Static properties of positive ions in atomic Bose-Einstein condensates

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The excess number of atoms around an ion immersed in a Bose-Einstein condensate is determined as a function of the condensate density far from the ion. We use thermodynamic arguments to demonstrate that in the limit of low densities the excess number of atoms is proportional to the ratio of the atom-ion and atom-atom scattering lengths. For denser systems we calculate the excess number from solutions of the Gross-Pitaevskii equation using a model potential that has a $1/r^4$ attraction coming from the polarization of the neutral atoms and a hard-core repulsion at short distances. We show that there exist in general many solutions to the Gross-Pitaevskii equation for a given condensate density, the maximum number of solutions being related to the number of bound states of the Schrödinger equation for the same potential. With increasing density, pairs of these solutions merge and disappear, implying a discontinuous change of the state of the system.

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I. INTRODUCTION

For the helium liquids, measurements on ions have served as a valuable probe of liquid properties. As examples we may mention the use of ions to put in evidence vortex lattices in rotating liquid ^{4}He and the measurement of ionic mobilities in superfluid ^{3}He to elucidate scattering processes. The first experiments on ions in an ultracold gas of ^{87}Rb atoms were reported by Ciampini *et al.* [1], who produced ions by irradiating a rubidium condensate with laser pulses which ionize atoms through one- and two-photon absorption processes.

Theoretically, the capture of atoms into weakly bound states of the atom-ion potential has been considered in Ref. [2]. In this paper we consider the structure of a positive ion in a Bose-Einstein condensate when there is no capture of atoms into bound states, and in particular we calculate the excess number of atoms associated with an ion. We shall demonstrate that this number is typically of order 10^2, either positive or negative.

The interaction between an atom and a positively charged alkali-metal ion (charge e), which are separated by a distance r, is given at large distances by the polarization potential caused by the electrostatic field $\mathcal{E}_{\rm es}$ due to the ion, $\mathcal{E}_{\rm es} = e/4\pi\epsilon_0 r^2$, which gives rise to a change in the energy of the neutral atom given by $V=-\alpha\mathcal{E}_{\rm es}^2/2$, where α is the polarizability of the atom. Writing the polarizability as $\alpha=4\pi\epsilon_0\tilde{\alpha}$, where $\tilde{\alpha}$ has the dimension of volume, the energy shift of an atom due to the ion becomes

$$V(r) = -\tilde{\alpha}\frac{e_0^2}{2r^4}, \tag{1}$$

where $e_0^2 \equiv e^2/4\pi\epsilon_0$. At short distances ($r \lesssim 10a_0$) the potential has a repulsive core. An important characteristic length, which we denote by β_4, may be identified by equating the kinetic energy $\hbar^2/2m\beta_4^2$ to the potential energy $V(\beta_4)$, resulting in

$$\beta_4 = \sqrt{\frac{\tilde{\alpha}}{a_0}\frac{m}{m_e}}. \tag{2}$$

Here m denotes the mass of a neutral atom, m_e is the electron mass, and $a_0 \equiv \hbar^2/m_e e_0^2 \sim 0.53$ Å is the Bohr radius. Using the measured values $\tilde{\alpha}=320a_0^3$ for ^{87}Rb and $\tilde{\alpha}=163a_0^3$ for ^{23}Na, one finds $\beta_4^{\rm Rb} \approx 7150a_0$ and $\beta_4^{\rm Na} \approx 2620a_0$. The quantity β_4 gives the distance from the ion beyond which the zero-energy atom-ion wave function ceases to oscillate, and it sets the scale of atom-ion scattering lengths, but their actual values depend on the details of the potential at short distances.

We begin by deriving from thermodynamics a general expression for the excess number of atoms around an ion and show that in dilute systems the excess number depends only on the ratio of the atom-ion and atom-atom scattering lengths. As we shall see, this approach suggests that the number of atoms associated with an ion is typically of the order of 10–100, but that it may be either positive or negative. In denser systems the excess number must be obtained from microscopic considerations, and we shall determine the structure of an ion immersed in a Bose-Einstein condensate at zero temperature, assuming that atom-atom interactions may be described within the framework of the Gross-Pitaevskii (GP) mean-field approach. We present solutions of the GP equation for a number of potentials which include a hard-core repulsion, an attractive square well, and one that resembles the atom-ion interaction, a hard core with a $1/r^4$ attraction at larger distances.

For a given inner boundary condition, the Schrödinger equation has only one solution for a given value of the energy. By contrast, the GP equation, because it is nonlinear, can have more than one solution for a given chemical potential. For potentials like the atom-ion one that can support two-body bound states, we shall find that at low densities there are $2\nu_S+1$ solutions of the GP equation, where ν_S is the number of bound states of the Schrödinger equation for the same potential. With increasing density, pairs of solutions merge and disappear until there is only a single solution with no nodes. We shall illustrate this behavior for two potentials, an attractive square well and one with an attractive $1/r^4$ tail. An important question is which of these solutions is physically relevant. At low condensate densities, one expects the wave function close to the ion to resemble the zero-energy solution of the Schrödinger equation, and to have ν_S nodes. This will be the case unless inelastic processes can populate lower-lying states. We find that with increasing condensate

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density, this solution ceases to exist. This indicates that the evolution of the state with density cannot be continuous even in the absence of inelastic processes.

