Effective-scattering-length model of ultracold atomic collisions and Feshbach resonances in tight harmonic traps

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We consider the problem of cold atomic collisions in tight traps, where the absolute scattering length may be larger than the trap size. As long as the size of the trap ground state is larger than a characteristic length of the van der Waals potential, the energy eigenvalues can be computed self-consistently from the scattering phase shift for untrapped atoms. By comparing with the exact numerical eigenvalues of the trapping plus interatomic potentials, we verify that our model gives accurate eigenvalues up to milliKelvin energies for single-channel *s*-wave scattering of ^{23}Na atoms in an isotropic harmonic trap, even when outside the Wigner threshold regime. Our model works also for multichannel scattering, where the scattering length can be made large due to a magnetically tunable Feshbach resonance.

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I. INTRODUCTION

Along with the development of laser cooling of atoms have come techniques for trapping the cold atoms, with tremendous advantages for experimental atomic physics. Just to name a few potent examples where trapping is necessary, the Bose-Einstein transition has been reached in several atomic species [1] (for reviews, see Ref. [2]), threshold scattering properties have been studied [3,4], molecules formed with the assistance of light [5–7], and quantum chaos [8,9] and quantum phase transitions [10] observed using optical lattices.

Atomic collisions play an essential role in most of these phenomena. In the past one could ignore the fact that these collisions take place in a trap, since trap sizes are very large in comparison with the sizes associated with atomic interactions. However, recent developments make it crucial to account for the effect of trap confinement on collisions when the atoms are held tightly in one, two, or three dimensions by optical lattices. For example, Greiner *et al.* [10] have observed a quantum phase transition from a superfluid to a Mott insulator within a three-dimensional optical lattice. Moreover, several low-dimensional transitions of cold bosonic systems have been conjectured. In two dimensions, the Kosterlitz-Thouless transition has been proposed [11], while in one dimension the Tonks-Girardeau gas should be possible [12,13]. Zero-temperature transitions have also been investigated theoretically for a rotating two-dimensional gas [14]. All of these transitions depend on atomic collisions, and for quantitative predictions the low-dimensional interactions must be understood.

Two proposals for quantum computing involve loading cold atoms into optical lattices, and using the interaction between the atoms as the switching mechanism [15,16]. In one type of quantum logic gate, two atoms are brought together and allowed to interact for a set time interval, resulting in different phase shifts depending on their hyperfine sublevels. A recent experiment [10] represents an important first step towards quantum logic applications, since it shows that a lattice can be initialized with uniform occupancy of lattice sites.

Another burgeoning area is the study of Feshbach resonances, and weakly-bound molecular states, in the interaction of two ultracold atoms. This has improved the knowledge of interaction parameters of alkali atoms and opened up the field of molecular condensates and three-body processes [17,18]. By tuning Feshbach resonances one can easily reach an interesting regime where the scale length associated with the scattered wave exceeds the trap width [19].

We address these problems by calculating the eigenvalues of two interacting atoms confined in a trapping potential. A popular method for representing cold atom interactions is to replace the exact interatomic potential by a δ-function pseudopotential proportional to the scattering length a,

$$\hat{V}=\frac{4\pi\hbar^2}{m}a\,\delta(\mathbf{r})\frac{\partial}{\partial r}r, \tag{1}$$

where m is the atomic mass and r is the interatomic separation [20–22]. An analytic solution for the eigenvalues of two atoms in an isotropic harmonic trap plus the pseudopotential Eq. (1) has been found [23]. However, some of us have previously shown that the use of this solution is limited to sufficiently weak traps such that the trap width is much larger than $|a|$ [19]. Here we reexamine this problem and propose a simple method of calculating the energies in an isotropic harmonic trap, which gives good quantitative results over a wide range of trap frequencies, even when $|a|$ is larger than the trap size. The essence of our model is to replace a with an energy-dependent effective scattering length. An advantage of our model is that once the energy-dependent scattering phase shift for a particular type of cold collision is known, either from experiment or from close-coupling calculations, it can be easily applied to obtain eigenvalues for traps of all frequencies. Conversely, if the eigenvalues are measured, information about collisions can be obtained.

