Foundations of Physics, Vol. 28, No. 4, 1998

Two Cold Atoms in a Harmonic Trap[1]

Thomas Busch,[2] Berthold-Georg Englert,[3] Kazimierz Rzążewski,[4] and Martin Wilkens[2]

Received January 21, 1997

Two ultracold atoms moving in a trap interact weakly at a very short distance. This interaction can be modeled by a properly regularized contact potential. We solve the corresponding time-independent Schrödinger equation under the assumption of a parabolic, spherically symmetric trapping potential.

1. INTRODUCTION

The interaction of ultracold atoms in a trap is a topic of intense research with applications ranging from collective phenomena in optical lattices[(1)] to the recently observed Bose–Einstein condensation of alkaline vapors.[(2)] The distinct feature which makes the interaction in these systems differ from the related scenario of ultracold collisions in free space is the presence of the trapping potential. Whereas in free space the pair interaction is probed via differential cross sections and collisional phase shifts, for example, these quantities lose meaning in the presence of a trapping potential since the confinement does not admit the construction of asymptotic in and out states. Instead, in a trap the interacting many-atom system is characterized by a discrete energy spectrum and possibly also by transition matrix elements, similar to the situation in molecular physics.

The many-body problem of trapped atoms is rather complicated, in particular when using a realistic atom–atom interaction. To avoid this

[1] Dedicated to the memory of Professor Asim O. Barut.

[2] Institut für Physik, Universität Potsdam, Am Neuen Palais 10, 14469 Potsdam, Germany.

[3] Sektion Physik, University of Munich, Theresienstr. 37, 80333 München, Germany; presently at Atominstitut der Österreichischen Universitäten, Stadionallee 2, 1020 Wien, Austria.

[4] Center for Theoretical Physics and College of Science, Polish Academy of Sciences, Al. Lotników 32/46, 02-668 Warsaw, Poland.

0015-9018/98/0400-0549$15.00/0

difficulty one commonly employs the shape-independent approximation in which the physical interaction is replaced by a pointlike potential of zero range.[5] For ultracold atoms such a replacement is well justified since their de Broglie wavelength is so large that the finer details of the physical interaction potential do not matter.

Whereas in one spatial dimension a zero-range potential is easily modeled by a simple δ-function,[4] in three dimensions the frequently employed $\delta^{(3)}(\mathbf{r})$ function must be treated with great care because the corresponding Hamiltonian is not self-adjoint.[5] In particular, any attempt is void which would aim at an exact diagonalization of such a Hamiltonian, since it would only reproduce the trivialities of the noninteracting theory.[6]

This notwithstanding we shall here diagonalize exactly the problem of two particles in a three-dimensional trap which interact via a pointlike potential. However, in order to ensure the self-adjointness of the corresponding Hamiltonian we shall use the so-called regularized δ-function $\delta^{(3)}_{reg}(\mathbf{r}) \equiv \delta^{(3)}(\mathbf{r})(\partial/\partial r)\, r$ to model the atom–atom pair interaction.[6] Within the domain of square integrable functions that are regular at the origin, this distribution acts in the same manner as the pure δ-function. The domain of a Hamiltonian of the general structure $-\nabla^2 + \delta^{(3)}_{reg}(\mathbf{r})$ is slightly larger though, as it also includes functions which diverge $\sim r^{-1}$ for $r \to 0$.[7] It is worth remembering that the regularized δ-potential has also been used in other contexts; let us just mention two historic papers: the work of Breit and Zilsel in nuclear physics[10] and Bersons' study[11] of the ionization of negative ions.[8]

2. THREE-DIMENSIONAL TRAP

A. Schrödinger equation

Assuming now an external isotropic harmonic oscillator potential, we use the following Hamiltonian to describe the motion of two atoms that interact with each other via a pointlike force:

$$H = -\tfrac{1}{2}\nabla_1^2 - \tfrac{1}{2}\nabla_2^2 + \tfrac{1}{2}r_1^2 + \tfrac{1}{2}r_2^2 + 4\pi a_0\, \delta^{(3)}_{reg}(\mathbf{r}_1 - \mathbf{r}_2) \tag{1}$$

[5] For a mathematical theory of pointlike interactions see Ref. 3.

[6] This regularization has been introduced by Fermi.[7] In more general terms, regularizations of zero-range potentials are discussed in Refs. 3, 5, and 8. If one wishes to avoid mathematical subtleties associated with regularization, one can regard zero-range potentials as limiting cases of separable potentials; some aspects thereof are treated in Refs. 4 and 9.

