

Anisotropic potential immersed in a dipolar Bose-Einstein condensate

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We study a three-dimensional Gross-Pitaevskii equation that describes a static impurity in a dipolar Bose-Einstein condensate. Our focus is on the interplay between the shape of the impurity and the anisotropy of the medium manifested in the energy and the density of the system. Without external confinement, properties of the system are derived with basic analytical approaches. For a system in a harmonic trap, the model is investigated numerically, using the split-step Crank-Nicolson method. Our results demonstrate that the impurity self-energy is minimized when its shape more closely aligns with the anisotropic character of the bath; in particular a prolate deformed impurity aligned with the direction of the dipoles has the smallest self-energy for a repulsive impurity. Our work complements studies of impurities in Bose gases with zero-range interactions and paves the way for studies of dipolar polarons with a Gross-Pitaevskii equation.

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I. INTRODUCTION

The question of how a system responds to perturbation (stress) is of general importance in physics, in particular, in cold-atom physics. Naturally, isotropic media are the most explored in this context. However, progress in realizing ultracold dipolar gases brings the perfect playground for going beyond isotropicity [1]. It becomes possible to investigate the effect of perturbations on quantum degenerate gases that are intrinsically anisotropic.

In this work we explore the effect of a static perturbation on an anisotropic medium by placing an impurity at the center of the dipolar Bose gas. The impurity can be an optically generated potential, which in principle can be of arbitrary shape in modern cold-atom experiments [2]. By calculating the ensuing properties, we gain insight into the differences between dipolar and nondipolar systems.

First, we study the Bose gas without external confinement. In this case the character of the system can be analyzed analytically at least within the local density approximation. We show that even an isotropic impurity leads to an anisotropic response, which reveals the nature of the Bose gas. Further, for an anisotropic impurity, the energy of the system depends strongly on the interplay between the direction of the dipoles and the shape and orientation of the impurity. The dipolar nature of the Bose gas is the most pronounced in the vicinity of the collapse, where the number of bosons displaced by the impurity becomes large. Second, we analyze an experimentally relevant system in a harmonic trap. We show that the results derived in the homogeneous setting still hold, advocating for an exploration of static impurities with dipolar gases in a laboratory.

Before proceeding further, we note a connection of our work to a field of mobile impurities in cold gases that has seen a number of advances recently [3–7]. The interactions between the impurity and the medium effectively alter the

impurity's properties from its vacuum properties as it is dressed by particles of the medium, turning it into a polaron. Though these are mobile particles, studies of heavy impurities typically lay the ground for understanding the corresponding energy spectra.

This paper is structured as follows: Sec. II describes the system and the modified Gross-Pitaevskii equation (GPE) used in the study. Section III presents analytical analysis of a Bose gas without external confinement. Section IV contains numerical simulations of the GPE, along with their discussion. Additionally, we include a study of the time dynamics that follow a sudden immersion of the impurity. This allows us to estimate timescales relevant for the experiment. A brief summary of the results and an outlook are given in Sec. V. Finally, we include two Appendixes with additional information.

II. FORMALISM

Hamiltonian. The Hamiltonian that describes the system of interest—a Bose gas with a static “impurity” potential—reads

$$H = \sum_{k=1}^N \left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial \mathbf{r}_i^2} + V_{\text{trap}}(\mathbf{r}_i) \right] + \sum_{i<j}^N V_c(\mathbf{r}_i - \mathbf{r}_j) + \sum_{i<j}^N V_d(\mathbf{r}_i - \mathbf{r}_j) + \sum_{i=1}^N V_i(\mathbf{r}_i), \quad (1)$$

where m is the mass of a boson, and $\mathbf{r}_i$ is the coordinate of the i th boson. The bosons are confined by the harmonic-oscillator trapping potential V_{trap} . They interact via the contact, V_c , and the dipole-dipole interactions, V_d , discussed below; the function V_i is the impurity-boson potential energy. To differentiate between V_{trap} and V_i , we note that the latter vanishes at infinity, $V_i(|\mathbf{r}| \rightarrow \infty) \rightarrow 0$.

To analyze the system, we shall rely on a mean-field approximation. Therefore, we can write the contact interaction

as $V_c(\mathbf{r}) = 4\pi\hbar^2 a \delta(\mathbf{r})/m$, where a is the scattering length [8,9]. The functional form of the dipole-dipole potential is

$$V_d(\mathbf{r}) = \frac{\mu_0}{4\pi} \frac{\mathbf{d}^2 - 3(\mathbf{d} \cdot \hat{\mathbf{r}})(\mathbf{d} \cdot \hat{\mathbf{r}})}{|\mathbf{r}|^3}, \quad (2)$$

where $\mathbf{d}$ is the dipole moment of the bosons, μ_0 is the vacuum permeability, and $\hat{\mathbf{r}}$ is the unit vector along the direction of $\mathbf{r}$. We shall use a system of coordinates in which the z axis is along $\mathbf{d}$, and write the dipole-dipole interaction in a more convenient form

$$V_d = \frac{C_{dd}}{4\pi} \frac{1 - 3\cos^2\theta_d}{r^3}, \quad (3)$$

where θ_d is the angle between $\mathbf{r}$ and $\mathbf{d}$. We have adopted the standard notation, $C_{dd} = \mu_0 d^2$, which helps us to introduce a relevant length scale (the “dipolar length”) as $a_{dd} = C_{dd}m/(12\pi\hbar^2)$ [10]. The Hamiltonian in Eq. (1) without V_i is well studied [10,11] theoretically. The focus of our paper is on the effect of the impurity.

Gross-Pitaevskii equation. To analyze the system, we rely on a mean-field ansatz, i.e., we assume that the ground state of the Hamiltonian can be approximated by a product state $\psi(\mathbf{r}_1)\psi(\mathbf{r}_2)\cdots\psi(\mathbf{r}_N)$ well. To find the function ψ , we solve the GPE

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi(\mathbf{r})}{\partial \mathbf{r}^2} + V_{\text{trap}}(\mathbf{r})\psi(\mathbf{r}) + gN|\psi(\mathbf{r})|^2\psi(\mathbf{r}) + N \int d\mathbf{x} V_d(\mathbf{r} - \mathbf{x})|\psi(\mathbf{x})|^2\psi(\mathbf{r}) = [\mu - V_i(\mathbf{r})]\psi(\mathbf{r}), \quad (4)$$

where $g = 4\pi\hbar^2 a/m$ reflects the strength of the contact interaction and μ is the chemical potential. Any solution to the GPE is subject to the normalization condition $\int d\mathbf{r} |\psi(\mathbf{r})|^2 = 1$.

In the next section, we present various approximations for analytical analysis of Eq. (4) in a homogeneous case. In Sec. IV we calculate the energies and densities in a trapped case. To this end, we solve the GPE using the split-step Crank-Nicolson method. Our numerical code is a modification of an open-source software described in Ref. [12].

