Repulsive polarons in two-dimensional Fermi gases

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Abstract – We consider a single spin-down impurity atom interacting via an attractive, short-range potential with a spin-up Fermi sea in two dimensions (2D). Similarly to 3D, we show how the impurity can form a metastable state (the “repulsive polaron”) with energy greater than that of the non-interacting impurity. Moreover, we find that the repulsive polaron can acquire a finite momentum for sufficiently weak attractive interactions. Even though the energy of the repulsive polaron can become sizeable, we argue that saturated ferromagnetism is unfavorable in 2D because of the polaron’s finite lifetime and small quasiparticle weight.

Introduction. – The Fermi gas with effectively repulsive, short-range interactions provides a model system in which to investigate magnetic instabilities of the Fermi liquid state. Of particular interest is the putative Stoner transition to itinerant ferromagnetism, which is driven purely by the repulsive interactions. Such a scenario can potentially be realized and investigated with ultracold, dilute gases of atoms [1]. However, recent cold-atom experiments in three dimensions (3D) have cast doubt on whether the Stoner transition can ever be realized in a strongly repulsive Fermi gas with short-range interactions [2]. The central issue is that strongly repulsive interactions in 3D can only be truly short-ranged if the underlying potential is attractive. This necessarily demands that any magnetic phase be metastable at best, since the true ground state will involve attractively interacting pairs of \(\uparrow\) and \(\downarrow\) fermions. In 3D, the ferromagnetic state is apparently never stable [2–4], thus a key question is whether this is also true in lower dimensions.

Lowering the dimensionality will strongly modify both the two-body scattering properties and the many-body properties. In 1D, it is in fact permissible to have purely repulsive contact interactions, but here the Lieb-Mattis theorem precludes any ferromagnetic ground state [5]. The situation is less clear in 2D, however, where one still requires an underlying attractive potential to generate strong, short-range repulsive interactions, but in contrast to 3D there is always a two-body bound state and the two-body scattering amplitude is energy dependent, even at low energies [6].

Fortunately, 2D Fermi gases have recently been realized in cold-atom experiments [7–13], making it an ideal time in which to investigate ferromagnetism in 2D. Theories based on a mean-field approach currently support the existence of itinerant ferromagnetism [14]. However, given the importance of quantum fluctuations [14], we ideally want to explore limits of the problem where the theory is more controlled. To this end, we consider the limit of extreme spin imbalance, where we have one spin-down “impurity” immersed in a Fermi sea of spin-up particles. Here, theoretical approaches based on simple variational wave functions [15,16] have proved to be extremely reliable in 3D when compared with experiments [17,18] and quantum Monte Carlo simulations [19,20]. Thus far, the ground state of the 2D impurity problem has been theoretically investigated [21–23], and it has even been suggested that recent 2D experiments have already observed single-impurity physics [24].

In this letter, we show how a \(\downarrow\)-impurity interacting attractively with a \(\uparrow\) Fermi sea in 2D can form a metastable state —the so-called “repulsive polaron”— with energy greater than that of the non-interacting impurity. Our focus is on equal masses \((m_\uparrow = m_\downarrow)\), given its relevance to current cold-atom experiments and ferromagnetism, but we also investigate how the repulsive polaron depends on the mass ratio \(m_\uparrow/m_\downarrow\). As the attraction is decreased, we find that the energy \(E_+\) of the repulsive polaron increases and eventually surpasses the Fermi energy \(\varepsilon_F\) of the spin-up Fermi sea. Moreover, we find that the repulsive polaron acquires a finite momentum for
sufficiently weak attraction. However, its decay to the ground-state “attractive” polaron is also enhanced when $E_+ \approx \varepsilon_F$, which suggests that saturated ferromagnetism is unlikely to exist in 2D, as we argue below.

