A fermionic impurity in a dipolar quantum droplet

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Abstract

In this article we develop the framework to describe Bose–Fermi mixtures of magnetic atoms, focusing on the interaction of bosonic self-bound dipolar quantum droplets with a small number of fermions. We find an attractive interaction potential due to the dipolar interaction with several bound states, which can be occupied by one fermion each, resulting in a very weak back-action on the bosons. We conclude, that these impurities might act as unique probes giving access to inherent properties of dipolar quantum droplets.

Keywords: quantum droplets, impurity, dipolar interaction, quantum gases, ultra-cold atoms, Bose–Fermi mixtures

Self-bound quantum droplets [1–4] are manifestations of exotic liquid-like states of matter. They are reminiscent of superfluid helium droplets, but exist at orders of magnitude lower densities. Dipolar quantum droplets arise in Bose–Einstein condensates of strongly magnetic atoms. A combined experimental [2, 5–8] and theoretical [1, 9–16] effort has recently revealed, that these droplets are stabilized by beyond-mean-field effects, but many questions about their dynamics and finite-temperature behavior still remain. In the case of helium droplets, remarkable insights and applications have been made possible by the immersion of impurities [17]. In this spirit, we investigate the interaction of magnetic fermionic dipolar impurities with a bosonic dipolar quantum droplet. Immersed in the droplet, these impurities are subject to an intrinsically attractive dipole–dipole interaction (DDI). Therefore, we study the behavior of Bose–Fermi mixtures with dominant DDI. In the limit of only a few fermions, we show that the Hamiltonian reduces to a simple Schrödinger equation with the interspecies interaction acting as a trapping potential for the fermions. Solving it, we find several anharmonically bound states. Due to the Pauli exclusion principle and the shallowness of the attractive potential we find that only a few fermions can be trapped. Thus, the few-fermion limit is intrinsically satisfied.

Starting within second quantization, the full Hamiltonian of the system $\hat{H} = \hat{H}_f + \hat{H}_b + \hat{H}_{bd}$ in its most general form is composed of the intraspecies contribution

$$\hat{H}_f = \frac{\hbar^2}{2m_f} \int \nabla \hat{\psi}_f^\dagger \cdot \nabla \hat{\psi}_f + \frac{1}{2} \int \nabla \nabla \hat{\psi}_f^\dagger \nabla \hat{\psi}_f \, U_{ff}(\mathbf{r} - \mathbf{r}') \, \hat{\psi}_f(\mathbf{r}) \, \hat{\psi}_f(\mathbf{r}')$$

(1)

for fermions and similarly for bosons, and the interspecies interaction

$$\hat{H}_{bd} = \frac{1}{2} \int \nabla \nabla \hat{\psi}_f^\dagger \nabla \hat{\psi}_b^\dagger \hat{\psi}_b \hat{\psi}_f \, U_{bf}(\mathbf{r} - \mathbf{r}') \, \hat{\psi}_b(\mathbf{r}) \, \hat{\psi}_f(\mathbf{r}')$$

(2)

The predominant interactions for ultra-cold dipolar atoms are the contact interaction, which can be written in pseudo-potential form $U_{\text{con}}(\mathbf{r}) = g \, \delta(\mathbf{r}) \, \frac{\partial}{\partial |\mathbf{r}|} |\mathbf{r}|$ with $g = 4\pi \hbar^2 a/m$ defined by the s-wave scattering length $a$ and the atomic mass $m$, as well as the DDI

$$U_{\text{dip}}(\mathbf{r}) = \frac{\mu_0 \mu_r^2}{4\pi} \frac{1 - 3 \cos(\theta)^2}{|\mathbf{r}|^3}$$

(3)

which is non-local due to its long-range character and defined
by the magnetic moment $\mu$ of the atom [21]. There is no contact interaction between fermions in identical spin states, but they are subject to the dipolar interaction [22].

We are particularly interested in the ground state of few fermions, where the number of fermions $N_f$ is small compared to the number of bosons $N_b \gg N_f$. This restriction leads to a few assumptions. First, we neglect any back-action of fermions on the bosonic many-body state. Second, scaling with atom number, the interspecies interaction is much stronger than the fermionic intraspecies DDI. Third, the bosons are subject to quantum depletion [23], which is small even for systems that are stabilized by quantum fluctuations [11, 12]. Therefore we neglect any interaction of depleted bosons with fermions and the DDI between fermions. For both effects we estimate the order of magnitude later.

