## Polarons and molecules in a two-dimensional Fermi gas

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We study an impurity atom in a two-dimensional Fermi gas using variational wave functions for (i) an impurity dressed by particle-hole excitations (polaron) and (ii) a dimer consisting of the impurity and a majority atom. In contrast to three dimensions, where similar calculations predict a sharp transition to a dimer state with increasing interspecies attraction, we show that the polaron *Ansatz* always gives a lower energy. However, the exact solution for a heavy impurity reveals that both a two-body bound state and distortions of the Fermi sea are crucial. This reflects the importance of particle-hole pairs in lower dimensions and makes simple variational calculations unreliable. We show that the energy of an impurity gives important information about its dressing cloud, for which both *Ansätze* give inaccurate results.

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Since interactions between atoms can be tuned to essentially any value, cold atomic gases provide a unique opportunity for studying experimentally many-body physics in regimes that cannot be realized in other systems. Recently, much attention has been given to the problem of a Fermi gas with a low concentration of a second species, a so-called highly imbalanced gas (see, e.g., [1–3]). One fundamental problem is the nature of the ground state of a single impurity atom in a Fermi gas. For weak interspecies attraction, the ground-state energy is well described in terms of a state with an impurity atom dressed by a single particle-hole excitation of the Fermi sea, often referred to as a "polaron" [4,5], while for strong attraction, a state based on a molecular picture gives a lower energy [6,7]. The transition between the two states is predicted to be sharp [6,8].

It is natural to ask whether this picture persists in lower dimensions. This is of theoretical interest since on general grounds one would expect quantum fluctuations, in this case the creation of many particle-hole pairs, to play an important role. In addition, the problem is on the verge of being investigated experimentally with the use of optical lattices [9]. In one dimension, a polaronic description gives qualitative agreement with known exact results [10]. In this Rapid Communication, we consider the case of two dimensions. We perform simple variational calculations based on the polaron and molecule pictures, and these predict that the polaronic state has the lower energy for all interaction strengths, in marked contrast to what happens in three dimensions. For an infinitely massive impurity, the problem may be solved exactly, and the results show that the actual ground state incorporates aspects of both pictures: A two-body bound state is present for all coupling strengths in addition to distortions of the continuum states. We show that the energy of an impurity gives important information about correlations in its vicinity and about mutual interactions between impurities at nonzero density.

*Model.* We consider a uniform two-dimensional (2D) Fermi gas of atoms of species a, to which is added a single impurity

$$H = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}}^{(a)} a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} + \sum_{\mathbf{k}} \epsilon_{\mathbf{k}}^{(b)} b_{\mathbf{k}}^{\dagger} b_{\mathbf{k}} + \sum_{\mathbf{k}\mathbf{k}'\mathbf{q}} \frac{v(q)}{V} a_{\mathbf{k}+\mathbf{q}}^{\dagger} a_{\mathbf{k}} b_{\mathbf{k}'-\mathbf{q}}^{\dagger} b_{\mathbf{k}'}$$

since *a*-*a* interactions may be neglected because of the Pauli principle. The single-particle eigenstates are  $\langle \mathbf{x} | \mathbf{k} \rangle = e^{i\mathbf{k}\cdot\mathbf{x}}/\sqrt{V}$ , where we take the system to be enclosed in a 2D box of volume  $V \equiv L^2$  with periodic boundary conditions. The single-particle energies are  $\epsilon_{\mathbf{k}}^{(\sigma)} = k^2/2m_{\sigma}$ , where  $m_{\sigma}$  is the mass of species  $\sigma$  (we take  $\hbar = 1$  throughout);  $a_{\mathbf{k}}(b_{\mathbf{k}})$ annihilates an a(b) atom in state  $|\mathbf{k}\rangle$ . The interaction is modeled as  $v(q) = g_2$  for particle momenta less than a cutoff value  $\Lambda$ and zero otherwise. The coupling  $g_2$  and the cutoff may be eliminated in favor of the two-body binding energy  $\epsilon_B \ge 0$ [11],

$$\frac{1}{g_2} = -\frac{1}{V} \sum_{|\mathbf{p}| < \Lambda} \frac{1}{\epsilon_B + \frac{\mathbf{p}^2}{2\mu}} = -\frac{2\mu}{4\pi} \ln\left(1 + \frac{\Lambda^2/2\mu}{\epsilon_B}\right), \quad (1)$$

with the reduced mass  $\mu = (m_a^{-1} + m_b^{-1})^{-1}$ . For  $\epsilon_B \ll \Lambda^2/2\mu$ , none of the results depend on the cutoff, and we take  $\Lambda \to \infty$  at the end of the calculation.