We note that the pseudopotential can be used to obtain approximate solutions for trapped colliding atoms in one dimension [24,12] and two dimensions [25]. It may be possible

to adapt our effective scattering length method to accurately treat scattering in ''cigar-'' or ''pancake-'' shaped traps.

The paper is organized as follows. In Sec. II we formulate the problem of atoms colliding in a tight spherical trap, and briefly review scattering theory. In Sec. III we motivate and explain the effective-scattering-length eigenvalue model, which is our main result. Limitations of the model are discussed. Section IV applies the model to single-channel scattering of ^{23}Na atoms in a trap, and shows good agreement with numerical calculations using the full interaction Hamiltonian. Section V demonstrates similar good agreement for the case of multichannel scattering. Specifically, we consider a magnetically-induced Feshbach resonance in Na_2. We compare, for a range of magnetic fields, exact numerical results from the five-channel close-coupled scattering problem with the model's eigenvalues. Finally, in Sec. VI we draw conclusions and consider more general traps and applications to many-body theory.

II. TWO ATOMS COLLIDING IN AN ISOTROPIC HARMONIC TRAP

We consider an isotropic harmonic trap described for atom $j=1,2$ at position $\mathbf{r}_j$ by

$$V_{\rm trap}(\mathbf{r}_j)=\frac{1}{2}m\omega^2 r_j^2, \tag{2}$$

where ω is the trapping frequency. Harmonic traps can be made by a variety of means. Very tight confinement is possible with a three-dimensional optical lattice. Typical experimental trap frequencies range from 50 kHz to 1 MHz. These optical dipole traps are much tighter than those obtained with magnetic fields. In a recent experiment [10], isotropic potentials at each site were produced from three optical standing waves of equal intensity.

For the isotropic harmonic trap, the two-atom Hamiltonian is separable in the center-of-mass and relative coordinates. Since the center-of-mass motion is just that of the well-known isotropic harmonic oscillator, we need only discuss the problem in the relative coordinates. The Hamiltonian is

$$H=-\frac{\hbar^2}{2\mu}\nabla^2+\frac{1}{2}\mu\omega^2 r^2+V_{\rm int}(r), \tag{3}$$

where $r=|\mathbf{r}_1-\mathbf{r}_2|$, $\mu=m/2$ is the reduced mass, and $V_{\rm int}(r)$ is the interatomic potential. In (relative) spherical coordinates, the trap states neglecting $V_{\rm int}(r)$ have energy eigenvalues

$$E_n^{(0)}=\left(2n+L+\frac{3}{2}\right)\hbar\omega, \tag{4}$$

where $n=0,1,2,\ldots$ is the radial quantum number and $L=0,1,2,\ldots$ is the partial-wave quantum number. We henceforth consider only s waves ($L=0$). The size of the ground-state trap wave function is characterized by

$$l=\sqrt{\frac{\hbar}{\mu\omega}}. \tag{5}$$

Typical trap sizes l for Na in the above mentioned trap frequency range are 30 nm to 130 nm.

The interatomic potential $V_{\rm int}(r)$ is characterized by a short-range region of strong chemical bonding and a long-range van der Waals potential,

$$V_{\rm int}\to -C_6/r^6, \tag{6}$$

and leads to a van der Waals scale length [26,4,27]

$$x_0=\frac{1}{2}\left(\frac{2\mu C_6}{\hbar^2}\right)^{1/4}. \tag{7}$$

For $r\ll x_0$ the scattering wave function oscillates rapidly due to the strong-interaction potential. In alkali ground-state interactions, C_6 is the same for all hyperfine states of a given atomic pair; consequently, x_0 is the same for all collision channels. In the case of Na_2 considered below, it is about 2.4 nm.