The plan of the paper is as follows. In Sec. II we present thermodynamic considerations. Section III contains a description of the asymptotic behavior of the condensate wave function far from the ion. In Sec. IV we consider two simple potentials to illustrate important general features of our results, and in Sec. V we analyze the case of a potential that, like the actual atom-ion potential, behaves as r^{-4} at large distances. We calculate the excess number of atoms from numerical solutions of the Gross-Pitaevskii equation for a given background condensate density. The concluding section, Sec. VI, discusses our main results. In an Appendix, we address the question of the validity of the Gross-Pitaevskii equation in the present context.

II. THERMODYNAMIC CONSIDERATIONS

We wish to calculate the excess number of particles associated with an ion. To define this quantity precisely, we imagine adding an ion to a condensate. This will generally change the density of atoms far from the ion by an amount that varies as $1/V$, where V is the volume of the system. A natural definition of the excess number of atoms ΔN associated with the ion is the number of particles that must be added to keep the atom chemical potential constant, since this will ensure that the properties of the condensate far from the ion are unaltered by the addition of the ion. In terms of the microscopic density of atoms $n(r)$ around the ion, the excess number is given by

$$\Delta N = 4\pi \int_0^\infty dr\, r^2 [n(r) - n_0], \tag{3}$$

where n_0 is the density of atoms at large distances from the ion.

This is analogous to what has been done earlier to calculate the excess number of ^{4}He atoms associated with a ^{3}He impurity in liquid ^{4}He [3]. We shall denote the energy per unit volume as $\mathcal{E}(n_a, n_i)$, where n_a and n_i are the number densities of atoms and ions, respectively. The chemical potential of the atoms is given by

$$\mu_a = \frac{\partial \mathcal{E}}{\partial n_a}, \tag{4}$$

and therefore the condition that this be unchanged by adding one ion and ΔN atoms is

$$\frac{\partial^2 \mathcal{E}}{\partial n_a \partial n_i} + \frac{\partial^2 \mathcal{E}}{\partial n_a^2} \Delta N = 0 \tag{5}$$

or

$$\Delta N = -\frac{\partial^2 \mathcal{E}}{\partial n_a \partial n_i} \bigg/ \frac{\partial^2 \mathcal{E}}{\partial n_a^2}. \tag{6}$$

When the density of ions is sufficiently low, $\partial \mathcal{E}/\partial n_i$ is equal to the energy change ϵ_i when one ion is added to the condensate, and therefore

$$\Delta N = -\frac{\partial \epsilon_i}{\partial n_a} \bigg/ \frac{\partial^2 \mathcal{E}}{\partial n_a^2}. \tag{7}$$

One may also calculate ΔN from the change ΔF in the thermodynamic potential $F = E - \mu_a N$ when a single ion is added to the system at constant μ_a. Here E is the total energy and N the total number of atoms. Since the number of atoms is given by

$$N = -\frac{\partial F}{\partial \mu_a}, \tag{8}$$

it follows immediately that

$$\Delta N = -\frac{\partial \Delta F}{\partial \mu_a}. \tag{9}$$

Provided the volume considered is large compared with the scale of the atom excess around the ion, ΔF will be independent of the volume.

Let us begin by making estimates for a dilute gas. Provided the scattering of atoms by atoms and of atoms by ions may be treated as independent binary events, the energy density may be expressed in terms of the scattering lengths associated with the atom-atom and atom-ion interactions. If ion-ion interactions are neglected, we may write

$$\mathcal{E}(n_a, n_i) = \frac{1}{2} U_{aa} n_a^2 + U_{ai} n_a n_i, \tag{10}$$

and therefore from Eq. (6) we obtain

$$\Delta N = -\frac{U_{ai}}{U_{aa}}. \tag{11}$$

The mean-field interaction constant U_{jl} for species j and l, which may be either atoms (a) or ions (i), is related to the scattering length a_{jl} by

$$U_{jl} = \frac{2\pi\hbar^2 a_{jl}}{m_{jl}}, \tag{12}$$

where $m_{jl} = m_j m_l/(m_j + m_l)$ is the reduced mass of the two particles. Our result can therefore be expressed as

$$\Delta N = -\frac{m_{aa}}{m_{ai}} \frac{a_{ai}}{a_{aa}}. \tag{13}$$

If, as in Ref. [1], the ion is obtained by photoionization of the condensate itself, the latter expression reduces to

$$\Delta N = -a_{ai}/a_{aa}. \tag{14}$$

To obtain an order of magnitude estimate of the excess number of atoms associated with an ion, we note that the characteristic scale for the magnitudes of atom-ion scattering lengths $|a_{ai}|$ is set by β_4, given in Eq. (2), while the scale for the magnitudes of atom-atom scattering lengths $|a_{aa}|$ is set by

$$\beta_6 = \left(2\frac{m}{m_e} C_6\right)^{1/4} a_0. \tag{15}$$

Here C_6 is the coefficient of r^{-6} in the van der Waals interaction, expressed in atomic units. Thus we arrive at the estimate

$$|\Delta N| \sim \frac{\beta_4}{\beta_6} \sim \left(\frac{m}{2m_e}\frac{\tilde{\alpha}^2}{C_6}\right)^{1/4}, \tag{16}$$

which is of order 35 for Rb and 25 for Na.

The fact that the excess number of atoms is so large indicates that it may well be a poor approximation to regard the ion as a free particle, with mass equal to the bare ion mass. Rather, the recoil of the ion will be suppressed by the other atoms surrounding the ion, and if $\Delta N \gg 1$ it will be a better approximation to regard the ion as being stationary. In that case the excess number of atoms will be given by

$$\Delta N = -\frac{a_{ai}(m)}{2a_{aa}}, \tag{17}$$

where the argument of a_{ai} indicates that the scattering length is to be evaluated for a reduced mass equal to the atom mass. Expression (17) gives a value for ΔN that is typically of the same order of magnitude as that given by Eq. (16). However, we stress the fact that the estimate for ΔN depends sensitively on the value of the effective mass of the ion, since the atom-ion potential has many bound states, and therefore relatively small changes in the reduced mass can result in large changes in the scattering length. Given that in the limit of low atom density the magnitude of the excess number of atoms is expected to be very much greater than unity, the result (14) will generally not give a realistic estimate even in that case.

