized state $k_F a_s^c = 1.112$ [3,8] is translated to 1.40 to compare with our result (2.35). Our result should be translated to 1.87 to compare with MIT experiment [3,8].
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