Interacting bosons in a nearly resonant potential well

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We establish that the ability of a localized trapping potential to bind weakly interacting bosons is dramatically enhanced in the vicinity of the threshold of formation of the single-particle bound state of the trap. Specifically, for repulsive particles and a superthreshold trapping potential the equilibrium number of bound bosons and the size of the ground state diverge upon approaching the single-particle threshold from above. For attractive interactions and a subthreshold trap, a collective bound state always forms for a sufficiently large number of bosons, despite the inability of interparticle attraction alone to form a two-body bound state.

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I. RESONANT BINDING

It is empirically known that a surprisingly large number of short-range interactions operating in Nature have resonant character: the two-particle attraction is either barely sufficient to form a two-body bound state or misses the binding threshold by a small amount. In nuclear physics, prominent examples include the neutron-nucleon and neutron–α particle attractions, which are nearly binding [1]. In atomic physics the same is true for interactions between the atoms of ^{3}He [2] and those of the spin-polarized hydrogen family [3]. At the same time two ^{4}He atoms form a weakly bound dimer whose binding energy is four orders of magnitude smaller than the depth of the ^{4}He-^{4}He potential well [4].

The proximity to the two-body binding threshold can be quantified by the *s*-wave scattering length, whose magnitude significantly exceeds the range of interparticle forces, thus implying an effectively long-range interaction [1]. This regime is fundamentally interesting because systems consisting of resonantly interacting particles may exhibit a series of effects that are independent of the microscopic details of the interaction between the constituents. One such phenomenon is the well-understood Efimov effect [5], which occurs in a system of three bosons where resonant two-body forces trigger formation of an arbitrarily large number of loosely bound levels in a three-particle system. Conclusive experimental observation of the Efimov physics became possible only recently in an ultracold gas of Cs atoms [6] because, in contrast to other nearly resonant systems found in Nature, the two-body scattering length and thus interparticle interactions in a cold gas can be precisely controlled by using Feshbach resonances [7]. This allowed the measurement of the dependence of the three-body recombination rate on the two-body scattering length, which contains signatures specific to the Efimov effect [8].

The goal of this paper is to establish the existence of a resonant effect which may also be observed in a cold bosonic gas: we will demonstrate that the number of particles bound by a nearly resonant potential well increases as the well is made more shallow, diverging exactly at the single-particle threshold. The fact that such an effect might exist is implied by variational analysis given in our previous work [9]. Similar to the Efimov effect, the ultimate origin of this counterintuitive behavior is an effectively large attraction range of the potential well. Whereas the Efimov effect requires an attractive part of the physical potential to bind three particles, the phenomenon discussed below takes place in the presence of interparticle repulsion.

In the laboratory, attractive wells have been realized using the optical dipole force [10], in which atoms are attracted to the intense region of a focused laser beam. Strong confinement in three dimensions can be obtained at the intersection of two beams, each typically having diameter of about 15 μm [11]. The binding properties of such traps can be tuned by adjusting the laser power. Even tighter traps can be achieved by using holographic techniques [12,13], optical superlattices [14], and near-field [15] and white-light techniques [16].

Additionally, tuning the parameters of such a localized potential placed next to the classical edge of a Bose-Einstein condensate might allow manipulation of a well-defined number of particles [9]; it also provides an additional context for studying the quantum many-body problem, as this involves the states of an interacting boson system. The experimental feasibility of such a setup was discussed in Ref. [9], as well as reasons why a tightly focused potential is needed.