**Methods.** In the following, we consider a two-component ($\uparrow$, $\downarrow$) 2D Fermi system with short-range attractive interactions, described by the Hamiltonian

$$H = \sum_{p\sigma} \epsilon_p^\sigma c_p^{\sigma\dagger}c_p^\sigma + \frac{g}{\Omega} \sum_{kpq} \epsilon_{kq}^{\uparrow} c_{kp}^{\uparrow\dagger} c_{p+q-k}^{\uparrow\dagger} c_{-q}^{\downarrow}, \quad (1)$$

where $\epsilon_p^\sigma = p^2/2m_\sigma$ (with $h \equiv 1$), $\Omega$ is the system area and $g$ is the bare coupling constant describing the interspecies contact interaction. In addition we note that, for fermions, the interaction is interspecies only since the exclusion principle forbids interspecies $s$-wave scattering. In 2D, the bare coupling strength can be related to the two-body binding energy $\varepsilon_B$, which is always present for attractive interactions in 2D, via [6]

$$\frac{1}{g} = \frac{1}{\Omega} \sum_{\varepsilon_B} \frac{1}{\varepsilon_B + \epsilon_p^\uparrow + \epsilon_p^\downarrow}. \quad (2)$$

The cut-off momentum $\Lambda$ can be sent to infinity at the end of the calculation.

To proceed, we adopt the variational polaron wave function introduced in ref. [15],

$$|P\rangle = \alpha_0^{(p)} c_{p\downarrow}^\dagger |FS\rangle + \sum_{kq} \alpha_{kq}^{(p)} c_{p+q-k\downarrow}^\dagger c_{k\uparrow}^\dagger |FS\rangle. \quad (3)$$

The first term on the r.h.s. describes a bare impurity and the second term takes into account one particle-hole pair excitation of the Fermi sea, $|FS\rangle$. The polaron ground-state energy is determined by minimising $\langle P|H|P\rangle$ while keeping $\langle P|P\rangle = 1$. The variational approach can also be generalized to study metastable excited states such as the repulsive polaron by instead minimising the action $\int dt \langle P|(i\hbar \partial_t - H)|P\rangle$—see, e.g., ref. [25] for further details. Equivalently, one can use the diagrammatic method in which the interspecies interaction is treated in the ladder approximation [26]. This yields the expression for the self-energy

$$\Sigma(p, E) = \sum_q \left[ \frac{\Omega}{g} \sum_k \frac{1}{E + i0^+ - E_{kq,p}} \right]^{-1}. \quad (4)$$

$E_{kq,p} = \epsilon_{p+q-k}^{\downarrow} + \epsilon_k^{\uparrow} - \epsilon_q^{\downarrow}$ and $E$ measures the energy change due to the addition of an impurity to the Fermi sea. Here, and in what follows, the hole and particle momenta are limited to $|q| < k_F$ and $|k| > k_F$, respectively, with $k_F$ the majority Fermi momentum. In principle, one can obtain a more accurate description by allowing more particle-hole pair excitations; however, it has been shown that one particle-hole pair excitation yields a good estimate in 3D, as we will discuss below.

From the self-energy (4), one can obtain the energy of the polaron by locating the quasiparticle pole,

$$\varepsilon = \frac{p^2}{2m_\downarrow} + \Sigma(p, \varepsilon). \quad (5)$$

Solutions of this equation are in general complex, the presence of an imaginary part indicating a finite lifetime of the quasiparticle. If the decay rate $\Gamma$ is much smaller than $Re\{\varepsilon\}$, the quasiparticle energy is given by

$$E = \frac{p^2}{2m_\downarrow} + Re\{\Sigma(p, E)\}. \quad (6)$$

We quantify the momentum dependence of the energy $E$ with the effective mass $m^* \equiv 1/[\partial^2 E/\partial p^2]|_{p=0}$. The quasiparticle weight is described by the residue

$$Z = |\alpha_0^{(p)}|^2 \simeq \left[ 1 - \frac{\partial Re\{\Sigma(p, E')\}}{\partial E'} \right]^{-1} \bigg|_{E'=E}. \quad (7)$$

The approximation becomes exact in the limit $\Gamma/E \to 0$. Equation (6) yields two solutions for the energy $E$. The negative energy solution $E_-$ corresponds to the attractive polaron studied in refs. [21,22]. For a weakly interacting system, the attractive polaron is the ground state of an impurity immersed in the Fermi sea. However, as the strength of the attractive interaction is increased, a bound diatomic molecule dressed by particle-hole excitations becomes energetically favorable [21]. Additionally, a solution of eq. (6) with positive energy $E_+$ exists as found in ref. [24]. The theory of this repulsive polaron was recently elucidated in 3D [27–29]. This metastable quasiparticle is dressed by a cloud of particle-hole pair excitations whose effect is, in contrast to the attractive case, a reduced majority particle density around the impurity [28]. However, the repulsive polaron is not the true ground state (indeed, it is not generally an eigenstate of the system) and thus it will eventually decay. Energy and momentum conservation restrict the possible decay modes: the simplest are into either an attractive polaron and a particle-hole pair or into a molecule, two holes and one particle [19,20,28], the first being the main source of decay in the region of interest as we shall argue below.

