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Interacting atoms under strong quantum confinement

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We calculate the energy-level shifts of a tightly confined trapped alkali-metal atom in the presence of a second trapped atom. A complete microscopic description of the interaction energy between the two atoms is used. This allows us to study tightly confined atoms near a Feshbach resonance and to evaluate the usefulness of the regularized δ-function potential approximation. We present results for sodium and cesium when confined in a spherically symmetric harmonic optical trap. Possible implications of the level shifts and collisional decoherence for quantum computing with atomic systems are given.

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I. INTRODUCTION

During the last 15 years the ability to hold and manipulate neutral atoms and ions with lasers has become a mature part of atomic physics. These laser cooling techniques have allowed, for example, the study of weakly bound vibrational levels of molecules formed from two neutral atoms [1], the determination of threshold atomic scattering properties [2,3], the study of neutral atoms in optical lattices [4,5], and the observation of macroscopic quantum phase transitions [6]. Moreover it is possible to confine one or two single Cs atoms in a magneto-optical trap [7] as well as produce near-unit occupancy of the cells in a three-dimensional optical lattice [8]. Atomic collisions play a crucial role in many of the phenomena associated with trapped cold atoms. For example, elastic collisions determine the mean field of a Bose-Einstein condensate, while inelastic collisions provide loss mechanisms, which can remove atoms from a Bose condensate or an optical lattice.

Understanding collisions under tight confinement conditions is especially important in view of the possibility of using collisions of neutral atoms in single cells of optical lattices to implement quantum logic gates [9–11]. First steps toward quantum computing [12] have been made by demonstrating elementary quantum gates via ion traps [13], cavity QED [14], and with nuclear magnetic resonance [15]. Although no experimental work has yet been done on trapped neutral atoms for quantum logic, a simple gate might be made using quantum bits, or qubits, which are formed from a superposition of two or more hyperfine sublevels of a ground-state alkali-metal atom confined in an optical lattice. In a quantum gate operation, two atoms are brought together and allowed to interact for a predetermined time interval. The resulting phase shift gained by the atom pair, which is conditional on the hyperfine sublevels involved, permits the desired quantum gate [9–11].

As the size of atom traps decreases, it becomes necessary to consider the effect of trap confinement on the collisions [16]. This paper therefore examines the interactions of two atoms confined in a spherically symmetric harmonic trap. In a trap interactions manifest themselves as a shift in the quantized energy levels of the two-atom system. We present quantitative calculations of the energy shift for two trapped Na or Cs atoms, taking into account the effects of both the full interaction Hamiltonian of the two atoms and the trapping potential. We compare the energy shifts from these full calculations to those calculated when the full atomic interaction potential is replaced by a regularized δ function:

$$V_{\delta}(\vec{r}) = 4\pi \frac{\hbar^2}{2\mu} a\,\delta(\vec{r})\,\frac{\partial}{\partial r} r, \tag{1}$$

where a is the two-body s-wave scattering length, μ is the reduced mass of the atom pair, and $\delta(\vec{r})$ is the three-dimensional δ function [17,18]. This δ function approximation of the full interaction Hamiltonian is widely and successfully used as a starting point for the derivation of the mean-field energy of weakly interacting Bose particles.

We will show that for scattering lengths a that are small compared to the spatial extent of the lowest harmonic oscillator wave functions the δ-function potential in Eq. (1) provides an excellent approximation for the energy shift. In fact for two interacting particles in a spherically symmetric harmonic trap the effect of the regularized δ-function potential and thus of the full interaction Hamiltonian on the eigenenergies is known analytically [18]. On the other hand, we show that when the scattering length and the spatial extent of the harmonic oscillator wave functions become comparable, the actual energy shifts and those predicted from Eq. (1) can be quite different. This is especially true if a magnetic field is used to tune a through a region where there is a Feshbach resonance.

Using the analytic expressions of the level shift, we also present an estimate of the phase shift associated with a gate operation and derive an estimate of the probability of a destructive ‘‘bad’’ inelastic collision during the time the gate is operating. We will show that the probability of a bad collision during the time the elastic collision phase is built up is independent of trap size and frequency and depends only on a ratio K/a, where K is the inelastic rate constant.