The perturbation induced by the ionic potential is very strong. Therefore the question arises of whether the customary assumption of an essentially zero range for the atom-atom interaction is valid. We address this point in the Appendix, where we argue that the corrections to the GP result should not be large for the properties of interest here.

III. MICROSCOPIC THEORY

We now turn to microscopic considerations. Since, as we shall see, the distortion of the condensate wave function in the vicinity of an ion extends to large distances from the ion and involves many atoms, we expect that the effective mass of an ion and its dressing cloud will be much larger than that of an atom, and we may regard the ion as being static. To describe the structure of the condensate in the vicinity of an ion we must therefore calculate the structure of the condensate in a static external potential given by the atom-ion interaction. Provided the length scale on which the condensate wave function ψ varies in space is sufficiently large, we may do this by employing the Gross-Pitaevskii equation with the interaction of atoms with the ion included as an external potential,

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(r) + U_0|\psi|^2\right]\psi = \mu\psi. \tag{18}$$

Here and in what follows we shall denote the chemical potential of an atom by μ, and for simplicity we have written $U_0 \equiv U_{aa} = 4\pi\hbar^2 a_{aa}/m$, since $m_{aa} = m/2$. We wish to find solutions that tend to a constant at large distances from the ion, and since the potential is spherically symmetric, these solutions depend only on the radial coordinate r. Thus Eq. (18) becomes

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + V(r) + U_0\frac{|\chi|^2}{r^2}\right]\chi = \mu\chi, \tag{19}$$

where $\chi = r\psi$.

The behavior of the condensate wave function at large distances depends on the nature of the potential $V(r)$. On linearizing the GP equation (18) and making use of the fact that the chemical potential is related to the condensate wave function ψ_0 at large distances by the relation $\mu = n_0 U_0$ where $n_0 = |\psi_0|^2$, one finds that the deviation

$$\delta\psi = \psi - \psi_0 \tag{20}$$

of the condensate wave function from its asymptotic value satisfies the linearized GP equation

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V(r) + 2U_0 n_0\right)\delta\psi = -V(r)\psi_0. \tag{21}$$

For potentials with a finite range, one may neglect the potential at large distances from the ion, and the deviation that vanishes for $r \to \infty$ is thus given by

$$\delta\psi \propto \frac{e^{-k_\xi r}}{r}, \tag{22}$$

where $k_\xi = \sqrt{2}/\xi$ and ξ is the healing length for the bulk condensate,

$$\xi = \frac{1}{\sqrt{8\pi a_{aa} n_0}}. \tag{23}$$

For a potential, such as the atom-ion potential, that falls off at large distances less rapidly than the solution (22), the behavior is different. The leading term in the solution for large r is then the Thomas-Fermi result ψ_{TF}, given by

$$V(r) + U_0|\psi_{\mathrm{TF}}|^2 = \mu, \tag{24}$$

which, for the atom-ion potential with asymptotic form given by Eq. (1), amounts to

$$n_{\mathrm{TF}}(r) = n_0 - \frac{V(r)}{U_0} = n_0\left(1 + \frac{(\xi\beta_4)^2}{r^4}\right) \tag{25}$$

or, to first order in V,

$$\psi_{\mathrm{TF}} \approx \psi_0 - \frac{V(r)}{2U_0\psi_0}, \tag{26}$$

where we have taken ψ_0 to be real. The density perturbation at large distances is seen to be always positive. Corrections to this result for smaller r may be calculated from Eq. (21) by neglecting the potential on the left hand side of the equation. The resulting differential equation may be written in terms of a function $\delta\chi$ defined by $\delta\chi = r\delta\psi$,

$$\left(-\frac{d^2}{dr^2} + k_\xi^2\right)\delta\chi = -\frac{2m}{\hbar^2} r V(r)\psi_0. \tag{27}$$

This differential equation may be solved exactly in terms of exponential integrals, the two linearly independent solutions

of the homogeneous equation being $\exp(-k_\xi r)$ and $\exp(k_\xi r)$. By inspection of Eq. (27) it is evident that the leading term for large r of the particular solution to the inhomogeneous equation is given by $\delta\chi = -(2m/\hbar^2 k_\xi^2) r V(r)\psi_0$, which yields the Thomas-Fermi expression (26). The correction to this result may be obtained from the exact solution, but it is simpler to iterate Eq. (27) by moving the term $d^2\delta\chi/dr^2$ to the right hand side and replacing χ in it by the Thomas-Fermi solution. This results in

$$\frac{\delta\psi}{\psi_0} = -\frac{2m}{\hbar^2 k_\xi^2} V(r)\left(1 + \frac{12}{k_\xi^2 r^2}\right). \tag{28}$$

The leading correction to the Thomas-Fermi result for $\delta\psi$ given in Eq. (26) is thus seen to be proportional to r^{-6}. Since we have already neglected the potential energy on the left hand side of Eq. (21), we cannot by this method obtain higher-order corrections to the particular solution than the one exhibited in Eq. (28).