The decay rate of the repulsive polaron sets the timescale at which the physics related to this excited state may be observed. In general, if the quasiparticle self-energy is known exactly, the rate may be calculated as $\Gamma = -Z_+ \text{Im}\{\Sigma(p, E_+)\}$. However, when the self-energy is approximate, a reliable estimate requires the lower lying states into which the quasiparticle can decay to be incorporated correctly. The self-energy obtained from the wave function (3) is unable to accurately capture the decay to an attractive polaron (described by the same wave function) and a particle-hole pair. Instead, we calculate the rate of decay to the attractive polaron following the idea of ref. [28]: Close to the quasiparticle
poles, the repulsive (+) and attractive (−) polarons are described by Green’s functions

\[ G_{\pm}(p, \omega) \sim \frac{Z_{\pm}}{\omega - E_{\pm} - p^2/(2m_{\pm}^*)}. \] (8)

The decay to the attractive polaron is dominated by processes which correctly match the energy difference \( \Delta E \equiv E_+ - E_- \). Thus, we estimate the decay rate by replacing the bare impurity propagator in the ladder summation by the pole expansion of the attractive polaron. In this manner we arrive at the expression

\[ \Gamma = -Z_+ 3m \sum_q \left[ \frac{\Omega}{g^2} - \sum_k \frac{Z_-}{\Delta E + i0^+ - E_{kq,p}} \right]^{-1}. \] (9)

The energy \( E_{kq,p} \) is obtained from \( E_{kq,p} \) by replacing \( m_1 \) with the effective mass of the attractive polaron, and the coupling constant \( g \) is adjusted to obtain ultraviolet convergence.

**Repulsive polaron.**—The properties of the repulsive polaron are parameterized by the dimensionless quantity \( \varepsilon_B/\varepsilon_F \), which gives a measure of the interaction strength. For strong attraction, \( \varepsilon_B/\varepsilon_F \gg 1 \), the repulsive polaron branch is only weakly perturbed by the two-body bound state which sits far below the continuum, and the repulsive polaron approaches the bare impurity state. Consequently, when \( \varepsilon_B/\varepsilon_F \to \infty \), the energy \( E_+ \to 0 \), the residue \( Z_+ \to 1 \) and the effective mass \( m^*_+ \to m_+ \), as depicted in figs. 1–3, respectively. Indeed, in this limit we find

\[ E_+/\varepsilon_F \simeq \frac{(m_1 + m_2)}{m_1 \log(\varepsilon_B/\varepsilon_F)} \] (10)

to leading order, which is consistent with previous perturbative calculations for equal masses [30]. The two-body decay rate \( \Gamma \) is also logarithmically suppressed for \( \varepsilon_B \gg \varepsilon_F \): From eq. (9), \( \Gamma \simeq \frac{m^*_+ (m_1 + m_2)^2}{m_1^2 (m_1 + m_2)} \frac{\pi Z_+ Z_- \varepsilon_F}{\log(\varepsilon_B/\varepsilon_F)^2} \), which approaches zero faster than \( E_+ \) as expected (note that in this limit \( Z_+ \propto \varepsilon_F/\varepsilon_B \)). In this limit, we find that the rate \( \Gamma_{PM} \) at which the repulsive polaron can form a molecule is even smaller, like in 3D [28]. Conservation laws require the creation of an additional particle-hole pair, and Fermi antisymmetry leads to a suppression by a further \( \varepsilon_F/\varepsilon_B \) by the same argument as in 3D [31]. Thus the rate of the resulting three-body process is expected to approach zero at least as fast as \( \Gamma_{PM}/\varepsilon_F \sim (\varepsilon_F/\varepsilon_B)^2 \). Eventually, when the attractive polaron is no longer the ground state (e.g., above \( \varepsilon_B/\varepsilon_F \approx 10 \) for equal masses [21]), the pole expansion (8) breaks down for the attractive polaron and the repulsive polaron will predominantly decay into the molecular ground state.