III. HOMOGENEOUS SYSTEM

The Thomas-Fermi limit. We start by considering an infinite medium with $V_{\text{trap}} = 0$. We assume that the potential V_i changes “weakly and slowly” (see the discussion below for a weak impurity potential) so that we can employ the Thomas-Fermi approximation and solve the equation

$$V_i(\mathbf{r}) + g\delta n(\mathbf{r}) = - \int d\mathbf{x} V_d(\mathbf{r} - \mathbf{x})\delta n(\mathbf{x}), \quad (5)$$

where $\delta n(\mathbf{x}) = N|\psi(\mathbf{x})|^2 - n_0$ determines the density of the Bose gas in the presence of the impurity and $n_0 = N/\mathcal{V}$ is the average density, $n_0 = N \int d\mathbf{r} |\psi(\mathbf{r})|^2 / \mathcal{V}$ with $\mathcal{V}$ being the volume of the system. n_0 is also the density far from the impurity because $\delta n(\mathbf{r} \rightarrow \infty) \rightarrow 0$ as we will demonstrate below. This implies that n_0 fixes the chemical potential, i.e., $\mu = gn_0$ (it is independent of dipole-dipole interactions in a

homogeneous setting) [13]. In this section, we shall use $n_0^{-1/3}$ as the unit of length and μ as the unit of energy for presenting our findings in a dimensionless form.

Equation (5) has a nonlocal character, i.e., the density at any given position is determined in part by the density of its surrounding neighborhood. This makes it hard, if not impossible, to solve the equation in real space explicitly for a general form of the impurity potential (though see [14] for solutions in some special cases). At the same time, linearity of Eq. (5) with respect to δn allows us to find its Fourier transform $\delta \tilde{n}(\mathbf{k}) = \int d\mathbf{r} \delta n(\mathbf{r}) e^{-i\mathbf{k} \cdot \mathbf{r}}$ easily:

$$\delta \tilde{n}(\mathbf{k}) = - \frac{\tilde{V}_i(\mathbf{k})}{g + \tilde{V}_d(\mathbf{k})}, \quad (6)$$

where $\tilde{V}_i$ and $\tilde{V}_d$ are Fourier transforms of the impurity and dipole-dipole potentials, respectively. In the case of the dipole potential, $\tilde{V}_d(\mathbf{k}) = C_{dd}(\cos^2\alpha - 1/3)$ [10,15] with α being the angle between $\mathbf{d}$ and $\mathbf{k}$. This expression can be conveniently rewritten using the second Legendre polynomial, $\tilde{V}_d(\mathbf{k}) = 2C_{dd}P_2(\cos\alpha)/3$.

The density in real space can be written in integral form as

$$\delta n(\mathbf{r}) = - \frac{1}{g(2\pi)^3} \int d\mathbf{k} \frac{\tilde{V}_i(\mathbf{k})}{1 + 2\varepsilon_{dd}P_2(\cos\alpha)} e^{i\mathbf{k} \cdot \mathbf{r}}, \quad (7)$$

where $\varepsilon_{dd} = a_{dd}/a$ is a dimensionless ratio that determines the relative importance of dipolar physics. In particular, the system is unstable against a collapse if ε_{dd} is larger or equal to one [10]. Notice that the density is anisotropic even if the impurity potential is isotropic.

To illustrate this, let us consider $\varepsilon_{dd} \rightarrow 0$ (weak dipole-dipole interactions). Using the plane-wave expansion [$e^{i\mathbf{k} \cdot \mathbf{r}} = 4\pi \sum_{l,m} i^l j_l(kr) Y_l^m(\hat{\mathbf{k}}) [Y_l^m(\hat{\mathbf{r}})]^*$ with Y_l^m being the spherical harmonics], we derive

$$\delta n(\mathbf{r}) \simeq - \frac{V_i(\mathbf{r})}{g} - \frac{\varepsilon_{dd} P_2(\cos\theta)}{g\pi^2} \int dk k^2 \tilde{V}_i(k) j_2(kr), \quad (8)$$

where j_l is a spherical Bessel function, and θ is the polar angle of $\mathbf{r}$. The first term here is the Thomas-Fermi profile for a nondipolar gas [8]. The second part is due to the dipolar character of the medium; we have used the isotropicity of V_i to simplify it.

The uncomplicated form of Eq. (8) will be modified for larger values of ε_{dd} . In particular, the density will include higher order harmonics, $P_{2n}(\cos\theta)$. We clarify this in Fig. 1 by comparing Eqs. (8) and (7) for a strong spherical Gaussian impurity, $V_i(\mathbf{r}) = \mu \exp(-n_0^{2/3} r^2)$, and different values of ε_{dd} . At small values of ε_{dd} , Eqs. (7) and (8) agree with each other, while becoming more different as the dipolar interaction becomes stronger. It is seen clearly that the Thomas-Fermi approach approximation has broken down in Fig. 1(b) as it produces a nonphysical density at small ($\theta \lesssim \pi/6$) and large ($\theta \gtrsim 5\pi/6$) angles. This is discussed in more detail at the end of this section. These two equations do, however, retain similar angular dependence at all values of ε_{dd} . From Fig. 1(a), where the results agree also quantitatively, we conclude that the density increases in comparison to the nondipolar solution, $\varepsilon_{dd} = 0$, in the direction perpendicular to z , i.e., in the xy plane. Indeed, it is easier to deform the system in this

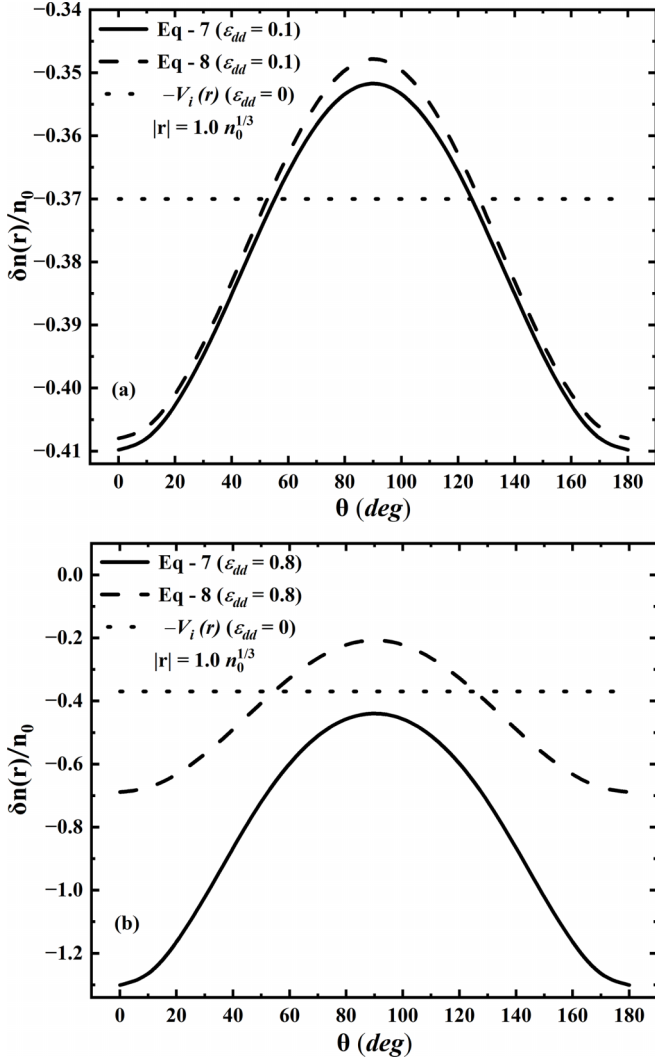


FIG. 1. Comparison of the results obtained from Eqs. (7) and (8) at different values of ε_{dd} , plotted with respect to the polar angle (θ), $\mathbf{r} = |\mathbf{r}|(\sin(\theta), 0, \cos(\theta))$. The value of the impurity potential is shown with a horizontal dotted line. Note that panel (b) makes it clear that Eq. (7) is not valid for large values of ε_{dd} as $\delta n/n_0 + 1$ must be non-negative (recall that $\delta n + n_0 = N|\psi|^2$).

direction because the corresponding phononic excitations are softer [10].