[7] Quite remarkably, these functions are neither in the domain of the kinetic energy operator $-\tfrac{1}{2}\nabla^2$ nor in the one of the potential energy operator $\delta^{(3)}_{reg}(\mathbf{r})$ alone, but only in the domain of the whole Hamilton operator.

[8] The two-dimensional analog of $\delta^{(3)}_{reg}$ has proved extremely useful in mathematical physics, as exemplified by Šeba's solution of a chaotic quantum billiard.[12]

where $\mathbf{r}_1$ and $\mathbf{r}_2$ are the position vectors of the two atoms. We are using harmonic-oscillator units, in which all energies are in units of $\hbar\omega$ and all lengths are in units of the extension $\sqrt{\hbar/(m\omega)}$ of the ground state of the trap. The strength of the interaction is characterized by the scattering length a_0 (in oscillator units) and the interaction potential is chosen to be the regularized δ-function.

Because of the quadratic form of both the kinetic energy and the external potential energy in Eq. (1), this Hamiltonian can be separated into a center-of-mass part and a relative part, $H = H_{\mathrm{CM}} + H_{rel}$ with

$$\begin{aligned} H_{\mathrm{CM}} &= -\frac{1}{2}\nabla_R^2 + \frac{1}{2}\mathbf{R}^2 \\ H_{rel} &= -\frac{1}{2}\nabla_r^2 + \frac{1}{2}\mathbf{r}^2 + \sqrt{2}\,\pi a_0\,\delta^{(3)}(\mathbf{r})\frac{\partial}{\partial r}r \end{aligned} \tag{2}$$

which can then be diagonalized separately. Here $\mathbf{R} = \sqrt{1/2}\,(\mathbf{r}_1 + \mathbf{r}_2)$ is the center-of-mass coordinate and $\mathbf{r} = \sqrt{1/2}\,(\mathbf{r}_1 - \mathbf{r}_2)$ is the relative coordinate.[9] One can see immediately that the eigenfunctions of the center-of-mass motion are the well known states of the harmonic oscillator. So one is just left with the problem of solving the Schrödinger equation for the relative motion,

$$\left(H_{osc} + \sqrt{2}\,\pi a_0\,\delta^{(3)}(\mathbf{r})\frac{\partial}{\partial r}r\right)\Psi(\mathbf{r}) = E\Psi(\mathbf{r}) \tag{3}$$

in which H_{osc} stands for the Hamiltonian of the three-dimensional, isotropic, harmonic oscillator. The two-particle problem has been reduced to an effective one-particle problem; we emphasize that the harmonicity of the trapping potential is essential for this reduction.

To solve the Schrödinger equation (3) analytically, we expand the unknown wave function $\Psi(\mathbf{r})$ into the complete set of the familiar wave functions $\varphi_n(\mathbf{r})$ of the harmonic oscillator,

$$\Psi(\mathbf{r}) = \sum_{n=0}^{\infty} c_n \varphi_n(\mathbf{r}) \tag{4}$$

Only $l = 0$ states enter the sum in (4) since all other states vanish at $\mathbf{r} = 0$. These $l \neq 0$ states do not "feel" the pointlike interaction and stay unperturbed.

[9] The true center-of-mass position is, of course, given by $\frac{1}{2}(\mathbf{r}_1 + \mathbf{r}_2) = \mathbf{R}/\sqrt{2}$ and the true position of atom 1 relative to atom 2 by $\mathbf{r}_1 - \mathbf{r}_2 = \sqrt{2}\,\mathbf{r}$. The unconventional factors of $\sqrt{2}$ are included so that the effective masses for the center-of-mass motion and the relative motion are the same.

We insert the expansion (4) into Eq. (3) and obtain ($H_{osc}\,\varphi_n = E_n\,\varphi_n$)

$$\sum_{n=0}^{\infty} c_n(E_n - E)\,\varphi_n(\mathbf{r}) + \sqrt{2}\,\pi a_0\,\delta^{(3)}(\mathbf{r})\,\frac{\partial}{\partial r}\,r\sum_{m=0}^{\infty} c_m\,\varphi_m(\mathbf{r}) = 0 \qquad (5)$$

The expansion coefficients c_n can be determined by projecting this expression onto $\varphi_n^*(\mathbf{r})$, which yields

$$c_n(E_n - E) + \sqrt{2}\,\pi a_0\,\varphi_n^*(0)\left[\frac{\partial}{\partial r}\left(r\sum_{m=0}^{\infty} c_m\,\varphi_m(\mathbf{r})\right)\right]_{r\to 0} = 0 \qquad (6)$$