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1We expect the impurity to act as a free particle for momentum \( k \gg k_F \). Instead of using a complicated dispersion for the attractive polaron (effectively letting \( m^-_+ \) depend on momentum), we note that the large \( k \) behavior is cut off by a corresponding term in the coupling \( g \) and adjust the coefficient in front of this term to cancel the ultraviolet divergence.

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Fig. 1: (Color online) Energy of the repulsive polaron as a function of \( \varepsilon_B/\varepsilon_F \) for different experimentally relevant mass ratios (thick): from top to bottom, \( m_1/m_2 = 40/6, 1, 6/40 \). Where these curves split, the dotted lines depict the zero-momentum energy while the lower branch traces the minimum of the polaron dispersion. We also display the asymptotic result (10) for equal masses (double-dash-dotted). At the bottom, the thin (black) lines are the energies of an infinitely massive impurity as obtained from the exact solution (solid) and the ladder approximation (dotted). As \( \varepsilon_B/\varepsilon_F \to 0 \), both of these approach \( \varepsilon_F \).

Fig. 2: (Color online) Inverse effective mass of the repulsive polaron for mass ratios \( m_1/m_2 = 40/6 \) (dot-dashed), 1(solid), 6/40 (dashed). Where \( m^*_+ < 0 \), a polaron with finite momentum will be energetically favorable. Reference [24] considered the equal mass case in the regime \( \varepsilon_B/\varepsilon_F \gtrsim 3 \) and their results agree with ours. Inset: \( (m_1 = m_2) \) momentum \( P^* \) which minimizes the energy of the polaron.

For decreasing \( \varepsilon_B/\varepsilon_F \), the energy \( E_+ \) initially steadily increases until it eventually exceeds \( \varepsilon_F \) (see fig. 1). The interaction at which this occurs depends sensitively on the mass ratio: For equal masses, the critical interaction \( (\varepsilon_B/\varepsilon_F)_c \simeq 2.7 \), while for \( m_1/m_2 \to \infty \) we have \( (\varepsilon_B/\varepsilon_F)_c \to \infty \), and for \( m_1/m_2 = 0 \) we have \( (\varepsilon_B/\varepsilon_F)_c = 0 \). Note that our result in the latter case is consistent with the exact solution [32], \( E_+ = \int_0^{\varepsilon_F} \frac{dy}{\pi} \cot^{-1}\left(\frac{1}{2} \log \frac{\varepsilon_B}{\varepsilon_F} \right) \) and

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in fact see in fig. 1 that \( E_+ \) is quite close to the exact energy, apart from where the exact energy is non-analytic near \( \varepsilon_B/\varepsilon_F = 0 \). Indeed, we expect our variational approximation (3) to be least accurate for the case of an infinitely massive impurity, where higher-order particle-hole excitations of the Fermi sea are expected to be more important [16].

For weak attraction, \( \varepsilon_B/\varepsilon_F \rightarrow 0 \), we find that the effective mass of the repulsive polaron diverges (fig. 2), signalling that the lowest-energy repulsive polaron has a finite momentum \( P^* \) beyond that point. This was also concluded from the shape of the spectral function calculated in ref. [24]. From the inset of fig. 2, we see that \( P^* \) smoothly evolves from 0 to \( k_F \) as \( \varepsilon_B/\varepsilon_F \rightarrow 0 \). This behavior is tied to the fact that, in this limit, the residue \( Z_+ \) decreases towards zero and the wave function evolves into a bare impurity at momentum \( p - k_F \) plus one \( \uparrow \)-particle excited from zero momentum to \( k_F \). This limit mirrors the repulsive-polaron solution for infinite impurity mass, where one removes a \( \uparrow \)-particle from the bound state formed from the zero-momentum state and places it at the Fermi surface. In terms of the wave function 3, the final state at \( \varepsilon_B/\varepsilon_F = 0 \) corresponds to \( \alpha_0 = 0 \) and \( \alpha_{kq} = \delta_{q,0} \delta_{k, -k_F} \), which is orthogonal to the attractive polaron (with \( Z_+ = 1 \)). Thus, in this limit, the energy is minimised when \( p = k_F \), giving \( E_+ = \varepsilon_F \). Contrast this with the \( p = 0 \) state, where \( E_+ = E_F (1 + m_+/m_\downarrow) \).