This paper is divided into the following sections. In Sec. II we will set up the problem of two interacting ground-state alkali-metal atoms in the absence of a confining potential. In Sec. III we introduce and give properties of the confining

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spherically symmetric harmonic optical potential. The harmonic nature allows for a separation of center of mass and relative degrees of freedom and the additional constraint of spherical symmetry leads to a separation of radial and angular degrees of freedom.

A simplified model of the interacting ground-state alkali-metal atoms in terms of regularized δ-function interactions is presented in Sec. IV. Section V describes results for two trapped doubly polarized sodium and cesium atoms. The calculations show the marked differences between two limiting cases. For Na the vibrational level spacing of the short-range interaction potential is much larger than that of the trapping potential, while for Cs they can be comparable.

In Sec. VI we present results for two confined Na atoms that are both in their lowest hyperfine state and are in the presence of an external magnetic field B. A Feshbach resonance for two such atoms exists near $B_{res}=91.0$ mT [3,16,19] and has profound effects on the magnetic field dependence of the eigenenergies.

Sections VII and VIII estimate the collisional phase shift for quantum logic gates and the relative effect of ''good'' elastic and ''bad'' inelastic collisions, respectively. The ratio of ''good'' to ''bad'' collisions is favorable if only spin-dipolar relaxation is possible, but unfavorable in the case of spin-exchange collisions, with the exception of the special case of ^{87}Rb atoms [20,21]. We provide conclusions in Sec. IX.

II. HAMILTONIAN

The Hamiltonian structure for two colliding ^2S alkali-metal atoms in the absence of a trapping potential is well known [16,20,22–24]. Here we only mention the most relevant features. In the absence of an external field the hyperfine states of a ^2S ground-state alkali-metal atom are labeled by $|f,m\rangle$, where f is the total atomic angular momentum and m its projection on the z axis in the laboratory frame. In the presence of a magnetic field aligned along this z axis, f is no longer a good quantum number and the hyperfine states are labeled $|a\rangle,|b\rangle, \ldots$ in order of increasing internal energy. Each state $|\alpha\rangle$ has a projection m_α along the z axis. The interaction between the atoms is described by the $X\,^1\Sigma_g^+$ and $a\,^3\Sigma_u^+$ adiabatic Born-Oppenheimer (ABO) potentials. During the collision this interaction mixes hyperfine states $|\alpha\beta\rangle$ where α (β) label states of atom $A(B)$. This leads to a set of coupled Schrödinger equations or a multichannel Hamiltonian for the relative motion with one channel for each allowed state $|\alpha\beta\rangle$. The multichannel Hamiltonian H is conveniently denoted as $H=T+V$, where T is the kinetic energy operator for the relative motion and V is the interaction potential matrix. As the atoms are ultracold and the two ABO potentials are independent of relative mechanical angular momentum ℓ, it is sufficient to assume s-wave or $\ell=0$ scattering between the atoms. The numerical scattering properties we present in the remainder of this paper are calculated using a Gordon propagator [25].

In this paper we are interested in trapping alkali-metal atoms in a specific hyperfine state. The first case is that of doubly polarized Na or Cs atoms. Since the electron and nuclear spin of the atoms are both aligned, the interaction potential between the atoms is given by the $a\,^3\Sigma_u^+$ potential. The doubly polarized collision is not the only collision that is solely described in terms of the $a\,^3\Sigma_u^+$ potential. For example, in Na the $B=0$ collision between a $|f=2,m=2\rangle$ and a $|f=1,m=1\rangle$ atom satisfies the same Hamiltonian.

