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., references 1, 2). 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” 3, 4, while for strong attraction, a state based on a molecular picture gives a lower energy 5, 6. The transition between the two states is predicted to be sharp 6, 7.

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 8, 9. In one dimension, a polaronic description gives qualitative agreement with known exact results 10. In this paper, 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 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 11 and weak longitudinal trapping. For densities low enough that only s-wave interactions are important, the Hamiltonian reads

$$H = \sum_k \varepsilon_k (a_k^\dagger a_k + \sum_{k'} \frac{v(q)}{\sqrt{V}} a_{k+q} a_{k'}^\dagger a_{k'} - q b_{k'}),$$

since $a-a$ interactions may be neglected because of the Pauli principle. The single-particle eigenstates are $(|x\rangle |k\rangle = e^{ikx}/\sqrt{V}$, 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 $\varepsilon_k (\sigma) = k^2/2m_\sigma$, where $m_\sigma$ is the mass of species $\sigma$ (we take $\hbar = 1$ throughout); $a_k (b_k)$ annihilates an $a (b)$ atom in state $|k\rangle$. 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 $\epsilon_B \geq 0$ 11,

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

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 6

$$\Psi_P = \left(\phi_0 b_0^\dagger + \sum_{|q| < k_F < |k|} \phi_{kq} b_{q-k}^\dagger a_k a_q\right) |N\rangle,$$
This plotted for comparison in Fig. 1. It gives the correct weak-coupling shown in Fig. 1. In the E, ǫ\_m = 2\pi/m where the density-dependent effective interaction \( \bar{\alpha} \) approximating \( \Delta \approx 0 \) reduces 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 for sufficiently strong attraction, 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

\[
\Psi_M = \sum_{|k| > k_F} \varphi_k b_{k}^\dagger a_{-k}^\dagger |N - 1\rangle,
\]

which corresponds to a correlated \( ab \) pair in states with momentum greater than \( k_F \) and a Fermi sea with \( N - 1 \) noninteracting 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),

\[
\frac{1}{g_2} = -\frac{1}{V \sum_{|k| < |k| < k_F}} \frac{1}{2m} (E_M + \epsilon_F),
\]

whose solution is

\[
E_M = -\epsilon_B + \frac{k_F^2}{2m_b}.
\]

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 (1) to describe a dimer with momentum \( p \) is \( \Psi_M(p) = \sum_{|k| > k_F} \varphi_k b_{k_p}^\dagger a_{-k_p}^\dagger |N - 1\rangle \), which leads to an equation similar to Eq. (4). The solution is

\[
E_M(p) - E_M(0) = \frac{p^2}{2M} - \frac{k_F^2}{2\mu} \left[ 1 + \left( \frac{M/m_b}{\rho \sigma_2} \right)^2 \right]^{-1},
\]
is the s-wave phase shift and $R_N$ when an impurity is added to the medium, because Pauli blocking of ladder diagrams is compensated by impurity–hole scattering \cite{14}. Our calculations show that the higher-order 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 \ref{5} in $D = 1, \ldots, 3$ (for equal masses) yields an energy of the form $E_M \simeq - \epsilon_B - \epsilon_F + \epsilon_D \epsilon_F (2 \epsilon_F / B)^{(D-2)/2}$ as $\epsilon_B \to \infty$. The last term corresponds to an upshift of the dimer energy due to Pauli blocking of the states $|q| < k_F$. 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 $\epsilon_B \to \infty$. The situation is dramatically different in lower dimensions. In $D = 2$, the density of states is constant and thus leads to an interaction-independent displacement of the vacuum energy by $2 \times \epsilon_F$, recovering the total shift $+ \epsilon_F$. This also illuminates why bare dimers should be even less favorable in 1D \cite{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 \cite{17}, we define the quantity $\nu = (\partial n_a / \partial n_b)_{n_a} = -(\partial \mu_a / \partial n_a) / (\partial \mu_a / \partial n_b)$, where $\mu_a$ is the chemical potential of a $a$-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 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, $\nu \simeq 2 / (2n_a / \epsilon_F)$, for $m_b = m_a$. For $m_b \to \infty$, we can infer that there is exactly one dressing atom as $\epsilon_B \to \infty$, $\nu \to 1$. This contrasts with the polaron ansatz, which for $m_b \to \infty$ predicts $\nu_F \to \eta = 0.14$ (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 $\nu_M = -1$, 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. By contrast, for strong attrac-
tion, 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 \(^{21}\).

Let us consider the case when the quasiparticles are fermionic. This could apply for weakly interacting fermionic impurities, but 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 \( \mathcal{E}(n_b) \approx \mathcal{E}(0) + \mathcal{E}_0(n_b) + E(B)n_b + \frac{1}{2}f n_b^2 \), 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 \( m^*_b \) modified by interactions, and the term \( n_b E(B) \) 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 \( f = \nu^2 \partial \epsilon_F/\partial n_a \). 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 \( n_a \to 0 \). 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 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 \( \Gamma_{\text{inc}}(\omega) \), which increases as \( (\omega - |E|)^{3/2} \) for \( \omega - |E| \ll \epsilon_F \) 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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