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, threshold scattering properties have been studied, molecules formed with the assistance of light, and quantum phase transitions 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. have observed a quantum phase transition from a superfluid to a Mott insulator within a three-dimensional optical lattice. Moreover, several low-dimensional phase transitions of cold bosonic systems have been conjectured. In two dimensions, the Kosterlitz-Thouless transition may occur, while in one dimension the Tonks-Girardeau phase should be possible. Zero-temperature transitions have also been investigated theoretically for a rotating two dimensional gas. 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. 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 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 ultra-cold atoms. This has improved the knowledge of interaction parameters of alkali atoms and opened up the field of molecular condensates and 3-body processes. By tuning Feshbach resonances one can easily reach an interesting regime where the scale length associated with the scattered wave exceeds the trap width.

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 delta-function pseudopotential proportional to the scattering length. An analytic solution for the eigenvalues of two interacting atoms in an isotropic harmonic trap plus the pseudopotential Eq. has been found. 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 the scattering length. The essence of our model is to replace 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 [21] and two dimensions [22]. It may be possible to adapt our self-consistent 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 self-consistent eigenvalue model, which is our main result. Limitations of the model are discussed. Section IV applies the model to single-channel scattering of one dimension [21,11] and two dimensions [22]. It may be made by a variety of means. Very tight confinement is possible with a three-dimensional optical lattice. Typical trap sizes for Na in the above mentioned trap frequency range are 30 nm to 130 nm.

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

\[
V_{\text{int}} \rightarrow -C_6/r^6,
\]

and leads to a van der Waals scale length,

\[
x_0 = \frac{1}{2} \left( \frac{2\mu C_6}{\hbar^2} \right)^{1/4}.
\]

For \( r \ll x_0 \) the scattering wavefunction 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 wavefunction for relative collision momentum \( \hbar k \) approaches

\[
\psi \rightarrow \frac{\sin(kr + \delta_0)}{\sqrt{kr}} \quad (8)
\]

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 \( \delta_0 \) by

\[
a = -\lim_{k \to 0} \frac{\tan \delta_0(k)}{k}. \quad (9)
\]

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

\[
k \ll \frac{\pi}{2|a|}. \quad (10)
\]

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
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. [1] by replacing $V_{\text{int}}$ 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 [14]! 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. (11) we are outside of the Wigner regime if $|a| > \pi/(2\sqrt{3})/l$.

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

### III. SELF-CONSISTENT MODEL

The improved model we propose relies on a generalization of the pseudopotential approximation for $V_{\text{int}}$ in Eq. (1). We introduce the energy-dependent pseudopotential operator [23]

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

(12)

where the **effective** scattering length is defined as

$$a_{\text{eff}}(E) = \frac{\tan \delta_0(k)}{k},$$

(13)

and the kinetic energy is related to the momentum by $E = \hbar^2 k^2/2\mu$. This operator gives the same asymptotic wavefunction, Eq. (8), as the full interaction potential $V_{\text{int}}$. The effective scattering length reduces to the usual one, Eq. (7), in the Wigner threshold regime. The phase shift in Eq. (13) does not need to be small in order to use Eq. (14). Even though the effective scattering length diverges when $\delta_0$ is an odd multiple of $\pi/2$, the wavefunction remains well-behaved.

Reference [20] found the eigenvalues of the trapped atoms interacting through the operator in Eq. (11) as the solutions of the equation,

$$\frac{a}{\Gamma} = f(E),$$

(14)

where the “intercept function” is

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

(15)

and $\Gamma$ 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

$$\frac{a_{\text{eff}}(E)}{l} = f(E)$$

(16)

self-consistently for the eigenvalues.

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 Eq. (16).

This model can be expected to break down if the trap becomes too tight. The interatomic potential $V_{\text{int}}$ becomes comparable to the trap potential near $r = \sqrt{lx_0}$. Hence the inner part of the wavefunction 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) $^{23}\text{Na}$ 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 $a = 3.2$ nm, and Figs. 3 and 4 show the effective scattering length as a function of energy. It increases with energy and diverges near $E/\hbar = 90$ 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 multi-channel phase shifts are calculated by applying the Gordon propagation method [20] with the best available scattering potentials for $\text{Na}_2$ [27].

The radial Schrödinger equation for the Hamiltonian Eq. (4) was solved numerically for the eigenvalues. For a detailed description of our numerical method using a discrete variable representation, see Ref. [28]. We take a trap frequency of $\omega/2\pi = 1$ MHz, for which $l = 29.6$ nm and $\hbar\omega/k_B = 48$ $\mu$K ($k_B$ is the Boltzmann constant). Such a tight trap should be feasible in a Na optical lattice.

We illustrate the graphical solution of the self-consistent model in Figs. 3 and 4. In each plot, the solid
curve represents the left hand side of Eq. (16), $a_{\text{eff}}/l$, while the dashed curve is the right hand side. The abscissae of the points where the curves intersect give the self-consistent 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 $E = a/l$; the corresponding eigenvalues differ significantly from both the exact and self-consistent ones.

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

The range of energies in Fig. 1 is centered near the energy at which $a_{\text{eff}}/l$ diverges. Even though $|a_{\text{eff}}| \gg l$, the self-consistent 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 the self-consistent 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 $a_{\text{eff}}$.