To further highlight the anisotropic character of Eq. (8), let us study the gradient of the density. In the contact case, we have $\nabla n = \mathbf{F}/g$, where the “force” is given by $\mathbf{F} = -\nabla V_i$. This simple law follows from conservation of chemical potential throughout the sample and the fact that the medium is isotropic, so that we cannot assign any tensor to it. For the dipolar medium the situation is different, and the gradient is given not only by the external force, but also by properties of the medium (e.g., internal strain), which are anisotropic and nonlocal.

Self-energy of the impurity. It is worth noting that Eq. (4) with the reduced mass instead of m can describe also a mobile impurity just as in a nondipolar case [16–21]. Therefore, even though our work focuses on the effect of static impurities, our results could also be useful for mobile impurities. Below

we use the densities in the Thomas-Fermi limit to calculate two paradigmatic properties typically studied for mobile impurities. First, we compute the self-energy of the impurity defined as the difference of the energies of the system with and without the impurity assuming a fixed chemical potential:

$$E_{\text{self}} = E[V_i] - E[V_i = 0], \quad (9)$$

where $E[V_i]$ is the energy of the system with the impurity potential V_i . This energy is one of the key characteristics for systems with impurities. The self-energy can be thought of as the chemical potential of the impurity or the change in energy of the bath due to the presence of the impurity [22]. Within our approach, E_{self} has the form (see Appendix A)

$$E_{\text{self}} = -\frac{gN^2}{2} \int \psi(\mathbf{x})^4 d\mathbf{x} + \frac{g\mathcal{V}n_0^2}{2} - \frac{N^2}{2} \int \psi(\mathbf{x})^2 V_d(\mathbf{r} - \mathbf{x}) \psi(\mathbf{r})^2 d\mathbf{r} d\mathbf{x}, \quad (10)$$

where $\mathcal{V}$ is the volume of the system. After straightforward calculations, we write this expression as

$$E_{\text{self}} = E_{\text{self}}^0 - \frac{1}{2g} \int \delta n(\mathbf{r}) V_d(\mathbf{x} - \mathbf{r}) V_i(\mathbf{x}) d\mathbf{r} d\mathbf{x}, \quad (11)$$

where $E_{\text{self}}^0 = n_0 \int V_i(\mathbf{r}) d\mathbf{r} - \frac{1}{2g} \int V_i^2(\mathbf{r}) d\mathbf{r}$ is the contribution to the energy that is independent of the dipolar nature of the Bose gas. Let us assume that the dipole-dipole interactions are weak (i.e., $\varepsilon_{dd} \rightarrow 0$), then we can estimate the dipolar contribution to the self-energy as

$$E_{\text{self}} - E_{\text{self}}^0 \simeq \frac{1}{2g^2} \int V_i(\mathbf{r}) V_d(\mathbf{x} - \mathbf{r}) V_i(\mathbf{x}) d\mathbf{r} d\mathbf{x}. \quad (12)$$

This equation clearly shows that the self-energy depends not only on the anisotropy of the dipole-dipole interactions, but also on the anisotropy of the impurity potential. Indeed, if the potential V_i is elongated along the z direction, then the right-hand side of Eq. (12) is negative. The opposite is true for the impurity potentials elongated along the x axis. We shall illustrate this dependence numerically in the next section for a trapped system.

Number of bosons in a “dressing” cloud. The number of bosons directly affected by the presence of the impurity can be estimated as follows [$\delta N = \int d\mathbf{r} \delta n(\mathbf{r})$; see Appendix A]:

$$\delta N = -\frac{\int d\mathbf{r} V_i(\mathbf{r})}{g\sqrt{3\varepsilon_{dd}(1-\varepsilon_{dd})}} \tan^{-1} \left[\sqrt{\frac{3\varepsilon_{dd}}{1-\varepsilon_{dd}}} \right]. \quad (13)$$

This expression shows that $|\delta N|$ is an increasing function of ε_{dd} , implying that the dipolar medium leads to a “more heavy” dress of the impurity. This can be most easily visualized by considering limiting cases. For weak dipole-dipole interactions, $\varepsilon_{dd} \rightarrow 0$, we derive

$$\delta N \simeq -\frac{1}{g} \int d\mathbf{r} V_i(\mathbf{r}) \left(1 + \frac{4\varepsilon_{dd}^2}{5} \right). \quad (14)$$

Note that this expression depends on the square of ε_{dd} , because the linear contribution from Eq. (8) averages out to zero.

In the vicinity of the collapse, $\varepsilon_{dd} \rightarrow 1$,

$$\delta N \simeq -\frac{\pi \int d\mathbf{r} V_i(\mathbf{r})}{2\sqrt{3}g\sqrt{1-\varepsilon_{dd}}}. \quad (15)$$

This result is likely beyond the limits of applicability of local-density approximation; see below. Still, it shows that the number of bosons in the dressing cloud becomes large close to collapse. For a mobile impurity, this should lead to strong renormalization of the effective mass in agreement with previous studies of dipolar Bose polarons [23–25]. The mass renormalization is, however, direction-dependent with the strongest effect in the xy plane, which cannot be captured by the angle-averaged quantity δN .

Limits of applicability of the Thomas-Fermi approximation. The Thomas-Fermi approximation is valid whenever the quantum pressure term, proportional to $\frac{\partial^2 \psi(\mathbf{r})}{\partial \mathbf{r}^2}$, can be neglected in Eq. (4). For a nondipolar gas that can be done when the impurity potential changes weakly on length scales given by the local healing length of the gas, $\xi \sim 1/\sqrt{gn(\mathbf{r})}$. Obviously the Thomas-Fermi approximation fails when the impurity potential is so strong that $n(\mathbf{r}) \rightarrow 0$, which happens for example in trapped gases close to the edges of the Bose-Einstein condensate (BEC) [8]. For a dipolar gas, one can generalize the condition above assuming that the healing length depends on the direction.

To illustrate this, let us study a weak impurity potential, namely, we consider Eq. (4) without a trap and $V_i \rightarrow 0$. We look for a solution ψ in the following form (cf. Ref. [26]):

$$\psi(\mathbf{r}) \simeq \frac{1 + f(\mathbf{r})}{\sqrt{V}}. \quad (16)$$

We assume that f is small and satisfies

$$\frac{\hbar^2}{2m} \nabla^2 f(\mathbf{r}) = 2\mu f + \frac{2\mu}{g} \int d\mathbf{x} V_d(\mathbf{r} - \mathbf{x}) f(\mathbf{x}) + V_i, \quad (17)$$

which allows us to find Fourier transform $\tilde{f}(\mathbf{k})$ as

$$\tilde{f}(\mathbf{k}) = -\frac{\tilde{V}_i(\mathbf{k})}{\frac{\hbar^2 k^2}{2m} + 2\mu + 2\frac{\mu}{g} \tilde{V}_d(\mathbf{k})}. \quad (18)$$

By comparing this equation to Eq. (6), we conclude that the Thomas-Fermi approximation is valid if the characteristic momenta of $\tilde{V}_i(\mathbf{k})$ are much smaller than $\sqrt{4\mu m/\hbar^2 \sqrt{1+2\varepsilon_{dd}P_2(\cos\alpha)}}$. For $\varepsilon_{dd} = 0$, this condition implies that the potential must change weakly on length scales given by the healing length, validating our assertion above. For a dipolar gas, this condition depends strongly on ε_{dd} and on the direction. In particular, for ε_{dd} close to one, $1 + 2\varepsilon_{dd}P_2(0)$ is small and the Thomas-Fermi approximation should be used with great care.