II. MODEL

We consider n interacting bosons of mass m in the presence of a well-localized attractive potential $U(\mathbf{r})$. We assume a system of sufficiently low density so that the range of interactions between particles need not be included as a parameter. Therefore we study the Gross-Pitaevskii (GP) energy functional [17]

$$E = n\int d^3x\left(\frac{\hbar^2}{2m}(\boldsymbol{\nabla}\psi)^2 + U(\mathbf{r})\psi^2 + \frac{g(n-1)}{2}\psi^4\right) \qquad (1)$$

subject to the normalization condition

$$\int \psi^2 d^3x = 1. \qquad (2)$$

Here we have assumed that the many-body wave function can be written as a product of the single-particle functions $\psi(\mathbf{r})$. The parameter g represents the short-ranged interaction

between the particles. The external potential $U(\mathbf{r})$ will be chosen in the form of an attractive "shell" of radius a:

$$U(\mathbf{r}) = -aV\delta(r-a), \tag{3}$$

because this is a simple form that will bind particles without having singular behavior in the wave function at the origin. The case of more realistic potentials will be discussed in Sec. VI. For the case of one particle, there is a single bound state for $V > V_c = \hbar^2/2ma^2$, and this condition will continue to be relevant for the many-body problem.

III. RESULTS FROM AN APPROXIMATE WAVE FUNCTION

The ground-state wave function minimizes the energy functional (1). We can deduce its general form from inspection. If the ground state is to be bound, it will have to be relatively large in the well-localized region where $U(\mathbf{r})$ is nonzero. At sufficiently large distances it is decreasing more rapidly than $1/r$, to ensure normalizability. It will pass from large to small in a way that keeps the gradient term small; this suggests $\psi \approx 1/r$ at intermediate distances. The effect of the interparticle repulsion [the last term in Eq. (1)] will be to suppress large values of ψ.

In a previous paper [9] these considerations led us to study the two-parameter trial wave function such that $\psi = C$ for $r < a$, and $\psi(r) = Ca \exp(-\alpha r + \alpha a)/r$ for larger r. We will briefly recapitulate the results. The form of the wave function for larger r is the exact wave function for a bound state of noninteracting particles, and will remain a good approximation to the interacting wave function at large r, where ψ^4 will be negligibly small. The wave function extends to a distance of order $1/\alpha$, which will be large for large n and also for V close to V_c. Thus we are particularly interested in the case of small α. Integration of Eq. (2) gives

$$4\pi\left(\frac{1}{2\alpha} + \frac{a}{3}\right)a^2C^2 = 1. \tag{4}$$

We note that for small α this reduces to $C^2 \approx \alpha/a^2$, rather than α^3 (i.e., the reciprocal of the "volume" of the wave function). This implies that the two length scales a and $1/\alpha$ both play roles; the limit $a \to 0$ cannot be taken. Equation (1) leads to

$$\frac{E}{4\pi n a^3} = \left(V_c - V + \frac{1}{2}\alpha a V_c\right)C^2 + \frac{2}{3}g(n-1)C^4 - 2g(n-1)\alpha a e^{4\alpha a}E_1(4\alpha a)C^4, \tag{5}$$

where $E_1(x)$ is the exponential integral [18].

Using Eq. (4) to eliminate mention of α, the leading terms of Eq. (5) are

$$\frac{E}{4\pi n a^3} = (V_c - V)C^2 + \pi\left(a^3V_c + \frac{2}{3\pi}g(n-1)\right)C^4. \tag{6}$$

Minimizing this expression with respect to C gives an estimate for the energy. Assuming $g > 0$ (i.e., the particles repel each other) gives for $V \geqslant V_c$

$$E = -\frac{n(V-V_c)^2}{V_c + 2g(n-1)/3\pi a^3}. \tag{7}$$

For large n this becomes independent of n, and the corresponding value of α is small. The energy at $n \to \infty$ is greater or less than the energy at $n=1$, depending on whether g is greater or less than $g_c = 3\pi a^3 V_c/2$. For g less than g_c, this would seem to indicate that the potential can bind an infinite number of particles (with a very swollen wave function); however, including the last term of (5) gives a shallow minimum for $g < g_c$, and then for large n the state is unstable against the unbinding of particles (i.e., it is within the continuum of a state with smaller n). Our main goal is to establish whether this minimum is real, and if this is the case, what is its behavior as the single-particle threshold is approached from above, $V \to V_c + 0$.