Both these states are eigenstates of the non-interacting Hamiltonian and thus the decay rate of the repulsive polaron approaches zero as \( \varepsilon_B/\varepsilon_F \rightarrow 0 \) (see fig. 3). Note that when \( m_+ < 0 \), the \( p = 0 \) state may excite a particle out of the Fermi sea to gain momentum \( P^* \). By evaluating the available phase space close to the divergence of \( m_+ \), the rate at which this process occurs is found to go as \( [E_+ (|p| = 0) - E_+ (|p| = P^*)]^{1/4} \), which implies that the \( p = 0 \) state is metastable with respect to the finite momentum repulsive polaron in this limit.

Similar finite-momentum excitations are encountered in the corresponding impurity problem in 1D. The Bethe Ansatz solution for attractive interactions and equal masses exhibits an excited "broken-pair" state with negative effective mass [33]. Here, the excitation’s lowest energy is always at momentum \( k_F \) and equals \( \varepsilon_F \). By contrast, the energy at \( p = 0 \) exceeds \( \varepsilon_F \), with a maximum of \( 2\varepsilon_F \) when the interactions are switched off, like in 2D. The Bethe Ansatz solutions are, of course, exact eigenstates of the 1D system and thus the decay rates for these excitations are zero. However, in 2D, the repulsive polaron is, at best, metastable outside of the limits \( \varepsilon_B/\varepsilon_F \rightarrow 0 \) and \( \varepsilon_B/\varepsilon_F \rightarrow \infty \), and indeed we see in fig. 3 that the decay rates are sizeable in the regime \( \varepsilon_B/\varepsilon_F \lesssim 10 \) for a range of mass ratios.

**Itinerant ferromagnetism.** – To examine how this impacts the existence of itinerant ferromagnetism in 2D, we start by assuming the presence of spin-polarized domains and then assessing the stability of these. In order to have stable, well-defined \( \uparrow \) and \( \downarrow \) domains, we require there to be an energy cost for transporting particles across the \( \uparrow - \downarrow \) interface. Thus, we require a repulsive polaron formed from a \( \downarrow \) (\( \uparrow \)) impurity to have energy greater than the Fermi energy of the \( \downarrow \) (\( \uparrow \)) domain. Assuming mechanical equilibrium, where the pressures of each domain are equal, we then obtain the stability condition \( E_+ > \varepsilon_F^{\uparrow}/\sqrt{m_\uparrow/m_\downarrow} (E_+ > \varepsilon_F^{\downarrow}/\sqrt{m_\downarrow/m_\uparrow}) \). For equal masses, this simply gives \( E_+ > \varepsilon_F \), which corresponds to \( \varepsilon_B/\varepsilon_F < 2.7 \) as described earlier. At first sight, this might suggest that ferromagnetism can exist in this regime; however, we see in fig. 3 that the decay rate \( \Gamma \) is large near \( \varepsilon_B/\varepsilon_F = 2.7 \) and amounts to a significant fraction of the Fermi energy. The large \( \Gamma \) corresponds to a large uncertainty in the energy of the repulsive polaron, thus allowing particles to tunnel across the interface and destabilize the domains even when \( E_+ > \varepsilon_F \). Once across, the particles quickly decay into attractive polarons, e.g. for the typical densities used in 2D experiments [10], a repulsive polaron with \( \Gamma \sim 0.1\varepsilon_F \) near \( \varepsilon_B/\varepsilon_F \sim 1.3 \) only has a lifetime of order 1 ms. Of course, the decay rate is eventually suppressed once \( \varepsilon_B/\varepsilon_F \rightarrow 0 \), leading one to suspect that ferromagnetism becomes possible in this limit. However, \( Z_+ \) is also heavily suppressed as \( \varepsilon_B/\varepsilon_F \rightarrow 0 \), which means that the particles will mostly tunnel directly into the attractive polaron state (the probability of tunneling into each polaron state is proportional to \( Z_+ \)). Thus, our results indicate that saturated ferromagnetism is highly unstable in 2D.