Finally, we mention another indication that the local-density approximation fails, which follows from the observation that $\delta n(\mathbf{r})/n + 1$ should be non-negative. Assuming repulsive spherically symmetric impurity with its maximum at the origin, the fulfillment of this condition can be checked by considering $\delta n(0)/n + 1$, which using Eq. (7) leads to

$$1 - \frac{\int dk \tilde{V}_i(k) k^2}{2\pi^2 \mu \sqrt{3\varepsilon_{dd}(1-\varepsilon_{dd})}} \tan^{-1} \left[\sqrt{\frac{3\varepsilon_{dd}}{1-\varepsilon_{dd}}} \right] \geq 0. \quad (19)$$

This condition clearly fails when the impurity potential is too strong, i.e., $V_i(0) \gtrsim \mu$, or when the system is close to the dipolar collapse, $\varepsilon_{dd} \rightarrow 1$. In both of these cases, the corresponding healing lengths diverge undermining the applicability of the Thomas-Fermi approximation. We illustrate this in Fig. 1 where a strong impurity potential and a relatively large value of ε_{dd} lead to $\delta n/n_0 + 1 < 0$ signaling the breakdown of the Thomas-Fermi approximation.

IV. TRAPPED SYSTEM

Guided by the results above, we now conduct a detailed analysis across a range of scenarios, which should help to identify the physics described in the previous section in a laboratory. To this end, we consider a harmonically trapped system of dysprosium atoms whose large dipolar length $a_{dd} \approx 130a_0$ puts them at the forefront of current experimental studies [1]. For simplicity, the trapping potential is assumed to be symmetric, with the form given by

$$V_{\text{trap}} = \frac{1}{2} m \omega^2 r^2, \quad (20)$$

where ω is the trapping frequency. The corresponding harmonic oscillator length is $L = \sqrt{\hbar/(m\omega)}$. In our numerical simulations, we use $L = 1\mu\text{m}$, which is representative of experimentally relevant values [27]. We set the number of atoms to $N = 2 \times 10^4$. The atomic scattering length is chosen to be $a = 150a_0$, which makes the gas stable ($a > a_{dd}$). This a is close to the background value in ^{162}Dy samples, otherwise our choice is rather arbitrary as a can be tuned using external magnetic fields; see, e.g., Ref. [1].

In Fig. 2 the density distribution of the dipolar gas in the absence of the impurity is shown in the xz plane, parallel to the plane of polarization. As expected [28,29], the graph demonstrates that the intrinsic interactions between the dipoles of the system make the system elongated along the z axis, the direction in which the dipoles are polarized. We stress that the trap itself is isotropic, so that the anisotropy observed in the density is purely from the interactions within the system (cf. Sec. III). For the considered parameters of the Bose gas, this anisotropy is weak close to the origin [see, e.g., the almost flat curve at $|\mathbf{r}| = 1\mu\text{m}$ in Fig. 2(b)], providing a suitable test bed for investigating the anisotropy induced by the impurity.

A. Introducing the impurity

We assume an impurity described by the potential

$$V_i(x, y, z) = V_0 \exp \left[-\left(\frac{x^2 + y^2}{a^2 L^2} + \frac{z^2}{b^2 L^2} \right) \right]. \quad (21)$$

Here a and b parametrize the width of the impurity potential in the transverse and longitudinal directions. The parameter V_0 determines the strength of the impurity potential. This parameter is positive in main part of this study, i.e., the impurity repels the bosons; see Appendix B for a brief discussion of the case with $V_0 < 0$. It was set to be $5\hbar\omega$ in our calculations, implying that the effect of the impurity is strong (nonperturbative); i.e., a number of collective modes can be excited in the Bose gas. The potential in Eq. (21) can be optically generated in a cold Bose gas [2], which would provide a physical realization of the impurity studied here in a laboratory [30].

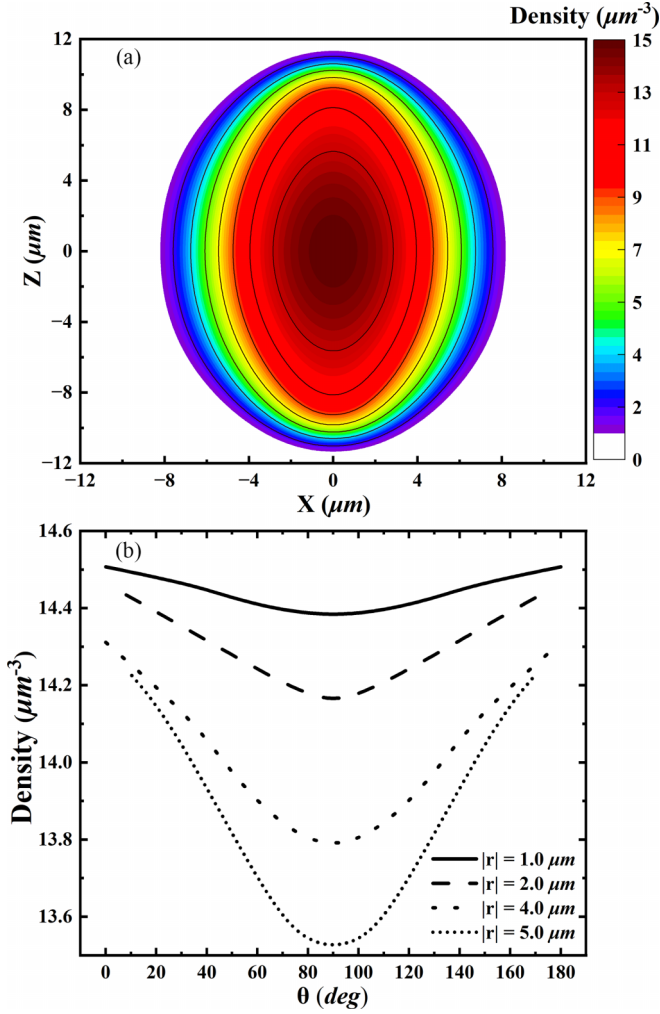


FIG. 2. Density distribution of the BEC in the absence of the impurity potential. (a) Density in the xz plane. (b) Density for a given value of $|r|$ as a function of the polar angle.