*Polaron.* We describe the state using the variational *Ansatz* [4]

$$\Psi_P = \left(\phi_0 b_0^{\dagger} + \sum_{|\mathbf{q}| < k_F < |\mathbf{k}|} \phi_{\mathbf{k}\mathbf{q}} \, b_{\mathbf{q}-\mathbf{k}}^{\dagger} a_{\mathbf{k}}^{\dagger} a_{\mathbf{q}}\right) |N\rangle, \qquad (2)$$

which describes an impurity atom *b* (here with zero momentum) dressed by a cloud of particle-hole excitations of the ground state  $|N\rangle$  of *N a* atoms. This state is an expansion of the true state in terms of numbers of particle-hole excitations, truncated at first order. Minimizing the energy functional for this *Ansatz* leads to equations for the energy of the state relative

1050-2947/2011/83(2)/021603(4)

atom of species b. The two species may be either different hyperfine states of the same element or different atomic species, in which case b may be bosonic or fermionic. The 2D confinement may be realized by a very tight trapping potential in the transverse direction [9] and weak longitudinal trapping. For densities low enough that only *s*-wave interactions are important, the Hamiltonian reads

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FIG. 1. (Color online) Energy *E* as a function of  $\epsilon_B$  for the polaron *Ansatz* (for the q = 0 approximation, see text) and the dimer *Ansatz*. For  $\epsilon_B < 2\epsilon_F$ , the dimer has momentum  $p_M \neq 0$ ; the thin straight line indicates the dimer energy at  $p_M = 0$ .

to the ground-state energy of N a atoms,  $E \equiv \langle H \rangle_{\Psi_P} - E_0^{(N)}$ , and the amplitudes  $\phi_{kq}$ :

$$E = \frac{1}{V} \sum_{\mathbf{q}} n_q T_{\mathbf{q}} \left( E + \epsilon_{\mathbf{q}}^{(a)} \right), \quad \frac{\phi_{\mathbf{kq}}}{\phi_0} = \frac{1}{V} \frac{T_{\mathbf{q}} \left( E + \epsilon_{\mathbf{q}}^{(a)} \right)}{E - \Delta \epsilon_{\mathbf{kq}}}.$$
 (3)

Here the *T* matrix  $T_{(\mathbf{q})}(E + \epsilon_{\mathbf{q}}^{(a)})^{-1} = g_2^{-1} - V^{-1} \sum_{|\mathbf{k}| < \Lambda} (1 - n_k)(E - \Delta \epsilon_{\mathbf{kq}})^{-1}$  plays the role of an effective interaction, with  $\Delta \epsilon_{\mathbf{kq}} \equiv \epsilon_{\mathbf{k}}^{(a)} - \epsilon_{\mathbf{q}}^{(a)} + \epsilon_{\mathbf{q}-\mathbf{k}}^{(b)}$ , and  $n_q \equiv \Theta(k_F - q)$  is the Fermi function, with  $k_F$  being the Fermi momentum. In the thermodynamic limit (keeping the majority density  $n_a = N/V = k_F^2/4\pi$  fixed), this becomes an integral equation, whose root *E* may be found numerically.

