Interaction Energy of Two Trapped Bosons with Long Scattering Lengths

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Abstract. I study two interacting bosons confined to a harmonic trap. The interaction is assumed to be of zero range, and expressed in terms of the s -wave scattering length. The energy shifts of the harmonic-oscillator states due to the atom-atom interaction are calculated analytically. It is found that for an ordinary potential the interaction energy depends only on the scattering length, while if the scattering length is modified by a near-threshold Feshbach resonance there is also a dependence on the width of the resonance.

1 Introduction

Experimental work on cold atoms and Bose-Einstein condensates are usually performed in atom traps where the confining potential has the shape of an harmonic oscillator. At the relevant temperatures and densities the atom-atom interactions may be characterized by the scattering length a alone, which typically is much longer than the range of the potential. Moreover, it has been demonstrated that the scattering length can be altered dramatically, even changing its sign, by using a magnetic field to tune a Feshbach resonance near the scattering threshold [1, 2, 3]. More recently Bose-Einstein condensation has also been achieved in optical lattices, where the size of the potential wells are comparable to the scattering length even without tuning [4]. It is therefore interesting to investigate the two-body interactions in the limit where the scattering length is comparable to the oscillator length a_{osc} of the harmonic potential. In particular, I compare the usual case when the scattering length is determined solely by the shape of a single-channel atom-atom potential to the case of scattering lengths modified by the presence of a Feshbach resonance.

2 Two boson scattering

We consider two bosons of mass m confined to a harmonic oscillator potential of frequency ω . The oscillator potential can be written as $m\omega^2/2(r^2/2 + 2R_{cm}^2)$,

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where r is the distance between the two bosons, and R_{cm} is the absolute value of the center of mass coordinate. Hence, the center of mass can be separated out. Assuming that the center-of-mass motion is not excited, the total energy of two non-interacting atoms with zero angular momentum is $E_{\text{tot}} = E + E_{cm} = \hbar\omega(2n + 3)$, where $n = 0, 1, 2, \dots$

2.1 Zero-range potential

Outside the range of the interaction potential the Schrödinger equation is

$$\left(-\frac{d^2}{dx^2} + x^2 - \eta\right)\psi(x) = 0, \quad (1)$$

where $x = r/(\sqrt{2}a_{\text{osc}})$, $a_{\text{osc}} = \sqrt{\hbar/m\omega}$, and $\eta = 2E/(\hbar\omega)$. The solution is given in terms of the confluent hypergeometric function M as

$$\psi(x) = e^{-x^2/2} \frac{1}{x} \left[c_1 M\left(\frac{1-\eta}{4}, \frac{1}{2}, x^2\right) + c_2 \sqrt{\eta} x M\left(\frac{3-\eta}{4}, \frac{3}{2}, x^2\right) \right], \quad (2)$$

where c_1 and c_2 are constants to be determined by the boundary conditions. In the limit $x \rightarrow \infty$ one has $M(a, b, x) \rightarrow (b)/ (a)x^{b-a} \exp(x)$, which gives the condition

$$\frac{c_1}{c_2} = -\frac{\sqrt{\eta}}{2} \frac{[(1-\eta)/4]}{[(3-\eta)/4]}, \quad (3)$$

in order for ψ to vanish at infinity. The boundary condition as $x \rightarrow 0$ is determined by the boson-boson interaction. In this limit the ψ goes over in the usual plane wave form

$$\psi(x) \rightarrow c_2 \left[\frac{\sin(px)}{x} + \tan \delta_0(k) \frac{\cos(px)}{x} \right], \quad (4)$$

where $p = \sqrt{2}ka_{\text{osc}} = \sqrt{\eta}$, and the s -wave phase shift is given by $\tan \delta_0(k) = c_1/c_2$. Inserting this expression for the phase shift in Eq. (3) we obtain the condition for quantization of the energy,

$$\tan \delta_0(k) = -\frac{\sqrt{\eta}}{2} \frac{[(1-\eta)/4]}{[(3-\eta)/4]}. \quad (5)$$

For a zero range potential $\tan \delta_0(k) = -ka$, where a is the scattering length, giving finally

$$\frac{a}{a_{\text{osc}}} = \frac{1}{\sqrt{2}} \frac{[(1-\eta)/4]}{[(3-\eta)/4]}. \quad (6)$$

This result has been obtained previously, using a different method, in Ref. [5].