First, to understand the effect of the static impurity on the BEC, we calculate the density of the Bose gas for various deformation ratios. Here the “deformation ratio” refers to a systematic variation in the values of a and b in Eq. (21), while keeping the volume of the impurity ($4\pi a^2 b L^3/3$, treating it as an ellipsoid) constant at $1 \mu\text{m}^3$. The volume integral of the potential, $\int d\mathbf{r} V_i(\mathbf{r})$, is then also constant at $3V_0 L^3 \sqrt{\pi}/4$. We showed in Sec. III that the volume integral of the impurity is a crucial property of the potential that determines the energy of the system for the homogeneous nondipolar BEC. Therefore, by fixing it we can more directly see the effect of the dipolar nature of the bath, i.e., we can isolate the effect of the last term in Eq. (11). (Note, however, that the interplay between the external trap and the impurity potential also plays an important role in the results presented in this section.) For the sake of simplicity, here we will mostly discuss results for $a = b$, $a = 3b/2$, and $a = 3b$.

Figure 3(a) illustrates the scenario of an isotropic impurity ($a = b$), as evidenced by the circular contours at the origin. The emergence of two central peaks shows the effect of the

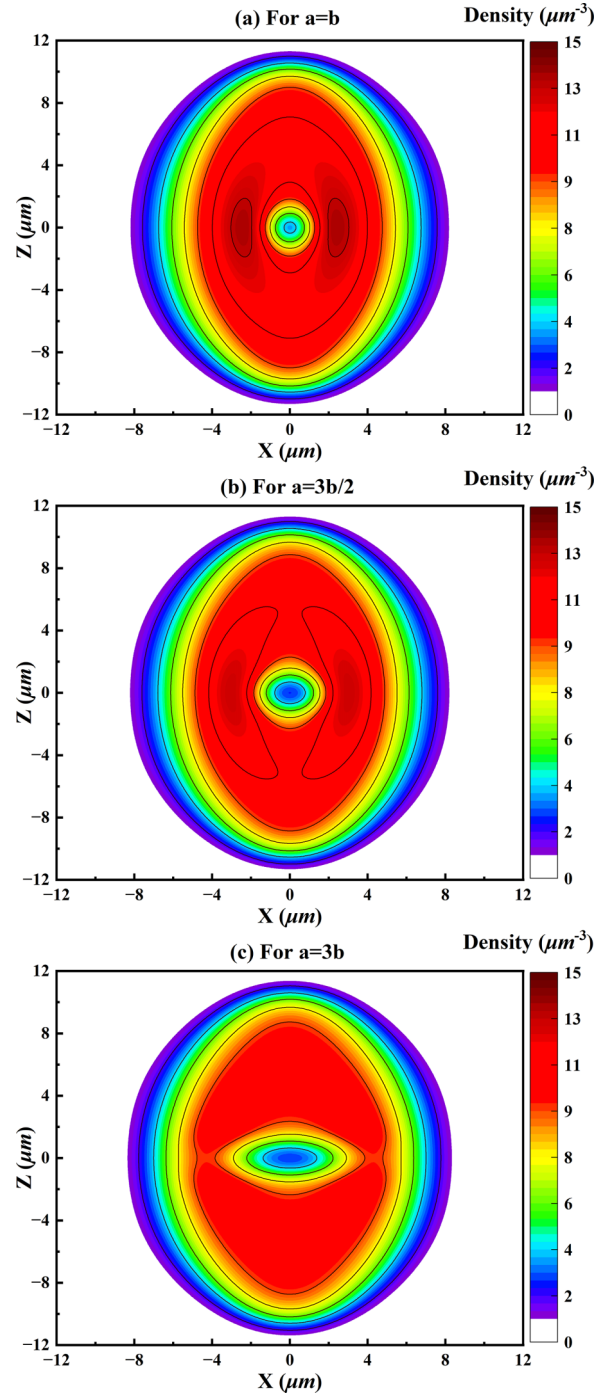


FIG. 3. Density of the system (BEC + static impurity) in the xz plane for different deformation ratios a/b ; cf. Eq. (21).

static impurity repelling the dipoles away from the origin. The peaks of the densities are located along the $z = 0$ lines in agreement with the discussion in Sec. III (see in particular Fig. 1). This figure shows a 2D cut of a 3D system, so one should bear in mind that instead of actual peaks in the density, the highest density exists in a torus around the z axis centered in the xy plane. Farther away from the impurity, the density is dominated by the harmonic trap (cf. Fig. 2).

Figures 3(b)–3(c) display results for anisotropic impurity potentials ($a \neq b$), with the impurity elongated along

the x axis, which induces a competition between intrinsic anisotropy of the system and anisotropy of the impurity. The elongation of the impurity dominates the properties of the dipolar gas at the origin. In particular, we see that contour plots of the density are elongated predominantly along the x axis in the vicinity of the origin.

In Fig. 3(c), which represents the maximum deformation analyzed in this study, the peak density regions now appear above and below the xy plane, though they appear much broader and diffuse than the other cases. The large deformation of the impurity has forced the system to reconstitute itself away from the xy plane and assemble in large caps separated along the dipolar axis. While the behavior far from the impurity remains similar to the previous cases, the system's response in the region of the impurity is clearly dependent on the precise shape and orientation of the impurity; the latter property we explore in the next section.

B. Orientation-dependent effects of impurity

To further analyze the interplay between the anisotropy of the impurity and the dipolar nature of the bath, in particular, the restoring of the dipolar symmetry far from the impurity, we examine the effect of rotating the impurity about the y axis. To achieve this, we employ a rotation matrix to change the functional form of the impurity potential in Eq. (21). As a result, we obtain

$$V_i = V_0 \exp \left[- \left(\frac{(x \cos \varphi + z \sin \varphi)^2 + y^2}{a^2 L^2} + \frac{(z \cos \varphi - x \sin \varphi)^2}{b^2 L^2} \right) \right], \quad (22)$$

where the angle φ is defined relative to the x axis. Neither the volume of the impurity ($4\pi a^2 b L^3 / 3 = 1 \mu\text{m}^3$) nor the volume integral of the potential is changed by rotation.

We present densities for 30° , 60° , and 90° fixing $a = 3b/2$ in Fig. 4. All these results exhibit similar features to those discussed in Fig. 3. Furthermore, they demonstrate the rotation of the density driven by the angle φ . For example, as the angle increases, the center appears to rotate and align with that particular angle. The density contours almost appear “stirred” though the impurity is static. The contours in the case of the top two panels also show the gradual evolution from the shape and orientation of the impurity to that of the bath. In the bottom panel, the impurity's elongation matches the elongation of the bath, so the center contours' orientation matches that of the edge contours. In addition, the maximal density regions become more focused as the major axis of the impurity gets closer to aligning with the polarization direction.

A superficial visual inspection of the density contours suggests that the maximum effect of the impurity potential occurs when the impurity's major axis is orthogonal to the polarization of the dipoles and decreases as they become more aligned. This remains true even for larger deformations of the impurity (not shown). To quantify this observation, we calculate the energy of the system below.