The second case we will discuss in detail is that of Na atoms in the lowest hyperfine state $|a\rangle$. For finite magnetic fields an accurate description of a collision between two $|a\rangle$ state atoms involves five coupled equations [16]. The corresponding five-channel Hamiltonian depends on both the $X\,^1\Sigma_g^+$ and $a\,^3\Sigma_u^+$ potential. At large internuclear separations only the $|aa\rangle$ state is accessible. The other four channels are asymptotically closed. In general these closed channels can lead to Feshbach resonances [26,16] in $|aa\rangle$ collision properties. In Na a Feshbach resonance is located at the threshold of the $|aa\rangle$ channel for an external magnetic field $B_{res}\approx 91$ mT. Here the four closed channels create a multichannel bound state that is coupled to the $|aa\rangle$ collision channel. The scattering length a for two freely scattering $|a\rangle$ state Na atoms is infinite at the resonance. In this situation the embedded bound state approaches the $|aa\rangle$ threshold from below for increasing magnetic field. This implies a positive a in Eq. (1) for magnetic fields just below the resonant magnetic field and negative a for magnetic fields just above.

III. TRAPPING POTENTIAL

Optical atom trapping potentials are periodic in optical lattices or can be more arbitrarily shaped. Nevertheless the deepest part of the well(s) can be approximated by a harmonic trapping potential. To simplify matters further we assume that each atom is held in a spherically harmonic trapping potential $U_{\text{trap}}(\vec{r}_i)=m\omega^2 r_i^2/2$, where $\vec{r}_i$ is the spatial position of atom $i=1$ or 2, m is the atomic mass, and ω is the trapping frequency. Then the separable Hamiltonian for the center of mass and relative motion of two atoms is

$$\left(-\frac{\hbar^2}{2M}\nabla_R^2+\frac{1}{2}M\omega^2R^2\right)+\left(-\frac{\hbar^2}{2\mu}\nabla_r^2+\frac{1}{2}\mu\omega^2r^2\right), \quad (2)$$

where $\vec{R}=(\vec{r}_1+\vec{r}_2)/2$, $\vec{r}=\vec{r}_2-\vec{r}_1$, $M=2m$ is the total mass and $\mu=m/2$ is the reduced mass. It is implicitly assumed that the trapping potential is the same for all the atomic hyperfine states.

The eigenvalues of Eq. (2) of the noninteracting atoms are well known. In fact after introducing a spherical coordinate system we have $E^{\text{trap}}=E^{\text{trap}}_{N,L}+E^{\text{trap}}_{n,\ell}$, where $E^{\text{trap}}_{N,L}$ is the energy in the center of mass motion, and $E^{\text{trap}}_{n,\ell}$ is the energy in the relative motion. Here L and ℓ are the orbital angular momentum for the center-of-mass and relative motion respectively, and

$$E^{\text{trap}}_{n\ell}=\left(\frac{3}{2}+2n+\ell\right)\hbar\omega, \quad n=0,1,2,\ldots \quad (3)$$

for either the center of mass or the relative motion.

For composite bosons the total wave function, which includes both (internal) spin as well as external degrees of freedom, must be symmetric under interchange of the atoms and this reduces the number of allowed orbital angular momenta for the *relative* motion. For two doubly polarized Na or Cs atoms and for $|a\rangle$ state Na atoms only even ℓ are present. Since the interaction between two atoms only depends on the relative coordinate, only the spectrum for the relative motion can be modified by this interaction. The remainder of this paper focuses on solving for the eigenpairs of the relative motion and emphasizes $\ell=0$ because of the ultracold energy assumed.

For convenience we introduce a scale length based on the trapping potential, which is a measure of the extent of the lowest harmonic oscillator wave functions

$$d=\sqrt{\frac{\hbar}{\mu\omega}}. \tag{4}$$

Hence the outer turning point of the lowest harmonic oscillator state, which is defined as $\mu\omega^2r^2/2=E^{\mathrm{trap}}_{00}$, is $\sqrt{3}d$. For optical lattices current experimentally accessible trapping frequencies $\nu=\omega/2\pi$ range from 50 kHz to 1 MHz for sodium and 10 kHz to 1 MHz for cesium. This corresponds to a d ranging from 150 nm to 10 nm for both atomic species. This should be compared to typical magnetic traps used for Bose condensed alkali-metal gases where trapping frequencies ν are on the order of 100 Hz corresponding to trap sizes of 1 μm.