For now, we will focus on the equal-mass case,  $m_{\sigma} \equiv$  $m = 2\mu$ . The energy  $E(\epsilon_B)$  obtained numerically is shown in Fig. 1. In the weak-coupling limit  $\epsilon_B \ll \epsilon_F \equiv k_F^2/2m$ , the energy  $E \simeq -2\epsilon_F / \ln(2\epsilon_F/\epsilon_B)$  decreases very rapidly with increasing  $\epsilon_B$ . This result can be interpreted as a meanfield shift  $E \sim n_a \bar{g}$ , where the density-dependent effective interaction  $\bar{g} = -4\pi/m \ln(n_a 4\pi \hbar^2/m\epsilon_B)$  is the leading term in  $T_{\mathbf{q}}$  for  $E, \epsilon_B \to 0$ . In the strong-coupling limit  $\epsilon_B \gg \epsilon_F$ , we find  $E \simeq -\epsilon_B - \eta \epsilon_F$ , with  $\eta \approx 0.26$ . Some analytical insight into these results may be obtained by approximating  $\Delta \epsilon_{\mathbf{kq}} = (\mathbf{k}^2 - \mathbf{k} \cdot \mathbf{q})/m$  by  $\mathbf{k}^2/m$ , as has proven qualitatively correct in the 3D case [12]. This "q = 0" approximation gives the equation  $E \approx n_a T_0(E) = -\epsilon_B \exp(2\epsilon_F/|E|) + 2\epsilon_F$ , whose solution is plotted for comparison in Fig. 1. It gives the correct weak-coupling limit; in the strong-coupling limit it yields  $E \simeq -\epsilon_B - 2\epsilon_F^2/\epsilon_B$ , which misses the term  $O(\epsilon_F)$ . We have also studied the case of arbitrary  $m_b$  and found that the mass dependence of the polaron energy is weak if energies are expressed in units of  $k_F^2/2\mu$ .

At first sight, it is somewhat surprising that for strong coupling the polaronic *Ansatz* leads to an energy close to that of a molecule in vacuum. In this limit, the overlap probability of  $\Psi_P$  with the noninteracting ground state is given by  $Z \equiv |\phi_0|^2 \simeq 2\epsilon_F/\epsilon_B$ , which tends to zero. Thus, the state is comprised mainly of holes and an *ab* dimer, as may be seen

## PHYSICAL REVIEW A 83, 021603(R) (2011)

from Eq. (2), and the coefficients  $\phi_{\mathbf{kq}}$  [Eq. (3)] reduce to the wave function for a molecule *in vacuo* plus a hole. The leading contribution to the energy is thus the energy of a molecule in free space since the hole has an energy of at most  $\epsilon_F$ .

*Molecule.* In three dimensions, it has been demonstrated that a simple variational wave function based on a molecular picture gives a lower energy than the polaron *Ansatz* (2) for sufficiently strong attraction [7], and we investigate whether this happens in two dimensions. In its simplest form, such an ab dimer with zero total momentum may be modeled using the trial state [7]

$$\Psi_M = \sum_{|\mathbf{k}| > k_F} \varphi_{\mathbf{k}} b^{\dagger}_{-\mathbf{k}} a^{\dagger}_{\mathbf{k}} |N-1\rangle, \qquad (4)$$

which corresponds to a correlated ab pair in states with momentum greater than  $k_F$  and a Fermi sea with N-1noninteracting atoms. Minimizing the energy functional leads to the following equation for the energy  $E_M$  (again relative to that of the *N*-particle Fermi sea):

$$\frac{1}{g_2} = -\frac{1}{V} \sum_{k_F < |\mathbf{k}| < \Lambda} \frac{1}{\frac{k^2}{2\mu} - (E_M + \epsilon_F)},$$
(5)

whose solution is

$$E_M = -\epsilon_B + \frac{k_F^2}{2m_b}$$

and  $\varphi_{\mathbf{k}} \propto \Theta(k - k_F)/(\epsilon_{\mathbf{k}}^{(b)} - E_M)$ . This result is simple because in 2D the density of states is independent of energy: The energy of the dimer is shifted by the kinetic energy of the lowest state not Pauli blocked. In this approximation, the bare zero-momentum dimer state is always energetically less favorable than the polaronic solution, and there is no sharp transition (Fig. 1), in contrast to the 3D case.