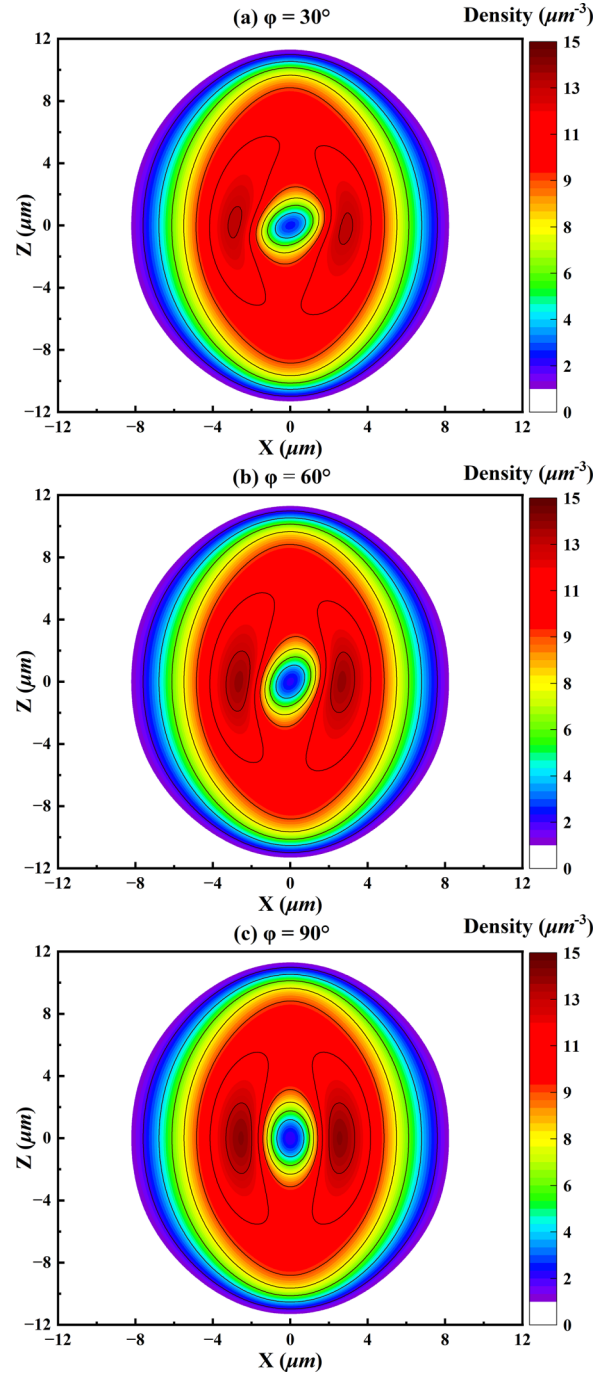


FIG. 4. Density of the system (BEC + static impurity) in the xz plane for different orientations of the impurity, i.e., for different values of φ ; cf. Eq. (22). The deformation ratio is $a = 3b/2$.

C. Self-energy of impurity

The results above show the interplay between the anisotropy of the impurity and the anisotropy of the medium in a trap. Quantifying this interplay by looking at the densities is difficult. Therefore, in this subsection we study the energy of the system. To quantify this effect, we calculate the self-energy (E_{self}) defined as in Sec. III. We expect this quantity to depend not only on the amount of deformation but also on the orientation of the impurity.

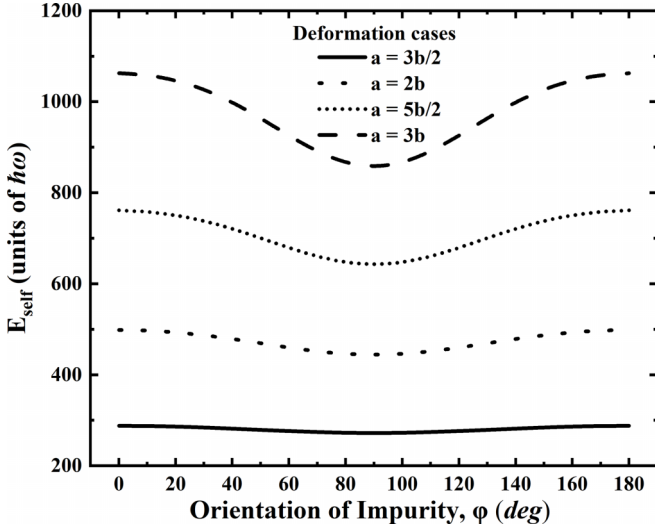


FIG. 5. Effect of rotation on the self-energy of the impurity for different deformation ratios. Recall that the orientation angle is defined with respect to the x axis and that the volume integral of the impurity $[\int d\mathbf{r} V_i(\mathbf{r}) = 3V_0 L^3 \sqrt{\pi}/4]$ is fixed; cf. Eq. (22).

In Fig. 5 the self-energy of the impurity for several deformation ratios is presented with respect to various orientation angles. The self-energy of the impurity-BEC system exhibits a nearly sinusoidal variation, showing a strong preference for the major axis of the impurity deformation to align along the z axis [cf. Eq. (12)]. The effect is solely due to the dipolar nature of the BEC and vanishes if $\varepsilon_{dd} = 0$. Larger deformation ratios exhibit very similar qualitative behavior, though quantitatively all the self-energies increase with increasing deformation.

We illustrate this in Fig. 6, which demonstrates the dependence of the self-energy on the major and minor axis ratio, a/b . This plot echoes what was seen in Fig. 5, in that the most energetically favorable impurity is the one with the most elongation along the polarization axis. The prolate ($a < b$)

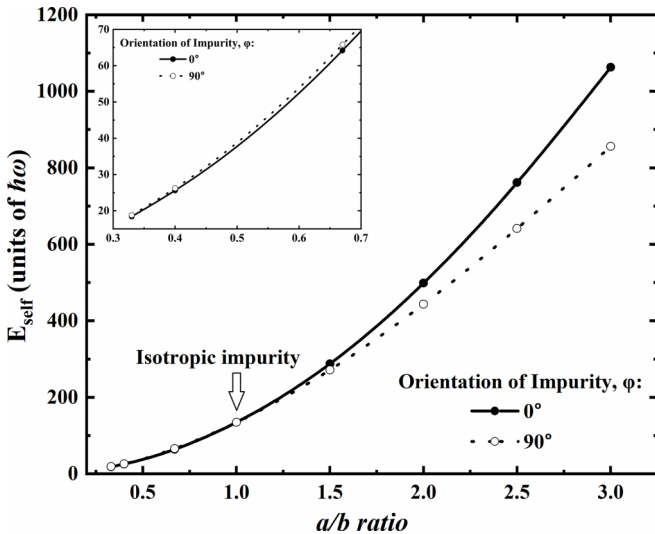


FIG. 6. Self-energies plotted as a function of the deformation ratio, a/b , for two orientations of the impurity potential in Eq. (22). The inset zooms in on small a/b ratios.

impurity allows more of the dipoles to be closer together in their favored head-to-tail configuration. Once the impurity becomes isotropic and then oblate ($a > b$), the self-energy increases more rapidly as the impurity's presence is increasingly disruptive to the dipolar gas. The dashed line in Fig. 6 shows the self-energy results for the systems where the impurity has been rotated by 90° . Here we see that for the oblate case, rotating the impurity decreases the self-energy. Since after rotating 90° , one of the impurity's major axes is now along the z axis, this result is not surprising. In the case of the prolate impurity, we observe the opposite in that the rotation increases the self-energy. The reasoning is the same since now the longest axis is along the x axis, though the difference is less dramatic than in the oblate case.