By keeping in the general solution only the exponentially decaying term we thus get the asymptotic result

$$\frac{\delta\psi}{\psi_0} \sim -\frac{V(r)}{2n_0 U_0}\left(1 + \frac{6\xi^2}{r^2}\right) + C\frac{e^{-k_\xi r}}{r}, \tag{29}$$

where C is an arbitrary constant.

For $r \to \infty$ the asymptotic behavior of the solution is always given by the TF result. However, whether or not this behavior is relevant for determining the structure of most of the cloud of atoms surrounding the ion depends on the relative size of the two characteristic lengths β_4 and ξ. On the one hand, for $\beta_4 \gg \xi$ most of the cloud will be described by the TF approxmation, and only at distances less than $\sim\xi$ will the exponential term become important. On the other hand, for $\xi \gg \beta_4$ (i.e., for low external density) the structure will be dominated by the exponential term, and the TF tail will become important quantitatively only at very large r. At shorter distances from the ion, the mean-field energy becomes small compared with the atom-ion potential and the GP equation reduces to a good approximation to the Schrödinger equation.

IV. SIMPLE MODEL POTENTIALS

Before presenting results for the attractive $1/r^4$ potential we begin by examining two simpler model potentials, a repulsive hard-core and a spherical well potential.

A. Hard-core potential

Consider an interacting Bose-Einstein condensed gas in the presence of a repulsive hard-core potential of radius R. This model may be treated analytically in both the small- and large-core-radius limits. The solution to the GP equation at large distances from the ion is given by Eq. (22),

$$\psi \simeq \sqrt{n_0}\left(1 + C\frac{\exp(-k_\xi r)}{r}\right). \tag{30}$$

If one assumes that this expression holds for all r greater than R, we can determine the constant of proportionality C by imposing the boundary condition $\psi(R) = 0$. This gives $C = -Re^{k_\xi R}\sqrt{n_0}$. For r close to R this has the form of the scattering solution for the Schrödinger equation, $\psi = 1 - R/r$. In fact, for $R/\xi \ll 1$ this solution becomes essentially exact, since this function fails to satisfy the GP equation only in the region where $r \simeq R$, and in this region the total change in the slope $d\chi/dr$ of the radial wave function is small and may be neglected. As an illustration of this fact, we calculate the excess number of particles, which is given by Eq. (3), and find

$$\Delta N = 4\pi n_0 \int_R^\infty dr\, r^2\left(-2R\frac{e^{-k_\xi(r-R)}}{r} + R^2\frac{e^{-2k_\xi(r-R)}}{r^2}\right) - \frac{4\pi n_0 R^3}{3}$$
$$= -4\pi n_0\left(R\xi^2 + \frac{3R^2\xi}{2\sqrt{2}} + \frac{R^3}{3}\right). \tag{31}$$

For $\xi \gg R$, this reduces to

$$\Delta N = -\frac{R}{2a_{aa}}. \tag{32}$$

Let us now compare this result with the one derived on the basis of thermodynamic arguments. For a hard-core potential the scattering length coincides with the core radius. Since we have assumed the ion to be stationary, its effective mass is taken to be infinitely large, and therefore the reduced mass for the ion and an atom is m, rather than the value $m/2$ one obtains for an ion and an atom with equal masses. Thus, this result is in precise agreement with Eq. (13).

When the core radius is much larger than the healing length, the wave function reaches its asymptotic value on a length scale that is short compared to R. In Eq. (19) we can therefore replace the factor $1/r^2$ appearing in the nonlinear term by the constant $1/R^2$ and we are left with an effectively one-dimensional GP equation whose solution is

$$\psi = \sqrt{n_0}\tanh\frac{r-R}{\sqrt{2}\xi}, \quad r \geqslant R, \tag{33}$$

and zero otherwise, as may be seen by inspection. The excess number of particles is given by

$$\Delta N = -\frac{4}{3}\pi R^3 n_0 - \frac{R^2}{\sqrt{2}a_{aa}\xi}, \tag{34}$$

where the leading term is due to exclusion of atoms from the core.

B. Attractive square well

We next consider a more physical potential, an attractive well:

$$V(r) = -\frac{\hbar^2 k_0^2}{2m}, \quad r < R, \tag{35}$$

$V(r) = 0$ otherwise. Like the actual atom-ion potential, this can have bound states for the two-body problem. With this potential we shall be able to examine how solutions of the GP equation disappear as the condensate density increases. The GP equation (19) reads

$$\left[-\frac{1}{2}\frac{d^2}{dr^2}-\frac{k_0^2}{2}\theta(R-r)+4\pi a_{aa}\left(\frac{|\chi|^2}{r^2}-n_0\right)\right]\chi=0 \quad (36)$$

[where $\chi=r\psi$ and $\theta(x)$ is the step function] and the scattering length for this potential is

$$a=R\left(1-\frac{\tan k_0R}{k_0R}\right). \quad (37)$$

Since this equation is nonlinear, there can be multiple solutions for the same boundary conditions (i.e., the same bulk density n_0). As we will show in the following, for small n_0 it has $2\nu_S+1$ solutions, where ν_S is the number of nodes of the zero-energy Schrödinger solution ψ_S or, equivalently, the number of bound states of the Schrödinger equation. In the low-background-density limit, inside the well the solution with the maximum number of nodes approaches ψ_S, i.e., $\psi(r)\propto\sin(k_0r)/r$, while outside it tends toward the uniform density n_0 with the asymptotic behavior given in Eq. (22), $\delta\psi(r)\propto\exp(-k_\xi r)/r$.