The question arises whether dimers with nonzero momentum have a lower energy. The extension of (4) to a dimer with momentum **p** is  $\Psi_M^{(\mathbf{p})} = \sum_{|\mathbf{k}| > k_F} \varphi_{\mathbf{k}}^{(\mathbf{p})} a_{\mathbf{k}}^{\dagger} b_{\mathbf{p}-\mathbf{k}}^{\dagger} |N-1\rangle$ , which leads to an equation similar to Eq. (5). The solution is

$$E_M(p) - E_M(0) = \frac{p^2}{2M} - \frac{k_F^2}{2\mu} \left[ 1 + \left(\frac{M/m_b}{pa_2}\right)^2 \right]^{-1}, \quad (6)$$

where  $\epsilon_B \equiv \hbar^2/2\mu a_2^2$  defines the 2D scattering length  $a_2$ . For  $\epsilon_B > \frac{k_F^2}{2\mu} \frac{m_a}{m_b}$ , the dimer energy is minimal for p = 0. For  $\epsilon_B < \frac{k_F^2}{2\mu} \frac{m_a}{m_b}$ , however, a dimer at  $p = p_M \neq 0$  is favorable because the kinetic-energy increase is outweighed by the reduced Pauliblocking shift.<sup>1</sup> For concreteness, consider the equal-mass case: The dimer momentum  $p_M = 2\sqrt{k_F a_2 - 1}/a_2$  changes smoothly from  $p_M = 0$  (at  $\epsilon_B = 2\epsilon_F$ ) to  $p_M \rightarrow k_F$  as  $\epsilon_B \rightarrow \epsilon_F/2$ , where the energy reaches the continuum threshold  $E_M = 0$  (Fig. 1). In that regime,  $E_M = -\epsilon_F + 2\sqrt{\epsilon_B}(\sqrt{2\epsilon_F} - \sqrt{\epsilon_B})$ . Thus, the bare dimer is energetically unfavorable compared with the polaronic *Ansatz* for any coupling strength. To obtain more insight, we now examine an exact solution.

<sup>&</sup>lt;sup>1</sup>Although the lowest-energy dimer has nonzero momentum, its velocity vanishes by definition,  $\partial_p E(p_M) = 0$ .

## POLARONS AND MOLECULES IN A TWO-DIMENSIONAL ...

Infinite-mass limit. We consider the case where the impurity atom is very massive,  $m_b \gg m_a$ . In addition to being exactly soluble by use of Fumi's theorem [13], this is also relevant to experiments with atomic mixtures (e.g., Li and Yb [14]). The massive impurity may be treated as a static defect, which has two effects on the Fermi gas: It creates a two-body bound state with energy  $-\epsilon_B$ , and it also shifts the energy levels in the continuum. In any number of dimensions, the energy shift of an s-wave level in the continuum is given by  $-k\delta_0(k)/m_a R$ , where  $\delta_0(k)$  is the *s*-wave phase shift and *R* is the radius of the sphere containing the Fermi gas. The density of s-wave levels per unit interval in k is  $\pi/R$ . The total energy change when an impurity is added to the N-atom system is

$$E = -\epsilon_B - \frac{1}{m_a \pi} \int_0^{k_F} dk \, k \delta_0(k). \tag{7}$$

In 2D, the scattering phase shift is given by  $\cot \delta_0(k) =$ 

 $\ln(k^2/2m_a\epsilon_B)/\pi$  in the zero-range limit [11]. For large  $\epsilon_B$ ,  $\Delta E \equiv E + \epsilon_B \simeq -\epsilon_F + \frac{\epsilon_F}{\ln(\epsilon_B/\epsilon_F)}$ . The leading term corresponds to the fact that the phase shift is close to  $\pi$ , and consequently, each of the continuum s levels has become close to the next lower one in the absence of the impurity, thereby lowering the energy by  $\epsilon_F$ . The logarithmic term may be thought of as an effective atom-dimer repulsion. This is in stark contrast to the result  $\Delta E_M = k_F^2/2m_b \rightarrow 0^+$  $(m_b \rightarrow \infty)$  obtained from the dimer Ansatz. Moreover, for the polaron in the heavy-impurity limit, we find numerically  $\Delta E \approx -0.14\epsilon_F + O(n_a^2)$ , which is much smaller in magnitude than the exact result,  $-\epsilon_F$ .