For collisions of atoms in the absence of a trapping potential, the asymptotic s-wave scattering wave function for relative collision momentum $\hbar k$ approaches

$$\psi\to\frac{\sin(kr+\delta_0)}{\sqrt{k}r} \tag{8}$$

at large interatomic separation $r\gg x_0$. Another length scale that naturally appears for cold collisions is the scattering length, defined in terms of the s-wave phase shift δ_0 by

$$a=-\lim_{k\to 0}\frac{\tan\delta_0(k)}{k}. \tag{9}$$

The Wigner law regime is then defined by the range of momenta for which $\delta_0=-ka$ is a good approximation, i.e.,

$$k\ll\frac{\pi}{2|a|}. \tag{10}$$

The scattering length can take on any value between $+\infty$ and $-\infty$. As $|a|$ becomes large, the range of k for which the Wigner law applies becomes very small.

In view of typical trap sizes and van der Waals length scales, we need only consider the experimentally accessible regime, for which

$$x_0\ll l. \tag{11}$$

On the other hand, the scattering length can have a larger magnitude than the trap width l. This is especially likely if the scattering length is modified by means of a Feshbach resonance.

Our goal is to find a simple model for calculating the new energy eigenvalues of the trap when collisions are present. An analytical solution of this problem was presented in Ref. [23] by replacing $V_{\rm int}$ by the pseudopotential of Eq. (1). This

replacement assumes that the Wigner law is valid. However, we previously showed that the eigenvalues thus obtained are not always in agreement with numerical results [19]! Specifically, they are least accurate when $|a|$ approaches or exceeds l. One way to see this is that the energies of the unperturbed trap states are already large enough that the Wigner threshold law is invalid. For the unperturbed trap ground state $E=3\hbar\omega/2$ and hence the root-mean-square momentum $k=\sqrt{3}/l$. Therefore by Eq. (10) we are outside of the Wigner regime if $|a|>\pi/(2\sqrt{3})l$.

In the following section we will use the inequality Eq. (11) to motivate an effective-scattering-length model of cold collisions in the trap, that is valid at all relevant energies and scattering lengths.

III. SELF-CONSISTENT ENERGIES FROM THE EFFECTIVE SCATTERING LENGTH

The improved model we propose relies on a generalization of the pseudopotential approximation for $V_{\rm int}$ in Eq. (1). We introduce the energy-dependent pseudopotential operator [20]

$$\hat{V}_{\rm eff}=\frac{4\pi\hbar^2}{m}a_{\rm eff}(E)\,\delta(\mathbf{r})\,\frac{\partial}{\partial r}r, \tag{12}$$

where the *effective* scattering length is defined as

$$a_{\rm eff}(E)=-\frac{\tan\delta_0(k)}{k} \tag{13}$$

and the kinetic energy is related to the momentum by $E=\hbar^2k^2/2\mu$. This operator gives the same asymptotic wave function Eq. (8) as the full interaction potential $V_{\rm int}$. The effective scattering length reduces to the usual one Eq. (9) in the Wigner threshold regime. The phase shift in Eq. (13) does not need to be small in order to use Eq. (12). Even though the effective scattering length diverges when δ_0 is an odd multiple of $\pi/2$, the wave function remains well behaved.

Reference [23] found the eigenvalues of the trapped atoms interacting through the operator in Eq. (1) as the solutions of the equation,

$$\frac{a}{l}=f(E), \tag{14}$$

where the ''intercept function'' is

$$f(E)=\frac{1}{2}\tan\left(\frac{\pi E}{2\hbar\omega}+\frac{\pi}{4}\right)\frac{\Gamma\left(\frac{E}{2\hbar\omega}+\frac{1}{4}\right)}{\Gamma\left(\frac{E}{2\hbar\omega}+\frac{3}{4}\right)} \tag{15}$$

and Γ is the gamma function. To account properly for the scattering in tight traps, where the Wigner law may not apply at the trap energies, we need to replace Eq. (14) by one in which the left-hand side is energy dependent and solve the equation

$$\frac{a_{\rm eff}(E)}{l}=f(E) \tag{16}$$

self-consistently for the eigenvalues. (The term ''self-consistent'' here refers to the energy eigenvalue on both sides of the above equation, and should not be confused with its meaning in the context of Hartree-Fock approximations.)

One might ask, why does the idea of the pseudopotential still work outside the regime of the Wigner law? The answer is that the collision occurs on the very short length scale x_0, so the interatomic interaction potential is undistorted by the trap. This in turn means that the kinetic energy at which the effective scattering length needs to be evaluated is the eigenvalue itself, since the trap potential is negligible for $r<x_0$. Thus we were led to the self-consistent energy Eq. (16).