Consequently, the coefficients c_n are of the form

$$c_n = A\,\frac{\varphi_n^*(0)}{E_n - E} \qquad (7)$$

where the value of the n-independent numerical constant A is fixed by the normalization of $\Psi(\mathbf{r})$.[10] Upon inserting the ansatz (7) into (6) we arrive at

$$\sqrt{2}\,\pi\left[\frac{\partial}{\partial r}\left(r\sum_{n=0}^{\infty}\frac{\varphi_n^*(0)\,\varphi_n(\mathbf{r})}{E_n - E}\right)\right]_{r\to 0} = -\frac{1}{a_0} \qquad (8)$$

which determines the $l = 0$ eigenvalues of H_{rel} of (2). We note in passing that we are dealing here with the $r' \to 0$ limit of the Green's function solution discussed in Ref. 13.

B. Energy shifts

In order to simplify (8) the summation must be carried out first. This can be done by inserting the following representation of the harmonic oscillator s-wave functions

$$\varphi_n(\mathbf{r}) = \pi^{-3/4}\left[L_n^{(1/2)}(0)\right]^{-1/2} e^{-r^2/2} L_n^{(1/2)}(r^2) \qquad (\text{to } E_n = \tfrac{3}{2} + 2n) \qquad (9)$$

which leads to

$$\frac{1}{\sqrt{2\pi}}\left[\frac{\partial}{\partial r}\left(re^{-r^2/2}\sum_{n=0}^{\infty}\frac{L_n^{(1/2)}(r^2)}{n-\nu}\right)\right]_{r\to 0} = -\frac{1}{a_0} \qquad (10)$$

[10] Actually, the equality $|A|^2 = \sqrt{2}\,\pi a_0^2\,\partial E/\partial a_0$ holds with the functional relation (16) between E and a_0.

where $\nu \equiv \frac{1}{2}E - \frac{3}{4}$ is the noninteger analog of the principle quantum number n of the oscillator. The integral representation

$$\frac{1}{n-\nu} = \int_0^\infty \frac{dy}{(1+y)^2}\left(\frac{y}{1+y}\right)^{n-\nu-1} \tag{11}$$

which is valid for $n-\nu > 0$, shifts the n dependence of the sum in Eq. (10) from the denominator to an exponent,

$$\sum_{n=0}^{\infty} \frac{L_n^{(1/2)}(r^2)}{n-\nu} = \sum_{n=0}^{\infty} \int_0^\infty \frac{dy}{(1+y)^2}\left(\frac{y}{1+y}\right)^{n-\nu-1} L_n^{(1/2)}(r^2) \tag{12}$$

The summation variable n appears now only as the degree of the Laguerre polynomial and in the exponent so that we encounter one of the generating functions of the Laguerre polynomials, viz.

$$\sum_{n=0}^{\infty} L_n^{(1/2)}(x)\, z^n = (1-z)^{-3/2} \exp\left(\frac{xz}{z-1}\right) \tag{13}$$

Accordingly, we get

$$\begin{aligned}\sum_{n=0}^{\infty} \frac{L_n^{(1/2)}(r^2)}{n-\nu} &= \int_0^\infty \frac{dy}{\sqrt{1+y}} e^{-yr^2}\left(\frac{y}{1+y}\right)^{-\nu-1} \\ &= \Gamma(-\nu)\, U\left(-\nu, \frac{3}{2}, r^2\right)\end{aligned} \tag{14}$$

where the last step recognizes a standard integral representation of the confluent hypergeometric function U.[11] In view of the well-known behavior of $U(n, m, x)$ at $x = 0$, here:[12]

$$\Gamma(-\nu)\, U\left(-\nu, \frac{3}{2}, r^2\right) = -\sqrt{\pi}\left(\frac{2\Gamma(-\nu)}{\Gamma(-\nu-1/2)} - \frac{1}{r} + O(r)\right) \tag{15}$$

Eq. (10) thus reduces to

$$\sqrt{2}\,\frac{\Gamma(-E/2+3/4)}{\Gamma(-E/2+1/4)} = \frac{1}{a_0} \tag{16}$$

[11] See, for example, entry 13.2.5 in Ref. 14.
[12] Entries 13.1.3 and 13.1.2 in Ref. 14.