With increasing n_0, the mean-field repulsion between the atoms makes the effective potential shallower, which tends to push nodes of the wave function outward. At the same time, the increase in the chemical potential has the opposite effect on the nodes. What we find is that if the zero-energy solution of the Schrödinger equation has ν_S nodes, for low condensate densities the GP equation has one solution with no nodes, and *two* solutions with any nonzero number of nodes less than or equal to ν_S.

To demonstrate this, we analyze separately the behavior of the wave function inside and outside the well, and match them at some intermediate point, which for this particular potential we take to be the edge of the well. Specifically, we integrate out from the origin, where $\chi=0$, for different choices of the derivative of χ at $r=0$ and calculate ψ and ψ' at the boundary $r=R$. These trace a curve in ψ-ψ' space. Then we integrate inward from large distances, where the solution is defined by the proportionality constant C of the Yukawa asymptotic form Eq. (22). As C is varied, another curve in ψ-ψ' space is traced out. If the mean-field interaction could be neglected for $r<R$, the ratio $\psi'(R)/\psi(R)$ would not depend on the normalization of the wave function, and therefore the curve corresponding to the inner boundary would be a straight line through the origin. In the presence of atom-atom interactions, the ratio ψ'/ψ obtained by integrating outward traces out a spiral. For low n_0 this crosses the ψ' axis a number of times equal to the number of nodes the zero-energy solution of the Schrödinger equation has inside the potential. This follows from the observation that for low $\chi'(0)$ the solution will have the same number of nodes inside the potential as the zero-energy solution of the Schrödinger equation, while for very large values of $\chi'(0)$ the effects of the mean field will be so strong that the solution has no nodes inside the potential.

The corresponding plot obtained by integrating inward has two branches, depending on whether $\psi(r\to\infty)$ is positive or negative. Examples of the plots are given in Fig. 1 for parameters such that $\nu_S=3$. For low n_0, there are $2\nu_S+1$ intersections of the two sets of curves, corresponding to solutions of the GP equation. This is illustrated in Fig. 1(a). As n_0 increases, pairs of solutions with the same number of nodes merge and disappear, as shown in Fig. 1(b). Eventually, at sufficiently high values of n_0 only the nodeless solution survives.

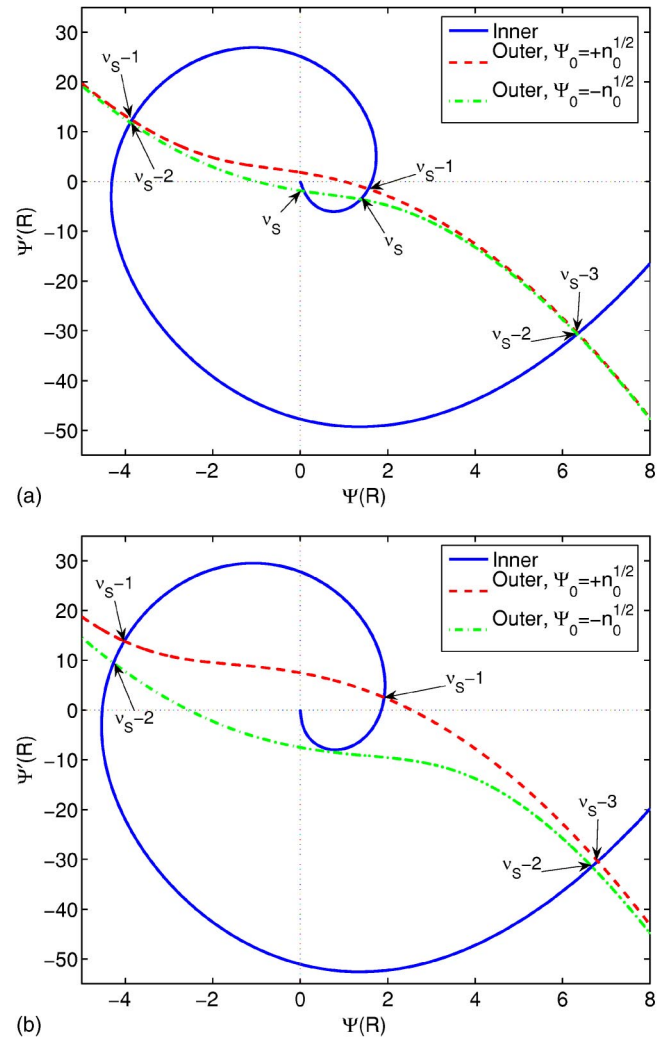

FIG. 1. (Color online) Behavior of $\psi(R)$ and $\psi'(R)$ for the solution inside the well (solid line) and outside it [dashed and dot-dashed lines for $\psi(r\to\infty)=\pm\psi_0$, respectively]. In the plots we have set $k_0R=9$, which gives three bound states for the Schrödinger equation. We measure energies in units of $\hbar^2k_0^2/2m$ and lengths in units of R. The calculations were performed for $U_0=0.45$ in these units, but results for other values of U_0 may be obtained by scaling, since for a given chemical potential, ψ and ψ' vary as $U_0^{-1/2}$. The symbols near intersections indicate the number of nodes of the solution, and for this case $\nu_S=3$. The upper panel (a) is for $\mu=0.45$, and the lower one (b) for $\mu=2.9$, just above the value $\mu=2.52$ at which the two solutions with three nodes merge and disappear.

In Figs. 1 and 2 we show how, on increasing the external density, the solutions with the highest number of nodes actually merge. For densities higher than this critical value, the only solutions are ones with a smaller number of nodes.