For sufficiently high trap levels, one can also understand Eq. (16) from a semiclassical perspective. The ratio of gamma functions asymptotically approaches $2/kl$ for $E\gg\hbar\omega$, and using the definition of effective scattering length Eq. (13), we can express the self-consistency condition as

$$\phi_{WKB}(E)=\pi(n+1)-\delta_0(E), \tag{17}$$

where as before $n=0,1,2,\ldots$ and

$$\phi_{WKB}(E)=\frac{\pi E}{2\hbar\omega}+\frac{\pi}{4}. \tag{18}$$

We may interpret Eq. (17) as the quantization of the Wentzel-Kramers-Brillioun phase of the wave function at the classical outer turning point, but the quantum defect $\delta_0(E)$ must first be subtracted to take into account the scattering at short distance.

Our model can be expected to break down if the trap becomes too tight. The interatomic potential $V_{\rm int}$ becomes comparable to the trap potential near $r=\sqrt{lx_0}$. Hence the inner part of the wave function where the scattering occurs is nearly the same as that without the trap when $x_0\lesssim\sqrt{lx_0}$, equivalent to Eq. (11). A different kind of limitation is that this model cannot predict bound states without our knowing the analytical continuation of the effective scattering length to negative energies.

IV. SINGLE-CHANNEL SCATTERING

The first problem we consider is that of doubly polarized (electron and nuclear spin up) ^{23}Na atoms colliding in the trap. In this case, there is only one scattering channel, governed by the $a^3\Sigma_u^+$ adiabatic Born-Oppenheimer potential. The scattering length is $a=3.4$ nm, and Figs. 1 and 2 show the effective scattering length as a function of energy. It increases with energy and diverges near $E/h=90$ MHz where $\delta_0=\pi/2$ (this corresponds to a local maximum of the s-wave cross section), and is negative immediately above this energy. In this work both the single- and multichannel phase shifts are calculated by applying the Gordon propagation method [28] with the best available scattering potentials for Na_2 [29].

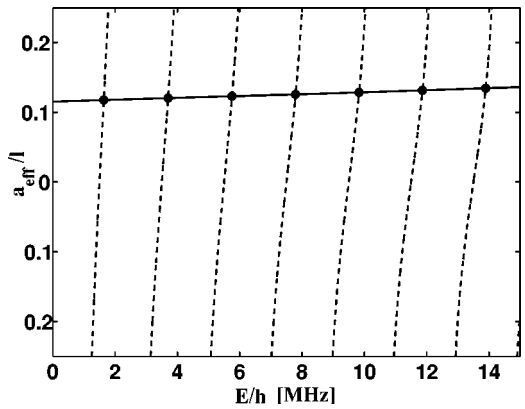

FIG. 1. Effective scattering length (solid curve) and intercept function $f(E)$ (dashed) versus energy for doubly polarized ^{23}Na in a 1 MHz trap. The energies at which the two curves intersect give the model eigenvalues. The circles show the actual positions of the exact numerical eigenvalues along the curve of the intercept function.

The radial Schrödinger equation for the Hamiltonian Eq. (3) was solved numerically for the eigenvalues. For a detailed description of our numerical method using a discrete variable representation, see Ref. [30]. We take a trap frequency of $\omega/2\pi=1$ MHz, for which $l=29.6$ nm and $\hbar\omega/k_B=48$ μK (k_B is the Boltzmann constant). Such a tight trap should be feasible in a Na optical lattice.