To begin with, this equation is valid for $E < \frac{3}{2}$ only [recall the restriction of (11) to $\nu < n$] but its range of validity is immediately extended to all $E \neq \frac{3}{2} + 2n$ by analytical continuation.

Upon combining Eqs. (4), (7), (9), and (14) we observe that the $\ell = 0$ solutions of the Schrödinger equation (3) are given by

$$\Psi(\mathbf{r}) = \tfrac{1}{2}\pi^{-3/2} A e^{-r^2/2} \Gamma(-\nu)\, U(-\nu, \tfrac{3}{2}, r^2) \tag{17}$$

One verifies without effort that this obeys (3) for $r > 0$ independent of the value of $E = 2\nu + \frac{3}{2}$, but the $\delta^{(3)}$ singularities at $r = 0$ cancel each other only for those E values for which (16) holds.

The left-hand side of Eq. (16) has simple poles at the s-state energies $E = \frac{3}{2}, \frac{7}{2}, \frac{11}{2}, \ldots$ of the unperturbed oscillator, and zeros for $E = \frac{1}{2}, \frac{5}{2}, \frac{9}{2}, \ldots$. The left-hand side of (16) is therefore positive in the intervals

$$E < \tfrac{1}{2}, \qquad \tfrac{3}{2} < E < \tfrac{5}{2}, \qquad \tfrac{7}{2} < E < \tfrac{9}{2}, \ldots$$

and negative in the intervals

$$\tfrac{1}{2} < E < \tfrac{3}{2}, \qquad \tfrac{5}{2} < E < \tfrac{7}{2}, \qquad \tfrac{9}{2} < E < \tfrac{11}{2}, \ldots$$

These matters are illustrated in Fig. 1. For a positive scattering length, which is characteristic of the scattering by a repulsive interaction, the energy levels are shifted upward and for sufficiently large values of a_0 they saturate at a shift of $\Delta E = 1$. When the scattering length is negative the levels are shifted downward and saturate at a shift of $\Delta E = -1$.[13]

In the absence of the harmonic trapping potential, the three-dimensional regularized δ-potential gives rise to a single bound state if the scattering length a_0 is positive;[14] the corresponding binding energy $1/a_0^2$ tends to ∞ as $a_0 \to 0^+$.[15] Owing to the trapping potential this state is now shifted upward in energy. We note that both for $a_0 < 0$ and for $a_0 > 0$ the ground state of the system lies below the one of the unperturbed system.

The velocity dependence associated with the $\partial/\partial r$ differentiation thus leads to a counterintuitive feature of the regularized δ-potential: For $a_0 > 0$ it behaves like an attractive interaction as far as bound-state properties are concerned, but it scatters like a repulsive potential. And for $a_0 < 0$ matters are reversed—no bound state, but scattering as if an attractive interaction

[13] Incidentally, the equality reported in footnote 10 requires $\partial E/\partial a_0 > 0$.

[14] Since we are employing oscillator units this bound state is recovered from (16) in the limit $-E \gg 1$ when the left-hand side equals $\sqrt{-E}$.

[15] In the same limit the wave function of this bound state $\Psi \sim e^{-\sqrt{2}\, r/a_0}/r$ has a vanishing overlap with any (a_0-independent) square-integrable wave function.

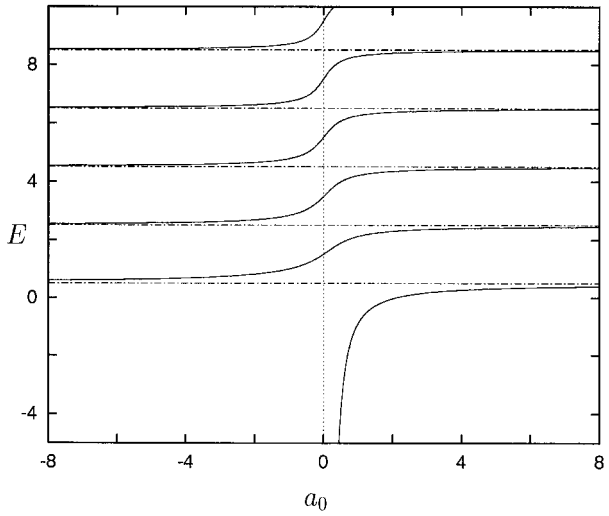

Fig. 1. Spectrum of the $l = 0$ states in the two-particle system with a regularized zero-range interaction in three dimensions. The solid lines (——) represent the solutions for E of (16) in their dependence on the strength of the interaction as measured by the scattering length a_0. The broken lines (—·—·—) indicate the asymptotic values that are reached for $a_0 \to \pm\infty$.

were at work. The limit $a_0 \to 0^+$ exhibits the anomaly *in nuce*: the binding energy grows without bound and the scattering cross section vanishes.