Despite its short-range character, the model given above captures the main features of the solutions of the GP equation for the atom-ion potential, which is long ranged. We

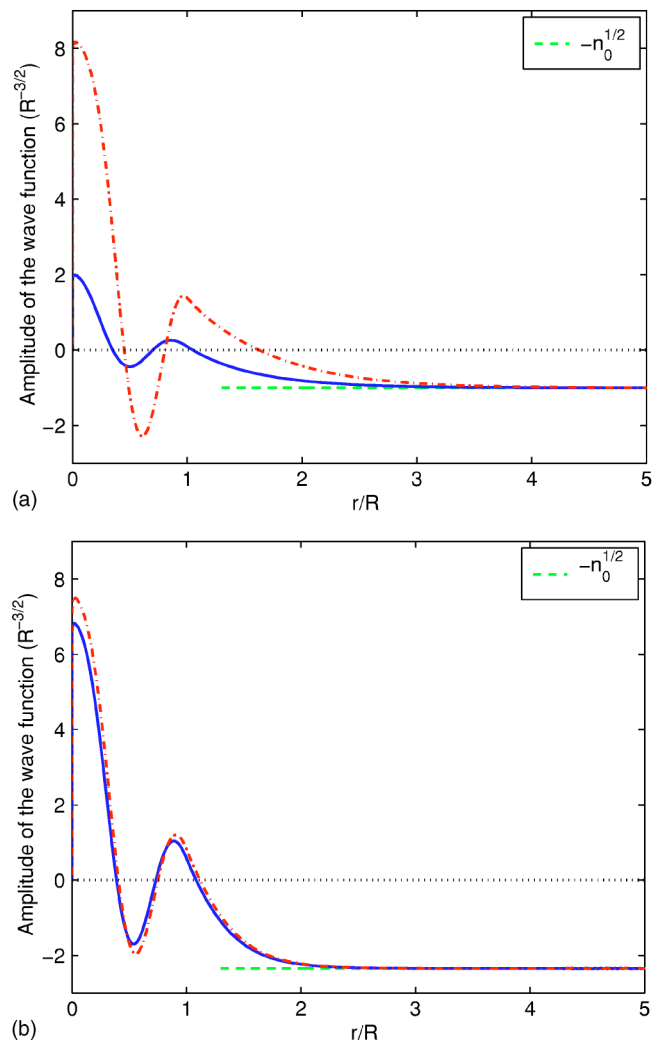

FIG. 2. (Color online) Two solutions of the Gross-Pitaevskii equation for the attractive square well potential. k_0R and U_0 are the same as in Fig. 1. For the upper panel, the chemical potential is 0.45, as in Fig. 1(a), while for the lower one it is 2.5, just below the value at which the solutions merge. The solutions both have three nodes, and are the first to merge as the chemical potential increases.

note that the discontinuous behavior does not occur in a one-dimensional model.

V. THE r^{-4} POTENTIAL

We now turn to a more realistic potential with the same r^{-4} behavior as the actual atom-ion interaction at large distances. For definiteness, we consider parameters appropriate for a ^{87}Rb condensate, and we take $a_{aa}=100a_0$. At large distances, we take the atom-ion potential to be given by Eq. (1) with $\tilde{\alpha}=320a_0^3$. The wave functions are sensitive to the short-range behavior of the potential, but we may obtain illustrative results by cutting the $1/r^4$ potential off by a hard core of radius R. Since many atoms are bound to the ion, we assume the ion to be static and set $m_{ai}=m$. The atom-ion scattering length of such potential may be calculated in the WKB approximation, and is given by [4]

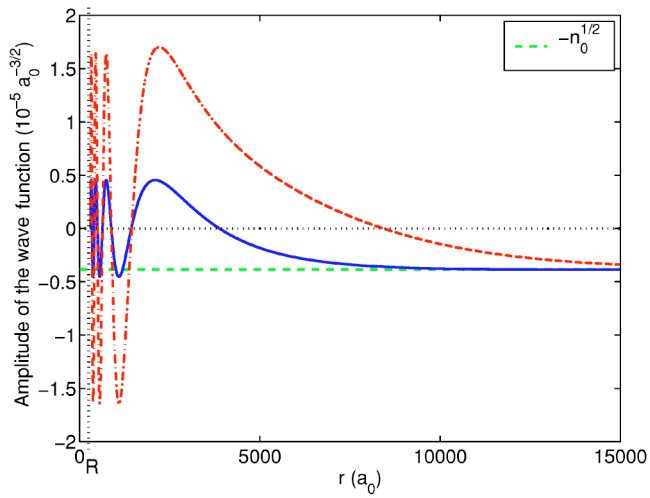

FIG. 3. (Color online) Condensate wave functions for the two uppermost states in the $1/r^4$ potential with the parameters given in the text for $n_0=10^{14}$ cm^{-3}. Both states have seven nodes, but the resolution of the figure is inadequate to exhibit the rapid oscillations for r close to R. The state that, in the dilute limit, becomes the zero-energy solution of the Schrödinger equation is given by the solid line.

$$a_{ai} = \beta_4 \cot\left[\frac{\beta_4}{R}\right]. \tag{38}$$

The number of bound states allowed by the potential can be estimated by increasing the potential strength from 0 to its actual value. A bound state appears each time the scattering length diverges, and therefore the number of bound states is given by

$$\nu_S = \mathrm{Int}\left(\frac{\beta_4}{\pi R}\right), \tag{39}$$

where Int(x) denotes the integer part of x. To model actual atom-ion potentials, a physically reasonable value of R would be $\sim 10a_0$. However, the properties of the wave function of most importance here are those at relatively large distances, $r \gtrsim 10^3 a_0$, so we take $R=300a_0$, since this should give us the correct physical behavior for the distances of interest. We do not expect the qualitative behavior of the wave function to depend on R, even though quantities like the scattering length do, and we have verified this numerically.