The two regimes for the interparticle strength (the cases $g > g_c$ and $g < g_c$) are in essence a small-n effect. The ground-state energy for two particles is greater or less than the energy for one, depending on whether the interaction parameter is large or small.

This shows that for $V > V_c$ there is an n-body bound state; however, the total energy for large n becomes independent of n, so that the chemical potential decreases to zero. This occurs because for small α the single-particle wave functions extend to large distances from the attractive center, making it correspondingly unlikely that two particles will be at the same place, so that the interparticle interactions can be effectively made as small as one likes (by tuning α). The effect depends on the way the size of the ground state scales with the number of bound bosons, and does not occur in lower dimensions [9].

IV. GROSS-PITAEVSKII EQUATION

The approach just outlined has the advantage that the mathematics is transparent, and yields results for the energy and wave function in which the role of the various parameters in the problem is explicit. It is a robust method that gives an upper bound on the exact ground-state energy. However, the results are only as good as the trial wave function. Therefore we will find the true minimum of Eq. (1) by numerical means. This gives the best possible wave function that can be written as a simple product of single-particle wave functions. In the process it verifies that the simple variational function is qualitatively correct, and puts the theory of resonant binding on a solid footing. Additionally we will show that nontrivial cooperative bound states also form for a subcritical well in the presence of a weak interparticle attraction.

In what follows we will choose $a=1$ and $V_c = \hbar^2/2ma^2 = 1$, which set the length and energy scales for the problem.

Taking a variational derivative of Eq. (1) gives the GP equation [17]

$$-\frac{1}{r}\frac{d^2}{dr^2}(r\psi) - V\delta(r-1)\psi + \gamma\psi^3 = \epsilon\psi, \tag{8}$$

where $\gamma = g(n-1)$. Unlike the case of the linear Schrödinger equation, the eigenvalue ϵ for which the GP equation (8) has

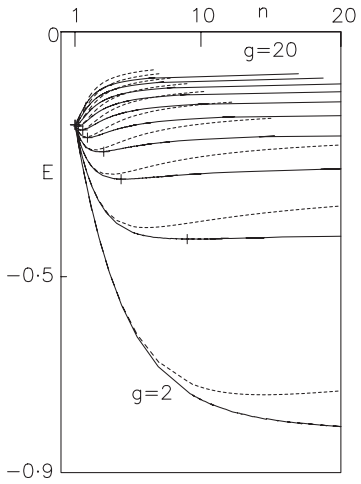

FIG. 1. Dependence of the ground-state energy on the number of particles n, for superthreshold well, $V=1.5$, and various values of the interaction parameter $g=2,4,6,\ldots,20$ (bottom to top). The solid line is the numerical solution to Eq. (8) substituted into Eq. (9); the dotted line is the minimum value of Eq. (5). Dimensionless variables defined in the main text are used.

a normalizable solution is not directly proportional to the minimum value of Eq. (1); however, they are related by

$$E = n\epsilon - \frac{1}{2}gn(n-1)B, \tag{9}$$

$$B = \int_0^\infty \psi^4 4\pi r^2 dr. \tag{10}$$

We solved Eq. (8) by integrating from $r=0$ with initial conditions $\psi=1$, $d\psi/dr=0$ and chosen values for V, γ, and ϵ. The integration was in the form of a power-law representation of $\psi(r)$ for $r<1$, which avoided the problems coming from the singular form of the GP equation at small r and gave accurate values for ψ and its derivative at $r=1$; thereafter, we used second-order Runge-Kutta integration with equal-sized steps in the variable $y=\sqrt{r}$. In general this gave a function that diverged to plus or minus infinity at large r. By tuning ϵ we could find the case for which ψ remained small at chosen large values of r. This condition defines the eigenvalue ϵ to high accuracy. Once a normalizable solution had been found, it was rescaled to satisfy the normalization condition (2). This also changes the value of γ, but not V or ϵ; only at the end of the calculation do we find what value of the particle number n the solution corresponds to.