With these assumptions, the bosonic many-body state is not modified by the presence of fermions. The former is then described by the extended Gross–Pitaevskii equation (eGPE) [9–12, 14] within the first beyond-mean-field correction [24], yielding the bosonic density distribution $n_b(r)$ and ground state energy $E_b$. For the interspecies interaction $H_{bf}$, we consequently replace the bosonic operator $\hat{\psi}_b(r)$ by the wavefunction $\psi_b = \sqrt{n_b(r)}$, which yields the Hamiltonian

$$\hat{H} = E_b + \int R \left[ \frac{\hbar^2}{2m_b} \nabla \hat{\psi}^+_b \cdot \nabla \hat{\psi}_b + \frac{1}{2} \hat{\psi}^+_b \hat{\psi}_b U_{bf}(R) \right] \quad (4)$$

with the Bose–Fermi interaction potential

$$U_{bf}(R) = g_{bf} n_b(R) + \int_{\text{3d}} \text{d} R' U_{\text{imp}}(R - R') n_b(R') \quad (5)$$

relying on the interspecies scattering length $a_{bf}$ defining $g_{bf} = 4\pi\hbar^2a_{bf}/m_b$². Finally, the remaining problem of equation (4) thus reduces to solving the stationary Schrödinger equation

$$\hat{H} = -\frac{\hbar^2 \Delta^2}{2m_b} + U_{bf}(R) \quad (6)$$

of a single particle in an external potential $U_{bf}(R)$.

As mentioned in the introduction, we are interested in the behavior of fermionic dipolar impurities interacting with a self-bound dipolar quantum droplet consisting of many bosonic atoms. Therefore we consider a number $N_{\text{qd}}$ of bosonic $^{164}\text{Dy}$ atoms with intraspecies scattering length $a_{bb} = 70a_0$ in accordance with recent measurements [25]. The magnetic moment $\mu = 9.93\mu_B$, $\mu_B$ being the Bohr magneton, relies on the electronic configuration and is thus constant across dysprosium isotopes. For these parameters, the critical atom number for the existence of a self-bound dipolar quantum droplet is $N_{\text{qd}} > N_{\text{crit}} \approx 975$, as calculated with the eGPE [2]. This way we also extract its density profile $n_b(R)$ having cylindrical symmetry with respect to the polarization axis $z$. In the next step, we calculate the interaction potential $U_{bf}(r,z) = U_{bf}(r)$ of equation (5) acting as an external trapping potential for the fermionic impurities. The necessary interspecies scattering length $a_{bf}$, describing the Bose–Fermi contact interaction, is not known for dysprosium. Yet, we expect to find a suitable combination of isotopes and magnetic field owing to the abundance of Feshbach resonances in lanthanide atoms [26]. For the purpose of this manuscript we consider $^{164}\text{Dy}$ with $a_{bf} = 70a_0$ for now. As sketched in figure 1(a), the resulting interaction potential resembles the droplet density distribution having radial symmetry and additionally attractive wings axially (red) and repulsive ones radially (blue) outside of the droplet (white ellipse). Furthermore, the trapping potential is highly anisotropic, as shown in figure 1(b), with a strong dependence of the potential depth $U_0 = U_{bf}(0)$ on the atom number $N_{\text{qd}}$. Owing to the incompressible character of the droplet, its peak density and thus $U_0$ saturate for $N_{\text{qd}} \gtrsim 10^4$ atoms, while it grows axially in this regime [11].

In order to analyze the potential $U_{bf}$ trapping the impurity, we Taylor-expand it at the center to obtain the trap frequencies $\omega_{r,z}$. Due to the anisotropy of the droplet the radial confinement is stronger than the axial one ($\omega_r \gg \omega_z$) and comparable to the potential depth $U_0 \gtrsim \hbar \omega_z$ for the parameter range discussed in the following. Therefore we expect only a single bound state radially, while there are likely multiple axial states. Thus, this is effectively a one-dimensional system.