We now describe numerical solutions of the GP equation that approach a constant density n_0 far from the ion. Just as for the finite-range potential considered in the previous section, there is generally more than one solution for a given value of the chemical potential, and for small external densities one expects $2\nu_S+1$. In Fig. 3 we show the wave functions corresponding to the two states with the highest number of nodes, namely, seven for the parameters chosen, in agreement with the quasiclassical result (39). The free energy, for a given condensate density n_0, is highest for the states with the highest number of nodes, and decreases as the number of nodes decreases.

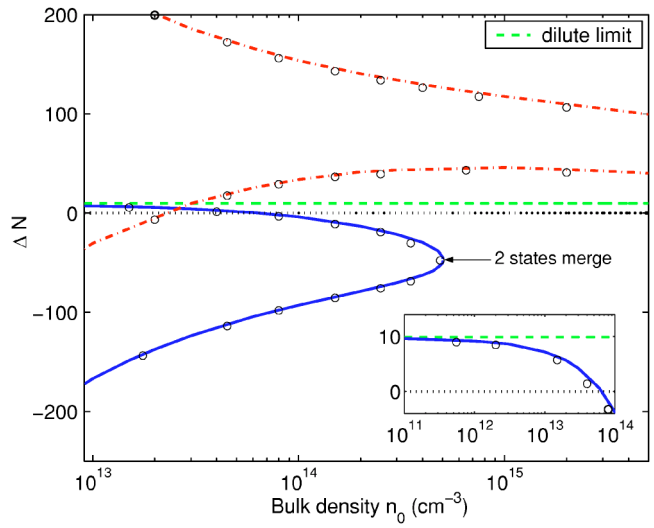

FIG. 4. (Color online) Excess number of atoms around a single ion as a function of the bulk density. The dashed line is the dilute limit appropriate for a fixed ion, $\Delta N = -a_{ai}/2a_{aa}$ ($R = 300a_0$ gives $a_{ai} \approx -1980a_0$ for an infinitely massive ion). Results are shown for the four uppermost levels for this potential (i.e., the two with seven nodes and the two with six nodes, indicated, respectively, by the solid and dot-dashed lines). The lines are obtained from Eq. (3), the circles from Eq. (9). The inset exhibits the behavior at lower densities.

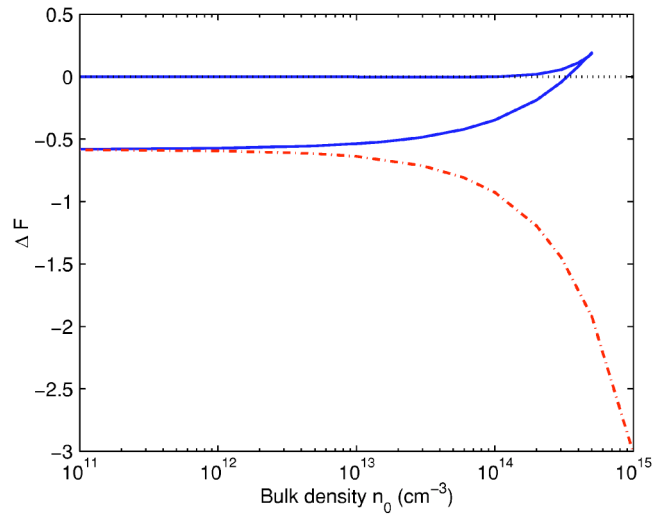

FIG. 5. (Color online) Difference in free energy for the states given in the previous figure: the solid lines are for the two states with seven nodes and the dot-dashed line for one of the states with six nodes. The free energy is measured in units of $10^{-5}\hbar^2/ma_0^2$. The other state with six nodes lies much lower, at around $\Delta F \approx -3 \times 10^{-4}\hbar^2/ma_0^2$.

In the absence of inelastic processes, we expect only the uppermost state of the ionic potential to play an important role in the capture process, since it is the only one with an appreciable overlap with the continuum wave function representing the unbound atoms [2].

The excess number of atoms is given in terms of the atomic density distribution by Eq. (3) or, alternatively, from the free energy $F = E - \mu N$ by Eq. (9). In Fig. 4 we show results obtained from our numerical simulations by both methods. In the limit of very low condensate density we get values for ΔN in accord with the thermodynamic arguments in Sec. II. The consistency of the two methods of calculation has been confirmed for core radii that give scattering lengths in the range $|a_{ai}| < 5000a_0$.

The figure shows that the excess numbers of atoms for two states with the same number of nodes become equal at the density above which the solutions no longer exist. This is to be expected, since the solutions become identical at this point. In the Appendix we use quasiclassical arguments to estimate the density at which solutions merge and disappear, and these are in good agreement with the numerical results. Fig. 5 exhibits the difference in free energy for the states given in Fig. 4.