A further observation is that for growing energy the level shift is saturating for smaller values of the scattering length, that is, for weaker interaction strengths. A numerical criterion is the slope of the linear a_0-dependence near $a_0 = 0$, where the solutions of (16) are approximately given by[16]

$$E \simeq \frac{3}{2} + 2n + \sqrt{2/\pi} \binom{n + 1/2}{n} a_0, \qquad (n = 0, 1, 2, \ldots) \tag{18}$$

Indeed, the slope grows proportional to $\sqrt{n}$. This is due to the fact that $\varphi_n(0)$, the s-state oscillator wave function at the center, increases with the principle quantum number n as $n^{1/4}$. So the zero-range interaction modeled by the regularized δ-function is getting more and more effective for higher

[16] In passing we note that a weak perturbation is characterized by $|a_0| \ll 1$, which indicates that the scattering properties of $\delta^{(3)}_{\text{reg}}$ are essential here, not the binding properties.

energy states.[17] Incidentally, this $n^{1/4}$ growth is the reason why one must evaluate the sum in (8) prior to the required differentiation.[18]

3. ONE-DIMENSIONAL AND TWO-DIMENSIONAL ANALOGS

These findings in three dimensions can be compared with the one-dimensional and two-dimensional analogs,[19] shown in Figs. 2 and 3. In all three cases the s-wave scattering amplitude is of the form $e^{i\theta}\sin\theta = (-i + \cot\theta)^{-1}$. For zero-range interactions the scattering phase θ has a particularly simple dependence on the wave number k, viz.

$$\cot\theta = \begin{cases} -(ka_0)^{-1} & \text{in three dimensions} \\ \dfrac{2}{\pi}\log(ka_0) & \text{in two dimensions} \\ ka_0 & \text{in one dimension} \end{cases} \tag{19}$$

The same relations hold for (almost) arbitrary finite-range interactions in the long-wavelength limit.

The scattering length a_0 is identified in this limit. The three-dimensional relation is quite familiar; the conventions we employ in one and two dimensions are exhibited in (19). They are such that matters are as similar as possible: (i) $\cot\theta$ increases with growing a_0; (ii) there is a bound state for $a_0 > 0$; (iii) its binding energy equals $1/a_0^2$.

An analysis that is closely analogous to the three-dimensional one can be performed in one and two dimensions as well. Remarkably, the shifted energies in the one-dimensional case are again determined by Eq. (16), except that now the unperturbed even-state energies $E = \frac{1}{2}, \frac{5}{2}, \frac{9}{2}, \ldots$ are obtained for $1/a_0 = 0$, not for $a_0 = 0$. In marked contrast to the three-dimensional case the values of the (even) wave functions at the center decrease as $n^{-1/4}$ here. In the limit of weak interaction strength ($1/a_0 \ll 1$) the one-dimensional analog of (18) reads

$$E \cong \frac{1}{2} + 2n - \sqrt{2/\pi}\binom{n - 1/2}{n}\frac{1}{a_0}, \qquad (n = 0, 1, 2, \ldots) \tag{20}$$

[17] The modeling of the physical interaction by a zero-range potential is an approximation which is valid as long as the interparticle de Broglie wavelength is larger than the range of the physical force. Consequently, this approximation is invalid if the relevant energies are too large.

[18] We also note this consequence: The coefficients c_n of (7) decrease like $c_n \sim n^{-3/4}$ for $n \gg 1$ and therefore the wave functions $\Psi(\mathbf{r})$ of (4) are not in the domain of H_{osc}. This remark is, of course, analogous to the one in footnote 7.

[19] In one dimension one has simply $V(x_1 - x_2) = -(2/a_0)\,\delta^{(1)}(x_1 - x_2)$; matters are more complicated in two dimensions because of logarithmic singularities.[3, 12]

Indeed, the slope decreases proportional to $\sqrt{n}$ with n. Hence, with growing energy the saturation takes place at larger values of the interaction strength $1/a_0$. These remarks are confirmed by Fig. 2.