The exact result shows that the ground state has a bound two-body state and that levels in the continuum are modified. It therefore incorporates aspects of both the polaron and the dimer pictures. The missing ingredient in the trial states we have used is components with a higher number of particlehole pairs: This is treated only to first (zeroth) order in the polaron (dimer) Ansatz. In the language of perturbation theory, the T matrix employed in the polaron Ansatz is calculated in the ladder approximation and thus contains only particleparticle and hole-hole scattering. However, it is known that the T matrix for scattering of a fermion from a massive impurity is essentially independent of the presence of the medium because Pauli blocking of ladder diagrams is compensated by impurityhole scattering [15]. Our calculations show that the higherorder impurity-hole scattering processes change  $\Delta E$  to leading order from  $-0.14\epsilon_F$  (for one particle-hole pair) to  $-\epsilon_F$  in the exact result.

However, the bare-dimer picture worked reasonably well in 3D, predicting a molecular transition in agreement with Monte Carlo results. To understand this paradox, let us look at the role of dimensionality in the dimer problem. Solving (5) in D = 1,2,3 (for equal masses) yields an energy of the form  $E_M \simeq -\epsilon_B - \epsilon_F + c_D \epsilon_F (\frac{2\epsilon_F}{\epsilon_B})^{(D-2)/2}$  as  $\epsilon_B \to \infty$ . The last term corresponds to an upshift of the dimer energy due to Pauli blocking of the states  $|\mathbf{q}| < k_F$ . In D = 3 the upshift vanishes in the limit  $\epsilon_B \gg 2\epsilon_F$ : This is because the density of states  $\rho(\epsilon) \propto \sqrt{\epsilon}$  vanishes at low energies, so that the contribution from Pauli blocking for  $\epsilon < 2\epsilon_F$  has a negligible weight for  $\epsilon_B \rightarrow \infty$ . The situation is dramatically different in

PHYSICAL REVIEW A 83, 021603(R) (2011)



FIG. 2. (Color online) Number of majority atoms  $\nu$  in the dressing cloud of an impurity as a function of  $\epsilon_B$ .

lower dimensions. In D = 2, the density of states is constant and thus leads to an interaction-independent displacement of the vacuum energy by  $2\epsilon_F$ , recovering the total shift  $+\epsilon_F$ . This also illuminates why bare dimers should be even less favorable in 1D [16], where the low-lying states have an even stronger weight  $\rho(\epsilon) \propto 1/\sqrt{\epsilon}$ , leading to a diverging upshift for strong coupling.

Dressing cloud of an impurity. Important information about the structure of the dressing cloud of an impurity may be extracted from the results for the energy. As is done in the theory of dilute mixtures of helium isotopes [17], we define the quantity  $v = (\partial n_a / \partial n_b)_{\mu_a} = -(\partial \mu_b / \partial n_a) / (\partial \mu_a / \partial n_a),$ where  $\mu_{\sigma}$  is the chemical potential of a  $\sigma$  atom. Physically, this is the number of a atoms in the dressing cloud of an impurity. The requirement that  $\mu_a$  be held fixed ensures that far from the impurity, the density of a atoms is unchanged by the addition of the impurity. For  $n_b \ll n_a$ , this number can be deduced from the single-impurity energy,  $\nu = -\partial E/\partial \epsilon_F$ , which is plotted in Fig. 2. As expected,  $\nu$  tends to zero in the weak-coupling limit,  $\nu \simeq 2/\ln(2\epsilon_F/\epsilon_B)$ , for  $m_a = m_b$ . For  $m_b \to \infty$ , we can infer that there is exactly one dressing atom as  $\epsilon_B \rightarrow \infty$ ,  $\nu \rightarrow 1$ . This contrasts with the polaron Ansatz, which for  $m_b \rightarrow \infty$  predicts  $\nu_P \rightarrow \eta \approx 0.14$  (following a peak near  $\epsilon_B = 2\epsilon_F$ ), illustrating that the single-particle-hole picture highly underestimates the impurity dressing. For comparison, the bare-dimer Ansatz predicts the unphysical result  $v_M = -1$ , amounting to a deficit of atoms in the dressing cloud due to Pauli blocking.