We illustrate the graphical solution of the effective-scattering-length model in Figs. 1 and 2. In each plot, the solid curve represents the left-hand side of Eq. (16), $a_{\rm eff}/l$, while the dashed curve is the right-hand side. The abscissae of the points where the curves intersect give the eigenvalues according to the model. One way of comparing with the exact numerical eigenvalues is to evaluate the intercept function $f(E)$ at these eigenvalues; these points are plotted as circles. The closer the circles lie to the intersection of the curves, the better the agreement. The exact numerical and model eigenvalues in Fig. 1 agree to better than $0.0016\hbar\omega$. Note that the solution of Eq. (14) is found from the intersection of $f(E)$ and the horizontal line a/l; the corresponding

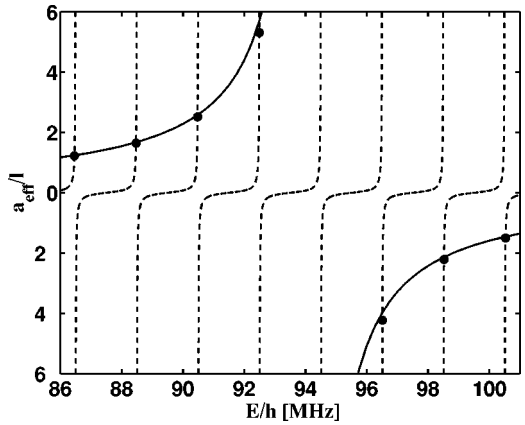

FIG. 2. Same as Fig. 1 but at a higher-energy range. Note that the effective scattering length diverges, but the model eigenvalues still agree with the exact numerical eigenvalues.

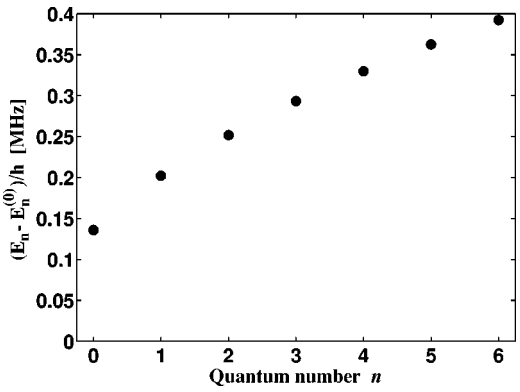

FIG. 3. Difference between eigenvalues for interacting and non-interacting, doubly polarized Na atoms in a 1 MHz trap versus quantum number n. The model and exact numerical eigenvalues are indistinguishable on the scale of this figure.

eigenvalues differ significantly from both the exact ones and the effective-scattering-length model.

The range of energies in Fig. 2 is centered near the energy at which $a_{\rm eff}/l$ diverges. Even though $|a_{\rm eff}|\gg l$, the model eigenvalues are still accurate. They agree with the exact ones to within $0.0018\hbar\omega$. Clearly this validates our model. We have also obtained eigenvalues for much higher trap frequencies, at which distortion of the collision potential is expected to cause our model to fail. At a trapping frequency 100 MHz, where $l=2.96$ nm$\approx x_0$, the error between the exact eigenvalues and those obtained from our model has increased to $0.045\hbar\omega$. The crucial interaction length scale for comparison to the trap size l is x_0, not the effective scattering length $a_{\rm eff}$.

The difference between the lowest seven eigenvalues and the corresponding harmonic oscillator eigenvalues given by Eq. (4) is plotted in Fig. 3 versus the quantum number n. The shift due to the interactions is a significant fraction of $\hbar\omega$ and should be observable in appropriate experiments. The dependence of the shift on the index for the lowest few eigenvalues is due mainly to the energy dependence of the gamma functions in Eq. (15), and only slightly due to the variation of the effective scattering length with energy. The solution for the eigenvalues in the semiclassical regime of Eq. (17), to first order in the effective scattering length, yields shifts

$$E_n-\left(2n+\frac{3}{2}\right)\hbar\omega=\frac{4}{\pi}\left(n+\frac{3}{4}\right)^{1/2}\frac{a_{\rm eff}}{l}\hbar\omega, \qquad (19)$$

explaining the approximately square-root dependence on quantum number n in the figure. On the other hand, for the higher eigenvalues in Fig. 2, the shifts in eigenvalues arise mostly from the rapid variation of effective scattering length with energy. Near the asymptote $a_{\rm eff}\to\infty$ the eigenvalues have increased by approximately $\hbar\omega$ compared with the unperturbed values.