In two dimensions the situation is somewhat more complicated. The scattering length is always positive, and the shifted energies are given by the solutions of

$$\psi(-E/2+1/2) = \log\left(\frac{1}{2a_0^2}\right) \tag{21}$$

where $\psi(\ )$ is the logarithmic derivative of Euler's Γ-function. In the vicinity of the unperturbed energies $E = 1, 3, 5, \ldots$, one has

$$E \cong 1 + 2n + 2\left[\log\left(\frac{1}{2a_0^2}\right)\right]^{-1}, \qquad (n = 0, 1, 2, \ldots) \tag{22}$$

so that the coupling strength is measured by $[\log(\frac{1}{2}/a_0^2)]^{-1}$. Here, the derivative of E with respect to the coupling strength does not depend on n in the weak-coupling limit. Figure 3 demonstrates the two-dimensional case.

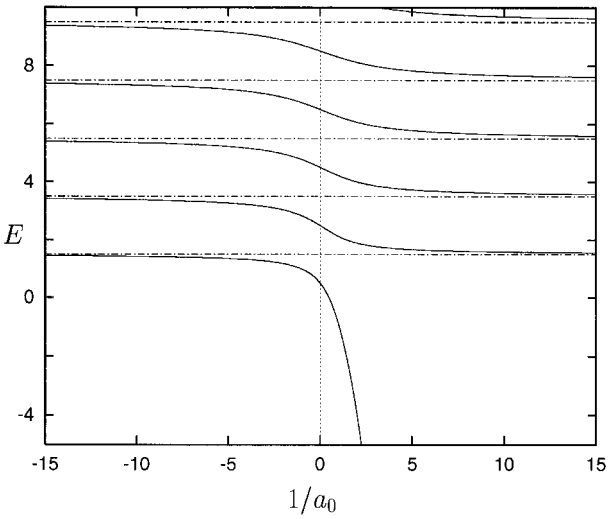

Fig. 2. Spectrum of the even states in the two-particle system with a zero-range interaction in one dimension. The solid lines (——) represent the solutions for E of (16) in their dependence on the strength of the interaction as measured by the inverse $1/a_0$ of the scattering length. The broken lines (—·—·—) indicate the asymptotic values that are reached for $1/a_0 \to \pm\infty$.

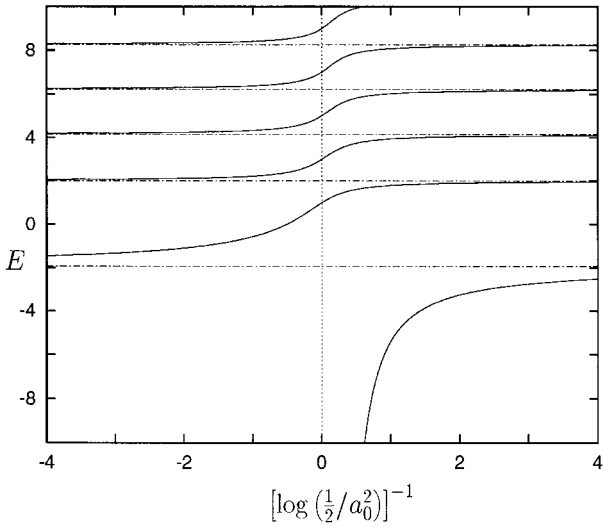

Fig. 3. Spectrum of the $m = 0$ states in the two-particle system with a zero-range interaction in two dimensions. The solid lines (——) represent the solutions for E of (21) in their dependence on the strength of the interaction which is given by $[\log(\frac{1}{2}/a_0^2)]^{-1}$ in terms of the scattering length a_0. The broken lines (—·—·—) indicate the asymptotic values $E = -1.923264$, 2.008166, 4.146997, 6.221442, 8.270587,... that are reached in the limit of very strong coupling.

4. SUMMARY

We have presented an analytical solution to the problem of two cold atoms with a zero-range interaction in a harmonic trap. We have thus added another example to the short list of solvable problems in quantum mechanics. In addition to its pedagogical value, the problem studied is of potential significance for the physics of ultracold vapors.

ACKNOWLEDGMENTS

We would like to thank C. Eberlein for bringing Ref. 4 to our attention. BGE expresses his gratitude for the hospitable environment provided by H. Paul and his group in Adlershof. KR and MW would like to thank J. Mlynek for the hospitality extended to them during their stay in Konstanz. KR gratefully acknowledges financial support by the Optik Zentrum Konstanz. TB and BGE each thank the Center of Theoretical Physics for supporting a visit to Warsaw.

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