The energies $E_{\text{tot}} = \hbar\omega(\eta + 3)/2$ obtained from the roots of Eq. (6) are displayed in Fig. 1. For zero scattering length the gamma function in the denominator of the right-hand side must diverge, i.e. $(3-\eta)/4 = -i$ ($i = 0, 1, 2, \dots$),

Figure 1. Energy as a function of a/a_{osc} (including the center-of-mass energy $3\hbar\omega/2$). The dashed line shows the energy for an unconfined bound two-body state $E_{\text{tot}} = 3\hbar\omega/2 - \hbar^2/(ma^2)$.

giving the energies of two non-interacting atoms. For small a/a_{osc} the interaction energy shows the familiar linear dependence on the scattering length

$$E_{\text{tot}} = 3\hbar\omega + 4\pi\hbar^2 a \rho / m, \quad (7)$$

where $\rho = (2n+1)!!/(n!2^n)(\sqrt{2\pi}a_{\text{osc}})^{-3}$ is the overlap density for two non-interacting bosons in the state n . In the opposite limit, when the scattering length becomes comparable to or larger than the physical size of the system, the interaction energy approaches a constant value. For an infinite scattering length the energy levels are given by $E_{\text{tot}} = \hbar\omega(2n+2)$, i.e. exactly in between the unperturbed levels.

It is also interesting to note that at $a/a_{\text{osc}} = 2.1$ the near-threshold two-body bound state acquires an energy larger than the center-of-mass energy, i.e. becomes unbound (although, of course, it is still bound by the harmonic oscillator potential). Hence, for confined bosons, the scattering length may be positive even if there is no two-body bound state.

2.2 Potential with finite range

For a potential with effective range r_e the modified expression for the phase shift is $\tan \delta_0(k) = -ka/(1 - r_e ak^2/2)$. The energy difference between a zero

range potential, and a potential with $r_e/a_{\text{osc}} = 10^{-3}$ is displayed for the lowest scattering state in Figure 2. As expected the effect is small, but we note that it does not vanish for $a/a_{\text{osc}} \rightarrow \infty$. In this limit the correction arising from the finite range of the potential is $\Delta E = \hbar\omega/4(4n+5)/(n+1)\rho^{1/3}r_e/a_{\text{osc}}$.

Figure 2. Difference in interaction energy between a potential with effective range $r_e = a_{\text{osc}}/1000$, and a zero-range potential, as a function of scattering length.

3 Long scattering length induced by a Feshbach resonance

The scattering length can be changed drastically if there is a Feshbach resonance close to the scattering threshold. Such a resonance may be present by chance, but it may also be tuned to a suitable energy through the application of a magnetic field, as has been demonstrated experimentally for ultracold atoms both in the condensed and non-condensed phase [1, 2, 3].

In an unconfined system the scattering phase shift modified by the presence of the resonance is [6]

$$\tan \delta(E) = \frac{\tan \delta_{\text{bg}}(E) + \Gamma/(2\epsilon)}{1 - \Gamma/(2\epsilon) \tan \delta_{\text{bg}}(E)}, \quad (8)$$

where δ_{bg} is the phase-shift in the absence of the resonance, and $\epsilon = E_{\text{res}} - E$ is the difference between the resonance and scattering energies. Similarly, since according to threshold laws the width has the form $\Gamma = \gamma k$, where γ is a constant, the scattering length is $a = a_{\text{bg}} - \gamma/(2E_{\text{res}})$.

The scattering properties at exactly zero collision energy are completely determined by the scattering length. Hence, in this case, it does not matter why the scattering length has a certain value. In particular, outside the range of the interaction potential, there is no difference between an ordinary scattering length and one that has been modified by the presence of a Feshbach resonance. In a confined system we are, however, not working at zero collision energy because of the zero-point motion. In section 2.2 it was demonstrated that for an ordinary scattering length, the change of the phase shift due to the finite collision energy causes only a very small effect on the interaction energy. For a scattering length modified by a Feshbach resonance, on the contrary, this effect is large. From Eq. (8) one sees that the energy scale for change in $\delta(E)$ is $\sim E_{\text{res}} \sim \gamma/a$. Hence, if γ is small and a is large, we expect deviations from the results in Section 2.1.