The above examples show that accurate eigenvalues can be obtained by using results of the single-channel scattering problem (without the trap), and solving Eq. (16). Our model

is good even when the effective scattering length is large compared to the trap width, provided the trap size is still larger than the van der Waals length scale.

V. MULTICHANNEL SCATTERING AND FESHBACH RESONANCE

In the preceding section, large ratios of effective scattering length to trap width were only possible for very high-lying levels. Here we want to discuss a situation where $|a_{\rm eff}|/l$ is arbitrarily large for the lowest trap levels. This can be experimentally realized for *s*-wave collisions using a magnetically-tuned Feshbach resonance.

We consider a Feshbach resonance in the collision of two ^{23}Na atoms in their lowest hyperfine level at a magnetic field near 90 mT [18,31,32]. The hyperfine states of the ^{23}Na atom diagonalize the Zeeman and hyperfine interaction and are labeled by $|a\rangle,|b\rangle,\ldots,|h\rangle$, starting from the lowest internal energy. For very low collision energy, *s*-wave collisions of two $|a\rangle$ atoms are represented by five symmetrized asymptotic collision channels, one of which is open, $|\{aa\}\rangle$, and four of which are closed, $|\{ag\}\rangle$, $|\{bh\}\rangle$, $|\{fh\}\rangle$, and $|\{gg\}\rangle$. The interaction between the atoms is mediated by the $X^1\Sigma_g^+$ and $a^3\Sigma_u^+$ adiabatic Born-Oppenheimer potentials. During the collision this interaction mixes hyperfine states and is described by a Hamiltonian coupling the above five channels [32]. A Feshbach resonance state at energy E_F is located at the threshold of the $|\{aa\}\rangle$ channel for a magnetic field $B_{\rm res}\approx 90.09$ mT. This resonance is a quasibound molecular eigenstate of the four closed channel problem. It can be formed from or decay to the $|\{aa\}\rangle$ open channel, to which it is coupled. As the magnetic field B is changed near $B_{\rm res}$, the resonance energy also varies with B,

$$E_F=\frac{\partial E_F}{\partial B}(B-B_{\rm res}). \tag{20}$$

The analytic theory of Feshbach resonances [33,34] shows that the phase shift δ_0 can be written as the sum of background and resonant scattering contributions,

$$\delta_0=\delta_{\rm bg}-\arctan\frac{\Gamma_F}{2(E-E_F-\Delta_F)}, \tag{21}$$

where Γ_F is the linewidth, Δ_F is a level shift induced by the coupling between the open and closed channels, and $\delta_{\rm bg}$ is the background phase shift. It follows that the effective scattering length Eq. (13) for the $\{aa\}$ channel is

$$a_{\rm eff}(E)=\frac{\frac{\Gamma_F}{2}-(E-E_F-\Delta_F)\tan\delta_{\rm bg}}{k\left(E-E_F-\Delta_F+\frac{\Gamma_F}{2}\tan\delta_{\rm bg}\right)}. \tag{22}$$

Up to the highest energy we will consider, $E/h\approx 5$ MHz, both Γ_F and $\tan\delta_{\rm bg}$ are proportional to $\sqrt{E}$, and Δ_F becomes constant. Moreover, Eq. (22) shows that the effective scattering length diverges near the energy

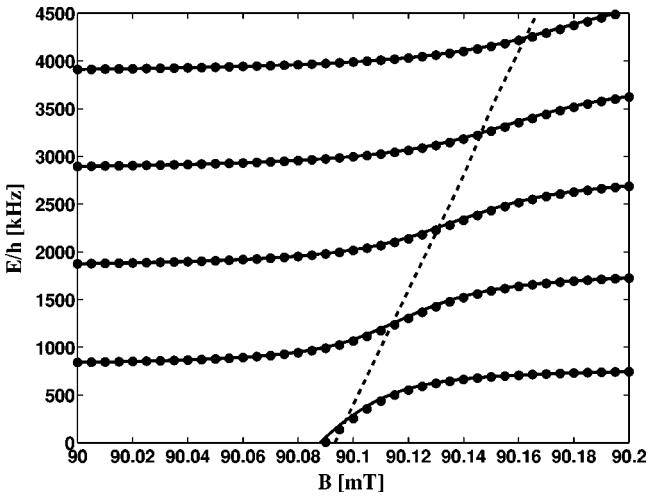

FIG. 4. Numerical (*circles*) and effective-scattering-length model (*solid curve*) eigenvalues versus magnetic field B for Na in a 500 kHz trap. The dashed line shows $E_{\rm div}$, where the effective scattering length diverges at a fixed value of magnetic field.