Another route to determining the existence of itinerant ferromagnetism is to start with a uniform 50/50 mixture of spins and then compare the formation rate of spin domains with the rate of decay into \( \uparrow - \downarrow \) pairs/dimers. In 3D,
previous theoretical studies [3,4] have shown that the decay into pairs always dominates, thus ruling out the spontaneous formation of ferromagnetic domains. Our stability argument, however, places a stronger restriction on ferromagnetism in 2D, namely that saturated ferromagnetism cannot exist even if fully polarized spin domains were to be artificially engineered.

A similar scenario holds for unequal masses. In figs. 1–3 we show the properties of a $^{40}\text{K}^{\text{Li}}$ impurity immersed in a $^{\text{Li}}^{40}\text{K}$ Fermi sea. In this case, we find the domain stability condition to be satisfied for $\varepsilon_B/\varepsilon_{F,\text{Li}} < 5.7$. However, again we find that the decay rate is prohibitively large and phase separation is not favored. Our results are derived under the assumption that the system is correctly described by the Hamiltonian (1). However, Feshbach resonances in this heteronuclear system are narrow [34] which changes the two-particle scattering properties. Studying this problem in detail is beyond the scope of this letter, but the enhanced closed-channel character close to a narrow resonance decreases the two-body decay rate of the repulsive polaron [35]. While in general the energy will also be lower, there may be an intermediate regime of parameter space which favors phase separation.

Our arguments may be extended to realistic experimental conditions where the atoms are subjected to a weak trapping potential in the 2D plane. The stability of the spin-polarized domains relies on mechanical equilibrium at the $\uparrow\downarrow$ interface. This constraint is local and thus the above considerations are also valid in the trapped system provided the trap changes smoothly enough so that the local density approximation holds. Additionally, the atoms are confined to quasi-2D by a strong transverse field characterized by the frequency $\omega_z$. For the equal mass case studied in ref. [10] with experimental parameters $\omega_z = 2\times 80 \text{ kHz}$ and $\varepsilon_F = 2\times 9 \text{ kHz}$, we have $\varepsilon_B \approx \varepsilon_F \ll \omega_z$, in the regime of interest for the question of possible ferromagnetism. Thus, we conclude that only the lowest transverse mode is occupied and the 2D approximation considered in this paper is valid.

**Concluding remarks.** – We now turn to the question of the accuracy of the variational wave function (3). In 3D, the energy and effective mass of the ground-state quasiparticle have been measured in refs. [17] and [18], respectively, and good agreement with the variational calculation [15,26] was obtained, even in the limit of strong interactions. The approach has been further validated by agreement with Monte Carlo simulations [20], while ref. [16] has argued that the accuracy of the wave function arises from a nearly perfect destructive interference of the contributions of states dressed by more than one particle-hole pair. This latter argument does not depend on dimension and indeed it can be shown that the ground-state energy from the variational approach agrees well with the exact Bethe Ansatz solution in 1D [36]. While the variational wave function allows an accurate calculation of ground-state properties of the system, it is, perhaps, less intuitive that this should be the case for a metastable polaron. Nevertheless, recent experimental and theoretical studies [35] of a $^{40}\text{K}^{\text{Li}}$ mixture in 3D have demonstrated that not only is the energy and residue of the repulsive polaron correctly captured in the equivalent diagrammatic approach, the decay rate is also well approximated by a technique similar to the one which led to eq. (9).

To conclude, we have calculated the quasiparticle properties of the repulsive polaron. We find that in the limit of weak attractive interactions the lowest lying repulsive polaron has finite momentum. These properties may be observed by radiofrequency spectroscopy [24]. However, the fast decay and small residue of these quasiparticles in the regime of strong repulsion indicates that spin domains will be unstable and precludes itinerant ferromagnetism in the same manner as in the 3D experiment [2]. Our results are also applicable to a bosonic impurity immersed in a Fermi sea and thus have implications for phase separation in 2D Bose-Fermi mixtures.

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