In order to obtain the bound states we calculate the spectrum of equation (6). Since the problem has cylindrical symmetry we expand on the basis set $\{\phi_{nlk}(r, \varphi, z)\}$ of the cylindrical harmonic oscillator, see appendix, and note that states with different $l$ quantum number are decoupled. Being in the radial ground state we restrict our analysis to the $l = 0$ components. To simplify calculations, we approximate the potential $U_{bf}(r,z) \approx U_{bf}(r) = U_{bf}(0,z)$, such that radial and axial contributions decouple. In the next step we compute the Hamiltonian matrix $\{\mathcal{H}\}$ with $\{\phi_{nlk}\}$ including radial (axial) quantum numbers $n = 0, 2, \ldots, 24$ ($k = 0, 1, \ldots, 59$) and $l = 0$. The number of basis vectors is chosen such that all...
contributions $\geq 10^{-2}$ to the calculated eigenenergies are considered. We obtain the latter by diagonalizing the Hamiltonian matrix and focus on bound state solutions $E_s < 0$ in the following. Figure 2 shows an example with $N_{\text{fd}} = 1500$ and $a_{\text{fd}} = 70 a_0$, where we find $N_{\text{bs}} = 12$ bound states. A few corresponding eigenstates $\psi_s$ are depicted as well. Qualitatively, these are similar to the well-known harmonic oscillator states and have $\phi_{00a}$ character. Thus the bound states are non-degenerate.

In the following we focus on the parameter range of $N_{\text{fd}} \leq 2000$ atoms and $a_{\text{fd}} = 50-120 a_0$. In this regime, the potential depth is large enough to accommodate several bound states, while it is well in the one-dimensional regime. At the same time the number of bound states $N_{\text{bs}}$ restricts the number of fermions in the system. Therefore the initial assumption $N_{\text{fd}} \gg N_{\text{bs}}$ neglecting an influence of fermions on the bosonic ground state is satisfied intrinsically. The number of bound states $N_{\text{bs}}$ is a direct measure of the trap depth for a known droplet. Therefore it increases with increasing droplet atom number $N_{\text{fd}}$ and decreasing Bose–Fermi scattering length $a_{\text{fd}}$, as shown in figure 3(a). The calculated energy $E_0$ of the ground state (solid lines) is verified by independent calculations via imaginary time evolution on a grid (dots), see figure 3(b). For $N_{\text{fd}} = 1500$ the spectrum $E_s$ of all bound states (dashed) is shown as well. The anharmonicity of the trapping potential $U_{\text{bd}}$ leads to a rich level scheme with a typical spacing of $\Delta E = E_{s+1} - E_s \approx 500$ Hz, that decreases to $\approx 200$ Hz towards the threshold. Experimentally, the level spectrum could be probed by driving transitions between bound states through harmonic modulation of $a_{\text{fd}}$ at the frequency $\Delta E/h$.

We now estimate the magnitude of the DDI between fermions, that we neglected so far. Although s-wave scattering is forbidden due to spin statistics, fermions can still interact via the dipolar interaction [22]. To estimate this effect, we compute the Hartree energy

$$E_{s,s'} = \frac{1}{2} \int \mathrm{d}r \int \mathrm{d}r' |\psi_s(r)|^2 U_{\text{bip}}(r - r') |\psi_{s'}(r')|^2$$

between the states $\psi_s$ and $\psi_{s'}$, occupied with one fermion each. For the conditions of figure 2 the energy shift $E_{0,1}$ between ground and first excited state is $\approx 20$ Hz, which is small compared to the level spacing $\Delta E$, as mentioned earlier. For other combinations of $s$ and $s'$ the values are even lower due to decreasing overlap of the wavefunctions. Therefore, the initial assumption of negligible dipolar interaction between fermions appears satisfied. Full Hartree–Fock calculations could allow to calculate the modifications to the orbitals due to the DDI when several fermions are present. However, the interaction of fermions with the bosonic quantum depletion has to be taken into account as well. In order to estimate it, we calculate the condensate depletion $\Delta n/n \approx 5\%$ [24] corresponding to $N_{\text{depl}} = 75$ depleted atoms for a droplet with $N_{\text{fd}} = 1500$. With $N_{\text{depl}} > N_{\text{bs}}$ and based on the prior estimate, this interaction can become sizeable. Thus, the energy due to interactions with the quantum depletion surpasses the fermion–fermion DDI interaction energy. Expanding on this idea, a fermionic impurity might be used to probe the quantum depletion. Yet, a more sophisticated theory like [27] is needed to describe and understand both effects properly, which is beyond the scope of this article.