D. Time dynamics

Another interesting question is how the system evolves once an impurity is introduced (going from Fig. 2 to Fig. 3). To study it, we start with the density solution of our system without an impurity and then utilize the real-time propagation of the split-step Crank-Nicolson method for our numerical solutions. The results of this can be seen in Fig. 7, where the density in 1D cross sections along the x and z axes are shown for an isotropic impurity. Results for the other impurities were similar to the isotropic case, so we discuss the time evolution without focusing on the different impurities. In Fig. 7 it can be seen how the density plunges in the center of the trap by first creating large peaks close to the origin, which then recede over longer times as more particles are pushed away from the repulsive impurity and vacate the center region of the trap. In both plotted directions, the density plunges all the way to zero in the center before rebounding back, and then repeating. The repeating pattern is due to the trap and was also seen in nondipolar trapped systems; see, e.g., Ref. [31].

An additional feature can be seen in the plots in the z direction. One can see a shoulder in the density peaks forming which separates into peaks seeming to show waves traveling outward along the $\pm z$ axes. This behavior is similar to what happens in a homogeneous nondipolar case (see, e.g., Ref. [32]) with a crucial difference that the dynamics in the x direction are different from that in the z direction. These waves appear to hit the trap boundary and then rebound and collapse eventually into a single peak as time increases. Recall that the spatial extent in the x direction (see Fig. 2) is not as large as that in the z direction, and thus the impurity induces this behavior only in the z direction. Finally, these results were obtained within the mean-field GPE framework, and further study involving beyond mean-field effects and/or finite temperature could be explored in the future.

V. CONCLUSION AND OUTLOOK

We have investigated the response of a dipolar medium to an implantation of a repulsive impurity at its center. We have observed a large distortion to the density of the medium, which indicates a preference for the dipoles to stay in their preferred head-to-tail configuration. This preference is reinforced by our results for self-energy, which we have examined as a function of the deformation of the impurity as well

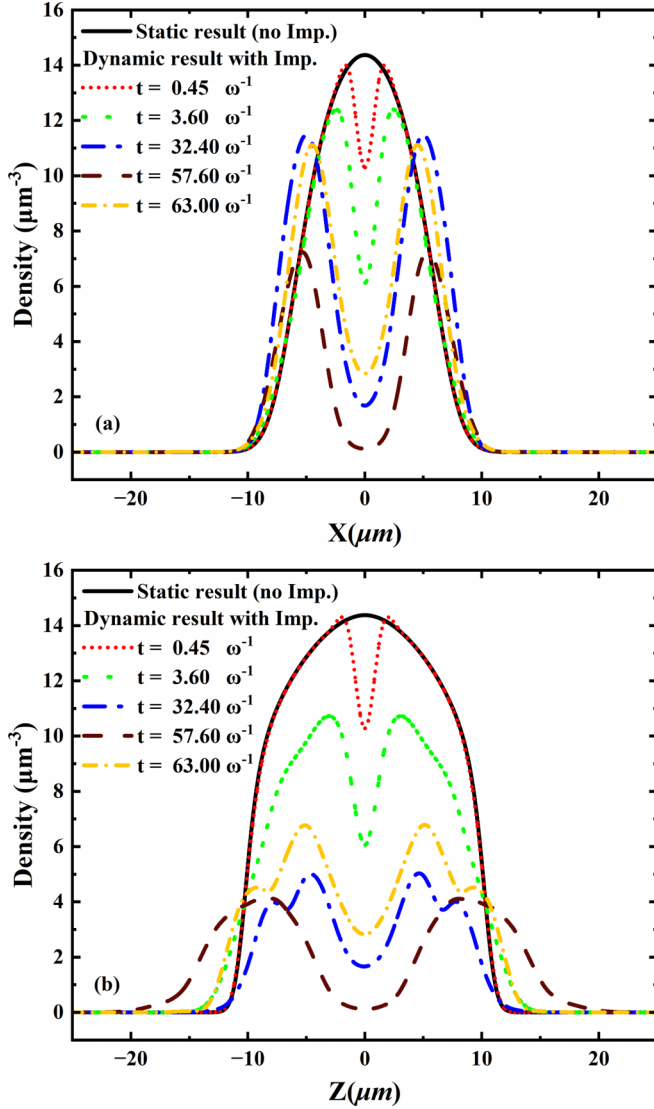


FIG. 7. Density profiles along the x axis (a) and z axis (b) for different amounts of time evolution. At $t = 0$, a dipolar BEC without an impurity has a spherical impurity implanted into it at the origin. The center density decreases until $t = 57.60 \omega^{-1}$, then begins to rebound. Note that the important timescale is defined by the frequency of the external trap, ω , which sets the smallest energy scale of the system. For the Dy system, which we use in our numerical simulations, $1/\omega \simeq 2.5$ ms.

as the orientation of the impurity. Future experiments with impurities in dipolar BECs would expect to see anisotropic density modulations in their atom-cloud images regardless of the type of impurity used. Mobile impurities, though smaller in size than the impurity potential of this work, should also lead to this behavior. It might be harder, however, to study the density modulations in this case as mobile impurities are free to move within the Bose gas distorting the signal. Our results pave the way for a number of possible follow-up studies, some of which we briefly outline below.

Mixtures. Mixtures of dipolar Bose gases with nondipolar Bose or Fermi gases have received relatively little attention in spite of their potentially rich physics [33,34]. Recent progress

in realizing quantum mixtures of dipolar gases [35] may, however, motivate further exploration of such systems.

Inadvertently, our results provide insight into properties of two-component mixtures. Arguably, the simplest mixture is an impurity system—a dipolar polaron [23–25]—that was mentioned already in Sec. III. The self-energy in Eq. (12) suggests that the induced impurity-impurity interaction becomes long-range. Indeed, assuming that the $V_i = v_1 + v_2$, where v_1 and v_2 correspond to two impurities, we derive the dipole-interaction-induced part of the mediated interaction as

$$V_{\text{eff}} \simeq \frac{1}{g^2} \int v_1(\mathbf{r}) V_d(\mathbf{x} - \mathbf{r}) v_2(\mathbf{x}) d\mathbf{r} d\mathbf{x}, \quad (23)$$

which, assuming that $v_j(\mathbf{r}) = g_j \delta(\mathbf{r} - \mathbf{a}_j)$, leads to $V_{\text{eff}} \simeq g_1 g_2 V_d(\mathbf{a}_1 - \mathbf{a}_2)/g^2$. This interaction is long-range in contrast to the well-known mean-field effective impurity-impurity interactions; see, e.g., [36–40]. In the future it will be interesting to investigate this potential in the vicinity of the collapse where the impurities strongly modify the bath, leading to strong mediated correlations.

Finally, we note that one can naively think of the impurity potential in Eq. (21) as of some zero-range-interacting Bose or Fermi gas that does not mix with the dipolar BEC; for conditions of miscibility of Bose-Bose mixtures see Ref. [41]. In this case our study provides some ideas for understanding immiscible two-component gases, where one of the gases (impurity) has only zero-range interactions. For example, Fig. 6 suggests that the density of this impurity gas will be shaped by the dipolar interaction.

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APPENDIX A: DERIVATION OF EQS. (11) AND (13)

First, let us outline a derivation of Eq. (10). We note that the energy within the mean-field approximation is given by

$$E = \mu N - \frac{gN^2}{2} \int \psi(\mathbf{x})^4 d\mathbf{x} - \frac{N^2}{2} \int \psi(\mathbf{x})^2 V_d(\mathbf{r} - \mathbf{x}) \psi(\mathbf{r})^2 d\mathbf{r} d\mathbf{x}, \quad (A1)$$

where ψ is the solution of the corresponding Gross-Pitaevskii equation. Without the impurity $\psi(\mathbf{x})$ is constant, whereas in the presence of the impurity it depends on the position. Equation (A1) together with Eq. (9) leads to Eq. (10). To derive Eq. (11), we use Eq. (5) together with the identity $\delta n(\mathbf{x}) = N|\psi(\mathbf{x})|^2 - n_0$ in Eq. (10).