The difference between the lowest seven eigenvalues and the corresponding harmonic oscillator eigenvalues given by Eq. (4) is plotted in Fig. 2 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. On the other hand, for the higher eigenvalues in Fig. 3 the shifts in eigenvalues arise mostly from the rapid variation of effective scattering length with energy. Near the asymptote $a_{\text{eff}} \rightarrow \infty$ 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 the self-consistent Eq. (16). Our self-consistent 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.

![FIG. 2. Same as Fig. 1 but at a higher energy range. Note that the effective scattering length diverges, but the self-consistent eigenvalues still agree with the exact numerical eigenvalues.](image)

V. MULTI-CHANNEL SCATTERING AND FESHBACH RESONANCE

In the previous 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 $|a_{\text{eff}}|/l$ is arbitrarily large for the lowest trap levels. This can be experimentally realized for $s$-wave collisions using a magnetically-tuned Feshbach resonance.
near which it is coupled. As the magnetic field is located at a Feshbach resonance state at energy $E_F$, the resonance energy also varies with $|\{aa\}$, where $\Gamma_F$ is the linewidth, $\Delta_F$ is a level shift induced by the coupling between the open and closed channels, and $\delta_{bg}$ is the background phase shift. It follows that the effective scattering length Eq. (13) for the $|\{aa\}$ channel is

$$a_{\text{eff}}(E) = \frac{\Gamma_F}{k} \frac{E_E - (E - E_F - \Delta_F) \tan \delta_{bg}}{E - E_F - \Delta_F + \frac{\Gamma_F}{2} \tan \delta_{bg}}. \quad (19)$$

Up to the highest energy we will consider, $E/h \approx 5$ MHz, both $\Gamma_F$ and $\tan \delta_{bg}$ are proportional to $\sqrt{E}$, and $\Delta_F$ becomes constant. Moreover, Eq. (19) shows that the effective scattering length diverges near the energy

$$E_{\text{div}} = \frac{E_F + \Delta_F}{1 + \frac{1}{2} \frac{\partial^2}{\partial E^2} (\Gamma_F \tan \delta_{bg})_{E \rightarrow 0}}, \quad (20)$$

The effective scattering length is positive below and negative above $E_{\text{div}}$, which is magnetically tunable according to Eq. (17). 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 $E_{\text{div}}$, which is plotted as the dashed curve in the $(E, B)$ plane in Fig. 4.

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

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 [7,29,38]. 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 $^3\Sigma_g^+$ and $^3\Sigma_u^+$ adiabatic Born-Oppenheimer potentials. During the collision this interaction mixes hyperfine states and is described by a Hamiltonian coupling the above five channels [38]. A Feshbach resonance state at energy $E_F$ is located at the threshold of the $|\{aa\}\rangle$ channel for a magnetic field $B_{\text{res}} \approx 90.09$ 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 $B_{\text{res}}$, the resonance energy also varies with $B$:

$$E_F = \frac{\partial E_F}{\partial B} (B - B_{\text{res}}). \quad (17)$$

The analytic theory of Feshbach resonances [18,31] shows that the phase shift $\delta_0$ can be written as the sum of background and resonant scattering contributions:

$$\delta_0 = \delta_{bg} - \arctan \frac{\Gamma_F}{2(E - E_F - \Delta_F)}. \quad (18)$$

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

$$a_{\text{eff}}(E) = \frac{\Gamma_F}{k} \frac{E_E - (E - E_F - \Delta_F) \tan \delta_{bg}}{E - E_F - \Delta_F + \frac{\Gamma_F}{2} \tan \delta_{bg}}. \quad (19)$$

Up to the highest energy we will consider, $E/h \approx 5$ MHz, both $\Gamma_F$ and $\tan \delta_{bg}$ are proportional to $\sqrt{E}$, and $\Delta_F$ becomes constant. Moreover, Eq. (19) shows that the effective scattering length diverges near the energy

$$E_{\text{div}} = \frac{E_F + \Delta_F}{1 + \frac{1}{2} \frac{\partial^2}{\partial E^2} (\Gamma_F \tan \delta_{bg})_{E \rightarrow 0}}, \quad (20)$$

The effective scattering length is positive below and negative above $E_{\text{div}}$, which is magnetically tunable according to Eq. (17). 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 $E_{\text{div}}$, which is plotted as the dashed curve in the $(E, B)$ plane in Fig. 4.

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

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 self-consistent eigenvalues were obtained by solving Eq. (16) graphically as in the single-channel case; the solutions versus magnetic field are the solid curves. The self-consistent 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 self-consistent eigenvalues always lie slightly above the numerical ones. Note that the self-consistent eigenvalues cross the \( E_{\text{div}} \) curve near \( E/\hbar \omega = 1/2, 5/2, 9/2 \ldots \) Another particular feature of the plot, which is correctly reproduced by the numerical solution, is that as \( B \) decreases the lowest trap state \( (E > 0) \) becomes the highest bound state \( (E < 0) \) for a magnetic field \( B < B_{\text{res}} \). This occurs where the effective scattering length is still finite and positive, since \( a_{\text{eff}}/l \approx 1.48 \) when \( E = 0 \) in Eqs. (15)-(16).

VI. CONCLUSION

We have shown how a self-consistent 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 Na both for a single channel collision and a multi-channel 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

In the future, we want to generalize the self-consistent 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. 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, colliding condensates, 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.

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