IV. PSEUDOPOTENTIAL APPROXIMATION

The low-energy scattering properties of two colliding atoms can be represented quantitatively by replacing the exact interaction potential $V(r)$ with a pseudopotential, which reproduces the s-wave ($\ell=0$) scattering length and cross section of two freely scattering ultracold atoms. This pseudopotential is given by

$$V_{\delta}(\vec{r})=4\pi\frac{\hbar^2}{2\mu}a\,\delta(\vec{r})\frac{\partial}{\partial r}r, \tag{5}$$

where a is a scattering length, and $\delta(\vec{r})$ the three-dimensional δ function [17,18]. This pseudopotential has a single bound state with $E^{\delta}<0$ for positive scattering lengths. Many-body theories such as those used in describing atomic Bose condensates [6] replace the exact interaction potential $V(r)$ with such a pseudo potential.

Reference [18] shows that the problem of two atoms in a spherically symmetric harmonic trapping potential interacting via a regularized δ-function potential can be solved analytically. They find that in the limit of large positive and negative scattering length a the bound state energies asymptotically approach $(1/2+2v)\hbar\omega$ for $v=0,1,2,\ldots$. Moreover, the eigenenergies are solely a function of the ratio a/d and $\hbar\omega$. To first order in $a/d\propto\sqrt{\omega}$ the bound states for s wave are

$$E^{\delta}_{v,\ell=0}\approx\left\{\frac{3}{2}+2v+\frac{2}{\sqrt{\pi}}\binom{v+1/2}{v}\frac{a}{d}\right\}\hbar\omega, \tag{6}$$

where ( ) is a combinatorial and $v=0,1,2,\ldots$. For $v=0$ and 1 this simplifies to $[3/2+(2/\sqrt{\pi})a/d]\hbar\omega$ and $[7/2+(3/\sqrt{\pi})a/d]\hbar\omega$, respectively.

The three-dimensional eigenfunctions $\Psi(\vec{r})$ for the regularized δ-function potential are singular at zero internuclear separation. In fact, they behave as $C(1-a/r)$ for $r\to0$ and hence the radial wave function $\chi(\vec{r})=r\Psi(\vec{r})\to C(r-a)$ for $r\to0$. Here C is a normalization constant. In essence the radial wave function is finite at $r=0$. For zero scattering length $\chi(r)$ naturally reduces to a radial harmonic oscillator wave function.

V. DOUBLY POLARIZED ALKALI-METAL ATOMS

The exact *radial* Schrödinger equation for the s-wave scattering of two trapped doubly polarized Na or Cs atoms is

$$\left(-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}+V(r)+\frac{1}{2}\mu\omega^2r^2\right)\chi(r)=E^{\mathrm{exact}}_{v,\ell=0}\chi(r), \tag{7}$$

where the single-channel potential V is equal to the $a\,{}^3\Sigma_u$ ABO potential of Na_2 and Cs_2, respectively, and defined such that $V(r)\to0$ when $r\to\infty$. In this case the radial wave-function $\chi(r)$ is always regular at the origin. We numerically solve Eq. (7) for bound states by using a discrete variable representation (DVR) [27] for the kinetic energy operator and potentials. In a DVR the potential is diagonal in r while the kinetic energy operator introduces coupling between all spatial grid points r. The corresponding eigenvalue problem is solved using standard diagonalization software.

Figure 1 shows the first two positive eigenenergies for doubly polarized sodium as a function of trapping frequency using the best known $\mathrm{Na}_2\,a\,{}^3\Sigma^+_u$ potential [28] which has a scattering length of $+3.3$ nm. The energies are in units of $h\nu=\hbar\omega$. Also shown are the eigenenergies of the δ function pseudopotential with $a=+3.3$ nm. The pseudopotential eigenenergies are in good to excellent agreement with the exact calculations. Notice that the ratio $a/d=0.36$ for a trapping frequency ν of 10 MHz.