We derive Eq. (13) using Eq. (7). Indeed, by definition,

$$\delta N = -\frac{1}{g(2\pi)^3} \int d\mathbf{k} d\mathbf{r} \frac{\tilde{V}_i(\mathbf{k})}{1 + 2\varepsilon_{dd} P_2(\cos \alpha)} e^{i\mathbf{k} \cdot \mathbf{r}}. \quad (A2)$$

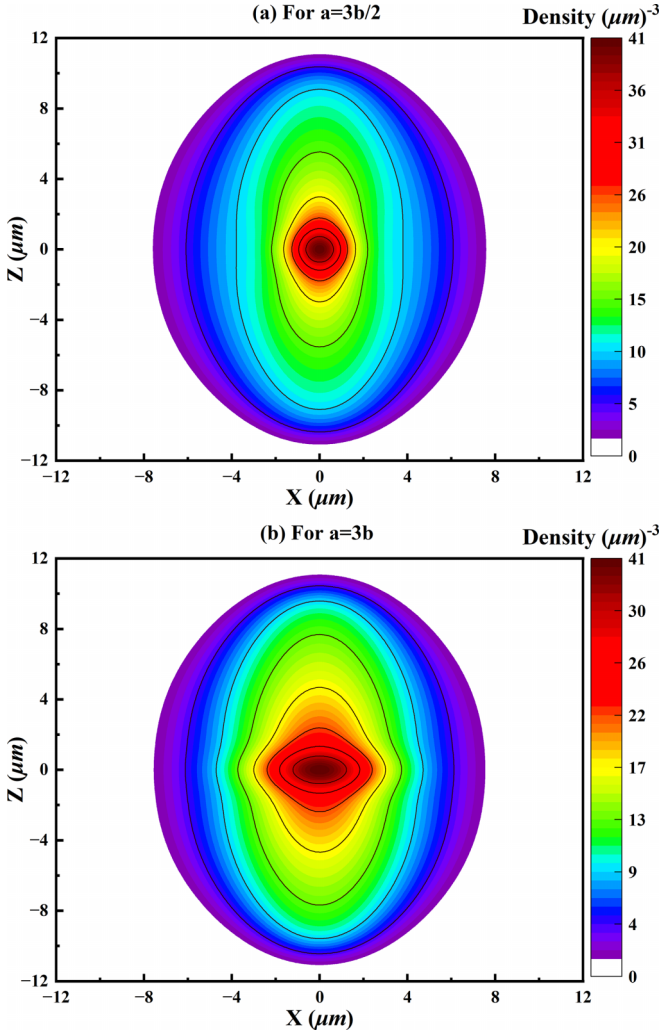


FIG. 8. Density contours in the xz plane for an attractive Gaussian impurity implanted into a dipolar BEC for two different deformation ratios a/b . The dipoles are polarized in the z direction.

Noticing that $\delta(\mathbf{k}) = \frac{1}{(2\pi)^3} \int d\mathbf{r} e^{i\mathbf{k}\cdot\mathbf{r}}$, we rewrite this expression as

$$\delta N = -\frac{\tilde{V}_i(0)}{g} \int d\mathbf{k} \frac{\delta(\mathbf{k})}{1 + 2\varepsilon_{dd}P_2(\cos\alpha)}, \quad (\text{A3})$$

where we assume that $\tilde{V}_i(0)$ is well defined. As the delta function is spherically symmetric, we can first take the integral over the α angle

$$\int_{-1}^1 \frac{dx}{1 + 2\varepsilon_{dd}P_2(x)} = \frac{2 \tan^{-1} \left[\sqrt{\frac{3\varepsilon_{dd}}{1-\varepsilon_{dd}}} \right]}{\sqrt{\varepsilon_{dd}(1-\varepsilon_{dd})}}. \quad (\text{A4})$$

Utilizing this expression, the fact that $\int k^2 dk \delta(\mathbf{k}) = 1/(4\pi)$ and $\tilde{V}_i(0) = \int d\mathbf{r} V_i(\mathbf{r})$, we derive the expression presented in Eq. (13).

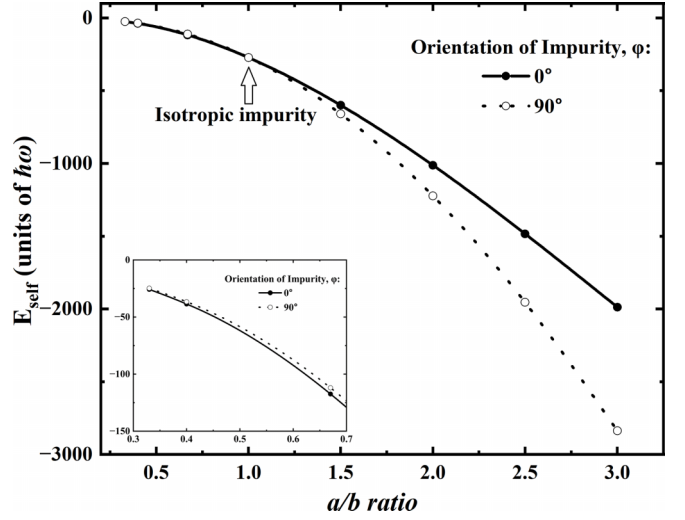


FIG. 9. Dependence of the self-energy as a function of the deformation of the impurity potential (expressed as the ratio a/b) for an attractive impurity. Inset: a close-up for small a/b ratios.

APPENDIX B: ATTRACTIVE IMPURITY

For an attractive impurity ($V_0 < 0$), particles will naturally be attracted to the center of the trap. We demonstrate contour plots for attractive impurities in Fig. 8 showing both an isotropic impurity and our extreme deformation, $a = 3b$. One can see the very large density peak in the center, which is over three times as dense as the maximum densities seen in the repulsive case. Like before, the system is three-dimensional, so this is an ellipsoid of maximum density in the center of the trap. Interestingly, just as in the repulsive plot, there appears to be a slight bump in the contour line as it crosses the x axis (at around $\pm 4 \mu\text{m}$) for the largest nonspherical case, though the bump goes in the opposite direction. In both the attractive and repulsive cases it makes sense. In the attractive case it goes outward indicating a slight bulge of larger density created by the attractive impurity, and it is the opposite in the case of repulsion.

In Fig. 9 we show the self-energy as a function of deformation plot analogous to Fig. 6. Here we see that, qualitatively, the plot looks the same except it is reflected over the x axis. The relationship between the 0° and 90° curves, however, remains the same with the rotated impurities, where the rotated curve is lower in energy for oblate impurities and higher for prolate ones. The magnitudes are also about twice that of the repulsive case for the solid curve. It is not surprising that adding any kind of attraction lowers the energy of the system, but this figure shows that an oblate impurity with one of its major axes along the polarization direction of the dipoles is the most stable. In the limit where the impurity becomes a disk, then it would match the shape of the contours in the top panel of Fig. 2, and thus matching the shape of the dipolar gas.

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