In the detailed calculations described so far we have focused attention on states with close to the maximum number of nodes. In particular, in the low-density limit and in the absence of inelastic processes that can cause the system to relax, one would expect the state of the condensate to be the one that close to the ion resembles the zero-energy solution of the Schrödinger equation. However, three-body processes can relax the system, thereby populating states with lower numbers of nodes. To calculate properties of such a system, one could start with a many-particle wave function of the Hartree-Fock type in which more than one single-particle state is occupied, and solve the Hartree-Fock equations. This is, however, beyond the scope of this paper because the density of atoms rises to values sufficiently high that the dilute gas approximation for the interaction energy employed in the GP approach fails at relatively large distances from the ion. To see this, we note that the density of atoms far from the ion will be given by the Thomas-Fermi approximation Eq. (25). The dilute gas approximation is valid provided $n|a_{aa}|^3 \ll 1$. This condition becomes

$$n|a_{aa}|^3 \approx \left| \frac{V(r)}{U_0} a_{aa}^3 \right| = \frac{\beta_4^2 a_{aa}^2}{8\pi r^4} \ll 1 \tag{40}$$

or

$$r \gg (\beta_4 |a_{aa}|)^{1/2}/2, \tag{41}$$

which for rubidium ($a_{aa} \approx 100a_0$) implies that the GP equation is valid only for $r \gg 400a_0$ for such states.

VI. CONCLUSIONS AND DISCUSSION

In this paper we have investigated solutions of the Gross-Pitaevskii equation for a Bose-Einstein condensate in the presence of a positive ion. We find that for low condensate densities, there are $2\nu_S + 1$ solutions for a given condensate density, where ν_S is the number of bound states of the Schrödinger equation. With increasing condensate density, pairs of states become degenerate and disappear, and the state of the system must change discontinuously. An interesting challenge is to find experimental evidence for such a behavior.

We have calculated the excess number of atoms around an ion, and find that for the state that resembles the zero-energy

solution of the Schrödinger equation it can be either positive or negative, depending on the sign of the atom-ion phase shift, and a typical magnitude is of order $\sim 10^2$. The spatial size of the density disturbance around an ion is set by $\beta_4 \sim 1\ \mu$m. Our estimates indicate that the Gross-Pitaevskii equation should give a reliable first approximation for the wave function of such states. For states with fewer nodes, the density of atoms may reach values high enough that the GP equation fails.

There are many outstanding problems. In most of the calculations we have assumed that the state of interest is that with the maximum possible number of nodes. More study is needed of inelastic processes that will cause atoms to relax to lower states [2]. Experimental studies will be valuable in providing guidance for future work.

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APPENDIX: VALIDITY OF APPROXIMATIONS

Here we examine the conditions under which it is a good approximation to replace the effective atom-atom interaction by the standard expression (12). Later we shall estimate the density below which the dilute gas result (13) would be expected to hold. For nonzero wave numbers k, the quantity that enters the expression for the energy shift is $-\delta/k$, where δ is the s-wave phase shift, rather than a [5]. Since a typical energy scale for changes in δ/k is set by $\hbar^2/2m\beta_6^2$, while the potential depth is given by $\tilde{\alpha}e_0^2/2r^4$, we expect that the scattering length approximation will fail when

$$\frac{\tilde{\alpha}e_0^2}{2r^4} \gg \frac{\hbar^2}{2m\beta_6^2} \quad \text{or} \quad r^4 \ll \beta_4^2\beta_6^2. \tag{A1}$$

The Gross-Pitaevskii approach should therefore be valid if the phase shift due to the region where $r \ll \overline{r} = (\beta_4\beta_6)^{1/2}$ is negligible. To estimate this phase shift, we make a semiclassical approximation to the GP equation. This gives for the total accumulated phase out to a distance r

$$\Phi(r) \approx \int^r dr' \sqrt{\frac{2m}{\hbar^2}[\mu - V(r') - n(r')U_0]}. \tag{A2}$$

Deep in the ionic potential, the wave function is given to a good approximation by the semiclassical result, which has an amplitude

$$\psi \propto (rp_{\rm cl}^{1/2})^{-1}, \tag{A3}$$

where $p_{\rm cl}(r) = [2mV(r)]^{1/2}$ is the classical momentum of a particle of zero total energy in the presence of the potential. For the r^{-4} potential, the amplitude of the wave function is therefore independent of r, and we may replace the mean-field energy to a first approximation by a constant $\tilde{n}U_0$, where $\tilde{n}$ is independent of r. Expanding expression (A2) in the deviation $n_0 - \tilde{n}$ we find

$$\Phi(r) \approx \Phi_0(r) + (n_0 - \tilde{n})\frac{2mU_0}{\hbar^2}\int_0^r dr' \frac{1}{2\sqrt{-2mV(r')/\hbar^2}}. \tag{A4}$$

Due to the mean-field interaction, the accumulated phase out to a distance $r \sim \overline{r} = (\beta_4\beta_6)^{1/2}$ is therefore changed by an amount

$$\delta\Phi(\overline{r}) \approx (n_0 - \tilde{n})a_{aa}(\beta_4\beta_6^3)^{1/2}. \tag{A5}$$

If we take the interior density to be of the same order of magnitude as that far from the ion, one finds

$$\delta\Phi(\overline{r}) \sim \frac{\beta_4^{1/2}\beta_6^{3/2}}{\xi^2}, \tag{A6}$$

where the healing length is defined in Eq. (23). Since under experimental conditions the healing length is typically comparable to β_4, while β_6 is two orders of magnitude smaller, this shows that the region close to the ion where the Gross-Pitaevskii equation fails is likely to be unimportant.

On the basis of the above calculation, we may also estimate the density below which the low-density result (13) is valid. Using the approximations above, we find that the total accumulated phase out to a distance $\sim\beta_4$, where the semiclassical treatment fails, is of order

$$\delta\Phi(\beta_4) \sim \frac{\beta_4^2}{\xi^2}. \tag{A7}$$

This indicates that changes to the accumulated phase can be significant under typical experimental conditions.

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