The change of the harmonic oscillator energies due to a Feshbach resonance can be studied using the following simple model. For simplicity I shall assume that the background scattering length $a_{\text{bg}} = 0$, so that the change of the energy levels is solely due to the presence of the resonance.

The Hamiltonian is split into three parts. First the initial-channel Hamiltonian H_i , which since $a_{\text{bg}} = 0$ is just the harmonic oscillator with s -wave eigenfunctions ϕ_n , and eigenvalues $E_n = \hbar\omega(2n+3)$. Secondly, the Hamiltonian in the molecular channel H_m , with the eigenfunction ψ_m and eigenvalue E_m , describing the molecular state, which is stable in the absence of couplings to other channels. Finally, there is the coupling V between the the initial and molecular channels, which turns the molecular state into a resonance, and shifts the energies E_n in the initial channel.

The harmonic oscillator states and the molecular state form a complete orthonormal basis for the total wavefunction,

$$\Psi = c_m \psi_m + \sum_{n=0}^{\infty} c_n \phi_n. \quad (9)$$

Denoting the non-diagonal elements of the Hamiltonian $\alpha_n = \langle \psi_m | V | \phi_n \rangle$ the total Hamiltonian takes the form

$$H = \begin{pmatrix} E_m & \alpha_1 & \alpha_2 & \cdots \\ \alpha_1 & E_1 & 0 & \cdots \\ \alpha_2 & 0 & E_2 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}. \quad (10)$$

Furthermore, the molecular state is assumed to have zero range, giving

$$\alpha_n = \frac{\phi_n(0)}{\phi_0(0)} \alpha_0 = \frac{1}{2^n} \frac{\sqrt{(2n+1)!}}{n!} \alpha_0. \quad (11)$$

For large n one has $\alpha_n \propto n^{1/4}$. Diagonalization of H then gives eigenenergies E as solutions of the equation

$$E = E_m + \sum_{n=0}^{\infty} \frac{\alpha_n^2}{E - E_n}. \quad (12)$$

The summation in Eq. (12) does, however, diverge since $\alpha_n^2 \propto \sqrt{n}$, and $E_n \propto n$ for large n . This is not a problem since E_m is not an observable. Instead we must take the coupling between channels into account and define the energy of the *resonance* as

$$E_{\text{res}} = E_m + \sum_{n=1}^{\infty} \frac{\alpha_n^2}{E_0 - E_n}. \quad (13)$$

In terms of the resonance energy E_{res} the energy eigenvalues are given by

$$E = \frac{\alpha_0^2}{E - E_0} + E_{\text{res}} + \sum_{n=1}^{\infty} \frac{\alpha_n^2 (E_0 - E)}{(E - E_n)(E_0 - E_n)}. \quad (14)$$

This sum converges since for large n the terms decrease as $n^{-3/2}$.

Figure 3. Energy of the lowest oscillator state as a function of scattering length in the presence of a Feshbach resonance, for different couplings α_0 between the resonance and the scattering states. Long dashes: $\alpha_0 = 10\hbar\omega$; short dashes: $\alpha_0 = \hbar\omega$; dash-dotted: $\alpha_0 = 0.1\hbar\omega$; solid: dependence without any resonance (see Section 2.1).

The solutions of Eq. (14) are displayed in Figure 3 for different values of the coupling α_0 between the resonance and the scattering states. The width of the resonance is related to the coupling through $\gamma = \sqrt{2\pi}\alpha_0^2 a_{\text{osc}}/(\hbar\omega)$. As expected, for very broad resonances the result approaches that in Section 2.1 without any resonance. For narrow resonances, on the other hand, the difference is substantial

even for small a/a_{osc} . When α_0 is small the contribution from the sum in Eq. (14) is negligible, and $E \sim E_0$ if $E_{\text{res}} < 0$, or $E \sim E_{\text{res}}$ if $E_{\text{res}} > 0$.

4 Conclusion

In this paper I have studied the interaction energy of two bosons trapped in a harmonic oscillator potential, when the scattering length is comparable in magnitude to the oscillator length of the potential. I have found that the energy levels approach a constant value when the scattering length is larger than the oscillator length. For an ordinary potential the energy is to a good approximation a function of the scattering length only. In the presence of a Feshbach resonance, however, the energy also depends on the width of the resonance. For very narrow resonances the energy is close to that of the unperturbed harmonic oscillator even for large scattering lengths. For broad resonances, on the other hand, the results approach those for scattering without any resonance.

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