Figure 1 shows how the ground-state energy varies with the number of bosons n, and compares the numerical solution of the GP equation, Eqs. (8) and (9), to the variational result [the minimum value of Eq. (5)]. The parameter $V=1.5$ and $g=2,4,6,\ldots,20$. The GP solution is always below the variational prediction, because it uses a better wave function.

Although the variational results differ quantitatively from the solution to the GP theory, qualitatively they are similar. We offer the following observations.

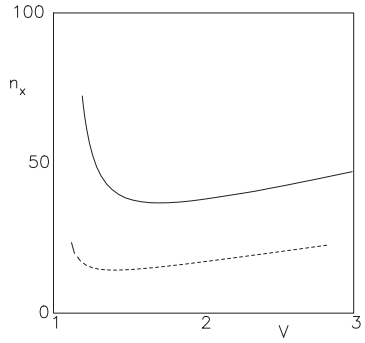

FIG. 2. Variation of n_x, the value of particle number n that minimizes the energy, with the strength V of the binding potential. The interaction parameter was taken to be $g=2$. The dotted line corresponds to the variational result.

(a) The energy is negative for all n, so that the attractive potential has a bound state with an infinite number of particles.

(b) For $g<g_c$, the energy has a very shallow minimum as a function of the number of particles. This implies that it will be difficult to attach a definite number of particles to a well by placing it in tunneling contact with a source (such as a condensate droplet): there is no equilibrium at all, or the number of particles bound will be large and very susceptible to small perturbations. The minimum in $E(n)$ is even less pronounced in the GP solution than it is in the variational result. We have indicated the apparent position of the minima, using the + graph marker.

(c) For $g>g_c$, the energy increases with the number of particles. Thus it is possible to bind a well-defined number of particles by letting the system equilibrate with a source. However, this scheme will work well only for a small number of particles: the plateau at large n will make the system insensitive to the number of particles.

In the variational study, we found a counterintuitive behavior for the value n_x at which the minimum of the total energy occurs: when g is below the critical value g_c, n_x becomes large, diverging as V approaches the binding threshold. This means that an arbitrarily large number of particles can be stably bound by making the potential weak. We have verified that this behavior is also exhibited by the solution to the GP theory. Here it is useful to observe that we are trying to find the minimum of the total energy both with respect to the parameter n and the normalized wave function ψ. Imposing the condition that the derivative of Eq. (1) with respect to n (with ψ fixed) is zero, and, combining the outcome with Eq. (9), we obtain a relationship

$$g = 2|\epsilon|/B. \tag{11}$$

Imposing this condition proved to be easier than trying to minimize E over n. We constructed Fig. 2 by finding normalized solutions to the GP equation (8) for various values of γ, and iterating until Eq. (11) holds.

Although our work demonstrates the existence of the effect of resonant binding only within the GP approximation, we expect that it is also present in the exact theory. As a nearly resonant well is made more shallow on approaching

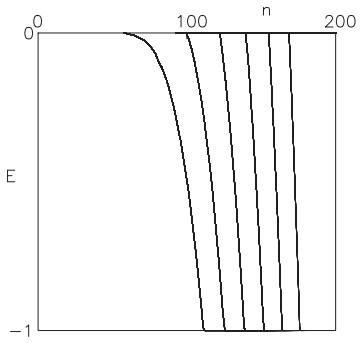

FIG. 3. Ground-state energy of weakly attractive bosons as a function of their number n, for various values of the binding potential amplitude V. The curves are all for the case $g=-0.1$, and the successive curves from left to right are for $V=1.00, 0.98, 0.96, 0.94, 0.92, 0.90$.

the single-particle binding threshold, the effective range of the central attraction increases, and the well binds an increasingly larger number of bosons. Therefore the microscopic details of the well are not expected to be of qualitative significance. The large range is responsible for the survival of the effect in the presence of weak short-range repulsion between the bosons because it allows the particles to take advantage of the central attraction while minimizing mutual contact interactions [19]. The interactions become more important as the well is made deeper, thus explaining the existence of the minimum in Fig. 2. For a sufficiently deep well the number of bound particles n_x increases as the well deepens, which is the normally expected behavior.