Nonzero impurity density. An intriguing question concerns the behavior at nonzero impurity density: Do the "dressed" impurity atoms behave as fermions, bosons, or neither of them? For weak attraction, it is not implausible that the dressed impurities have the same quantum statistics as bare ones. In contrast, for strong attraction, one may expect the basic degrees of freedom to be best described in terms of *ab* dimers, which are bosons for fermionic impurities and vice versa. On the basis of simple arguments, we cannot arrive at a definite conclusion about the statistics obeyed by the elementary excitations; to do so, it would be necessary to investigate

the importance of exchange processes in a system with two impurities.<sup>2</sup>

Let us consider the case when the quasiparticles are fermionic. This could apply for weakly interacting fermionic impurities and also for bosonic ones if they form a tightly bound dimer with a majority atom. We now show that the single-impurity findings have implications for the thermodynamic properties at nonzero concentration  $n_b/n_a \ll 1$ . The total energy density  $\mathcal{E}$  of such a Fermi liquid then reads  $\mathcal{E}(n_b) \simeq \mathcal{E}(0) + \mathcal{E}_0(n_b) + E(\epsilon_B)n_b + \frac{1}{2}fn_b^2$ , where  $\mathcal{E}(0)$  is the majority energy,  $\mathcal{E}_0(n_b) = \pi n_b^2 / m_b^*$  denotes the kinetic-energy density, with the effective mass  $m_{h}^{\star}$  modified by interactions, and the term  $n_b E(\epsilon_B)$  gives the energy reduction due to binding of independent quasiparticles. Even in the absence of direct interactions between b fermions, there is an induced interaction between them, mediated by the majority Fermi gas [18]. It turns out to be repulsive owing to the Pauli principle and is characterized by the Landau parameter  $f = v^2 \partial \epsilon_F / \partial n_a$ . Note that since in 2D the density of states  $\partial n_a / \partial \epsilon_F = m_a / 2\pi$ is constant, f is nonzero for  $n_a \rightarrow 0$ . We mention that for bosonic quasiparticles, the effective interaction follows in a similar fashion [19], the difference being that there is a direct s-wave interaction and that the induced interaction is attractive. However, how that influences the induced interactions

<sup>2</sup>Even if the polaron *Ansatz* gives the lower energy, one cannot conclude that the elementary excitations obey the same statistics as the impurity atom since the polaron state is dominated by a rather incoherent superposition of many dimer-hole configurations.

depends nontrivially on the degeneracy of the bosons and is left for future studies.

Finally, we mention that the properties of impurities can be probed using techniques similar to those in 3D. By exciting collective oscillations, the effective mass is accessible [3]. With increasing coupling, this tends to  $\infty$  for the polaron and to *M* for the dimer *Ansatz*. Another key tool is radio-frequency spectroscopy [2], where a *b* atom is transferred from its initial hyperfine level to an empty one via a pulse of frequency  $\omega$ . For a polaron, the transition rate  $\Gamma(\omega)$  decomposes into a quasiparticle peak  $\propto Z\delta(\omega - |E|)$ , indicating the polaron contribution, and an incoherent background  $\Gamma_{inc}(\omega)$ , which increases as  $(\omega - |E|)^{3/2}$  for  $0 \leq \omega - |E| \ll \epsilon_F$  and falls off as  $\omega^{-2}$  for  $\omega - |E| \gg \epsilon_F$  if final-state interactions are ignored. This contrasts with the dimer *Ansatz*, which yields  $\Gamma_M(\omega) \propto \Theta(\omega - |E|)/\omega^2$  without any quasiparticle peak.

In summary, using variational wave functions, we find no evidence for a sharp transition between the polaron and the molecular picture in two dimensions. Comparison with the exact result for a heavy impurity shows that both *Ansätze* lead to inaccurate results for the dressing cloud of the impurity in the strong-coupling limit. This reveals the key role of many particle-hole pairs, and it reflects the importance of quantum fluctuations in lower dimensions. We conclude that more work is needed to understand the nature of the ground state of an impurity with finite mass in a two-dimensional Fermi gas.

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