In conclusion, we derived the Hamiltonian of fermions interacting with a large number of bosons. Leaving the bosonic state unaffected due to the low fermion number, the problem reduces to a Schroedinger equation with an external
potential due to the Bose–Fermi interaction. We use this formalism to investigate the interaction of dipolar fermions with a dipolar self-bound quantum droplet. The resulting interaction potential closely resembles the elongated droplet density distribution with additional long-range features. For typical conditions of the droplet, the latter is attractive and we find a limited number of bound states. Since every state can only be occupied by a single fermion, we infer that neglecting a back-action on the bosonic droplet is justified, and the fermions act as impurities. These are effective one-dimensional systems due to the large aspect ratio of dipolar droplets.

Finally, this is the first step towards probing quantum droplets with impurities. With negligible back-action on the droplet, this should be possible non-destructively on the bosons, using recently developed single atom detection techniques [28]. Up to now, the droplet temperature has not been measured, because time-of-flight expansion, the standard tool for thermometry, does not work with self-bound objects. Since the fermionic impurities thermalize with the bosonic environment, the presented excitation spectrum should be subject to thermal broadening. This way, we expect to extract the temperature and other finite-temperature effects, e.g. thermal fluctuations aiding to stabilize self-bound droplets, as recently suggested [29, 30]. On the other hand, it is an open question whether self-evaporation towards zero temperature, that has been predicted for quantum droplets of Bose–Bose mixtures [1], also occurs in its dipolar counterpart.

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Appendix. Cylindrical harmonic oscillator

For convenience, we show the solutions \( \phi_{nlk} \) to the cylindrical harmonic oscillator, as used in the manuscript. The corresponding differential equation

\[
-\frac{1}{2} \Delta \phi + \left(\frac{1}{r^2} + \frac{2}{r} \partial_r + \frac{1}{r^2} \partial^2_\varphi + \partial^2_z\right) \phi = 0
\]  

(A.1)

with \( \Delta = \left(\partial^2_r + \frac{2}{r} \partial_r + \frac{1}{r^2} \partial^2_\varphi + \partial^2_z\right) \) is separated into an axial and radial equation with the ansatz

\[
\phi_{nlk}(r, \varphi, z) = R_{nl}(r, \varphi) Z_k(z)
\]  

(A.2)

yielding the energy eigenvalues \( E = \left(n + k + \frac{3}{2}\right) \).

The radial equation is a two-dimensional harmonic oscillator in polar coordinates

\[
-\frac{1}{2} \left(\partial^2_r + \frac{1}{r} \partial_r + \frac{1}{r^2} \partial^2_\varphi\right) + \frac{1}{2} r^2 - E_n \right) R_{nl}(r, \varphi) = 0
\]  

(A.3)

and is solved by the radial function

\[
R_{nl}(r, \varphi) = \sqrt{\frac{(\frac{n}{2} - \frac{1}{2})!}{\pi (\frac{n+1}{2})!}} e^{-\frac{r^2}{2}} e^{i\varphi} r^n L_{\frac{n+1}{2}}^{|n|}(r^2)
\]  

(A.4)

with \( n = 0, 2, 4, \ldots \) and \( l = -n, -n+2, \ldots, +n \). The eigenenergy is \( E_n = n + 1 \) with a degeneracy of \((n + 1)\) for a single \( n \) value.

The axial part is the well-known problem of the harmonic oscillator in one dimension

\[
-\frac{1}{2} \partial^2_z + \frac{1}{2} z^2 - E_k \right) Z_k(z) = 0,
\]  

(A.5)

that is solved by

\[
Z_k(z) = \sqrt{\frac{1}{\pi^{1/4} 2^{k} k!}} e^{-z^2/2} H_k(z)
\]  

(A.6)

obtaining eigenenergies \( E_k = k + \frac{3}{2} \) with \( k = 0, 1, 2, \ldots \).

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