Additionally, we argue that our results are immune to the effects of correlations neglected in the GP approximation. Indeed, the GP theory can be viewed as a variational method. Therefore the exact energy will be lower than our calculations indicate. What they do show is that near resonance the wave function can accommodate an unexpectedly large number of particles, because each particle manages to sample the attractive well without interacting with the other particles too strongly. The effect of correlations would be that the particles evade each other more effectively, and thus enhance the effect we predict.

The issue of validity of the GP theory was also addressed in Ref. [9], where the same problem was studied in general dimensions. Specifically, in one dimension a version of the problem in question was solved exactly by using Bethe ansatz methods, and the results were compared with the GP solution. Although the exact ground-state wave function is indeed not of the product (Hartree) type, in the limit of large particle number the exact ground-state energy turns out to be nearly identical to its GP counterpart. This example represents "the worst case scenario" as the effect of correlations is expected to be strongest in one dimension. Therefore we conclude that it is very likely that the GP theory is fully adequate in three spatial dimensions.

V. WEAKLY ATTRACTING PARTICLES

The variational analysis also predicts an interesting phenomenon for the case of weakly attracting particles in the presence of a potential that is too weak to bind a single particle ($g<0$ and $V\leqslant 1$). The second term of Eq. (6) is negative for sufficiently large n, pointing to the existence of a many-body bound state. For the particular case $V=1$, the critical value of the number of particles needed is given by $n_c=3\pi/2|g|$. When $V<1$, the minimum energy can be positive (indicating a metastable state), but becomes negative for sufficiently large n. The possibility of a cooperatively bound state of this sort was first pointed out by Migdal [20].

Figure 3 shows the results of numerical solution of the GP theory for the case of weakly attracting particles in the presence of a $V\leqslant 1$ potential. In agreement with the variational argument, collective bound states are seen to form for a sufficiently large number of bosons. Specifically, the farther away the binding threshold, the larger the number of bosons required to form a bound state.

VI. BEYOND THE MODEL

The δ-shell potential cannot be achieved experimentally. Thus one may ask how our results are relevant to the real world.

The variational results are quite general for a localized external potential. Since the trial wave function is constant for $r<a$, the external potential enters only through its average value

$$a^2V=-\int_0^\infty U(r)r^2dr. \tag{12}$$

The solution to the GP equation will be affected slightly. We can anticipate the effects by comparing the δ-shell problem to that of the attractive square well $U(r)=-W$ for $r<a$. Outside the well the GP equation is the same for the square well and the δ shell, and so the solutions (for given γ and ϵ) are the same; the only question is how the value for W corresponds to that for V. The condition that relates them is that the values of the logarithmic derivatives of the wave functions should be the same at $r=a$. For the δ shell, the solution to Eq. (8) (for $\gamma=0$) is $\psi=C\sinh(\sqrt{|\epsilon|}r)/r$, and is very nearly constant for the cases of interest; however, for the square well the solution inside (again for noninteracting particles) has the form $\psi=C\sin(\sqrt{W-|\epsilon|}r)/r$. The logarithmic derivative of this function takes on all values and there is an infinite set of values of W for which the match can be achieved. The effect of the particle interactions will be to somewhat suppress the accumulation of particles (places where ψ is large) and to push the consecutive bound states to larger values of W.

However, the feature of interest in the resonantly bound system is the number of particles that can be bound, and this is a property of the wave function at large distances. Thus we can expect that the differences between different external potentials can be absorbed into the definitions of V_c and g.

VII. CONCLUSIONS

To summarize, our work demonstrates that a superthreshold localized trapping potential can bind an unexpectedly

large number of weakly repulsive bosons while a subthreshold trap can trigger formation of a cooperative bound state of weakly attractive bosons even when the two-body attraction is insufficient to form a two-body state. These effects are insensitive to the microscopic details of the trapping potential and have their origin in the large effective range of the nearly resonant trapping potential. We hope that these results will be experimentally tested in the near future.

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