$$E_{\rm div}=\frac{E_F+\Delta_F}{1+\frac{1}{2}\frac{\partial}{\partial E}(\Gamma_F\tan\delta_{\rm bg})_{E\to 0}}. \tag{23}$$

The effective scattering length is positive below and negative above $E_{\rm div}$, which is magnetically tunable according to Eq. (20). However, instead of employing the analytic theory, at a given value of magnetic field we directly obtain the effective scattering length as a function of E from a numerical close-coupled scattering calculation with five channels. This enables us to extract the position of the divergence $E_{\rm div}$, which is plotted as the dashed curve in the (E,B) plane in Fig. 4.

We now examine the effect of the Feshbach resonance on trap eigenstates, assuming a trap with $\omega/2\pi=500$ kHz. We used the numerical discrete variable method for five channels to calculate the lowest eigenvalues of the trap states for a range of magnetic fields near the resonance. These eigenvalues are plotted as circles in Fig. 4. Solutions to the model eigenvalues were obtained by solving Eq. (16) graphically as in the single-channel case; the solutions versus magnetic field are the solid curves. The eigenvalues agree well with the numerical ones for all values of energy and magnetic field; the worst agreement, $<0.1\hbar\omega$, is for eigenvalues near the resonance position. The model eigenvalues always lie slightly above the numerical ones. Note that the model eigenvalues cross the $E_{\rm div}$ curve near $E/\hbar\omega=1/2,5/2,9/2\ldots$ Another particular feature of the plot, which is correctly reproduced by the model solution, is that as B decreases the lowest trap state $(E>0)$ becomes the highest bound state $(E<0)$ for a magnetic field $B<B_{\rm res}$. This occurs where the effective scattering length is still finite and positive, since $a_{\rm eff}/l\approx 1.48$ when $E=0$ in Eqs. (15) and (16).

VI. CONCLUSION

We have shown how a simple model can be used to calculate the eigenvalues of interacting atoms in an isotropic

harmonic trap. Our model involves solving an equation containing the effective scattering length for untrapped atoms, and the trap frequency. We compared our model with exact results for ^{23}Na both for a single-channel collision and a multichannel collision with a tunable Feshbach resonance. In both cases, the model can accurately treat tight traps, as long as the trap size is larger than the van der Waals scale length. Consequently we expect the model to apply to other atomic species. In particular, Cs would be an interesting case for which the scattering length is large in comparison with even modest trap sizes [35].

In the future, we want to generalize our model to more arbitrary trap potentials. There are two technical problems to be overcome. First, for atomic collisions in anisotropic harmonic traps, the relative coordinate equation does not separate; this implies that different partial waves are coupled via the anisotropy. A related point is that the scattering of higher partial waves can also be modeled by pseudopotentials [20]. Second, for anharmonic traps, the center-of-mass and relative atomic coordinates do not separate, and even more coordinates must be treated simultaneously. Anharmonic terms become important for low intensity optical lattices or for trap levels with many quanta of excitation.

One would expect to be able to use the effective scattering length in many-body problems, where the pseudopotential approximation has had widespread use. One would simply need to replace a by the effective scattering length. This should be especially useful and necessary for situations where a tunable Feshbach resonance is used to alter the interaction properties. There are a number of cases where the relative collision energy for a many-body system is well-defined, such as for condensates in optical lattices [10], colliding condensates [36,37], or cold gases of mixed fermionic species, where collisions occur at the Fermi energy. It should also be possible to incorporate inelastic collision loss channels by using a complex effective scattering length [36].

After completing this paper, we learned of a recent theoretical work [38] that has also treated the problem of two trapped atoms interacting through single-channel s-wave scattering. It introduces an energy-dependent pseudopotential and comes to similar conclusions.

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