Figure 2 shows the first two positive eigenenergies for doubly polarized cesium as a function of trapping frequency based on a $a\,{}^3\Sigma^+_u$ potential with a scattering length of -37 nm [29]. For very small trapping frequencies the corresponding δ function pseudopotential agrees with the exact calculations. However, for $\nu\gtrsim50$ kHz the pseudopotential does not agree with the exact calculation. The ratio $a/d=1$ for a trapping frequency of 100 kHz.

The difference in the applicability of the pseudopotential approximation for Na and Cs can be understood in terms of the range of validity of the Wigner threshold law. For two free particles the elastic cross section is given in terms of a scattering length only in the Wigner threshold regime, which extends up to wave vectors k, such that $k|a|\ll1$ or alternatively for collision energies, $E=\hbar^2k^2/(2\mu)\ll E_W$

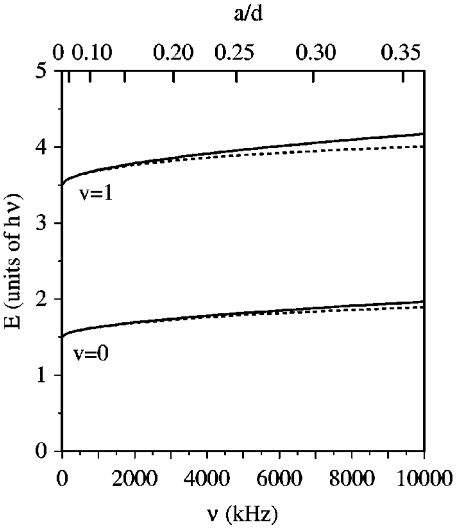

FIG. 1. The energy in the relative motion of two trapped interacting doubly polarized Na atoms as a function of trapping frequency $\nu=\omega/2\pi$. The figure shows the first two so-called trapped states. The full lines correspond to energies obtained from exact numerical calculations. The dotted lines correspond to solutions for a regularized δ-function interaction potential with $a=+3.3$ nm plus a trapping potential. The top axis shows the ratio a/d with $d=\sqrt{\hbar/\mu\omega}$.

$=\hbar^2/(2\mu a^2)$. However for a confined system the energy that determines this validity is the zero-point energy of the trapping potential. Consequently, the effect of the exact interaction potential on the lowest positive eigenstates of Eq. (7) can be expressed in terms of a scattering length when $\hbar\omega$ is much smaller than E_W. When this criterion is satisfied the pseudopotential is valid. For $a>0$ an equivalent explanation of the breakdown point of the pseudopotential approximation follows from an analysis of the binding energy of the last bound state of $V(r)$. This binding energy is approximately equal to $-\hbar^2/(2\mu a^2)$ and as long as this energy remains large compared to the zero-point energy of the trap, the Wigner threshold law criterion holds.

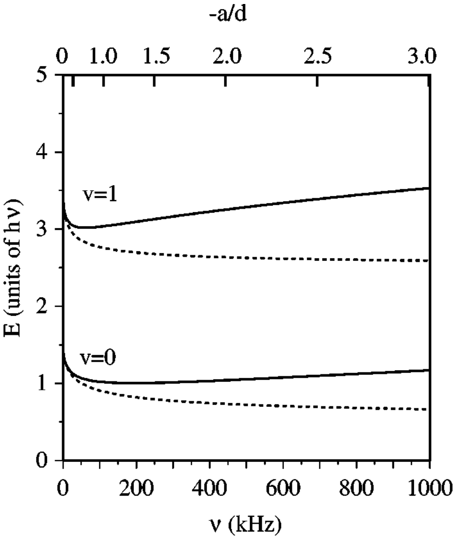

FIG. 2. The energy in the relative motion of two trapped interacting doubly polarized Cs atoms as a function of trapping frequency $\nu=\omega/2\pi$. The figure shows the first two so-called trapped states. The full lines correspond to energies obtained from exact numerical calculations. The dotted lines correspond to solutions for a regularized δ function interaction potential with $a=-37$ nm plus a trapping potential. The top axis shows the ratio $-a/d$ with $d=\sqrt{\hbar/\mu\omega}$.

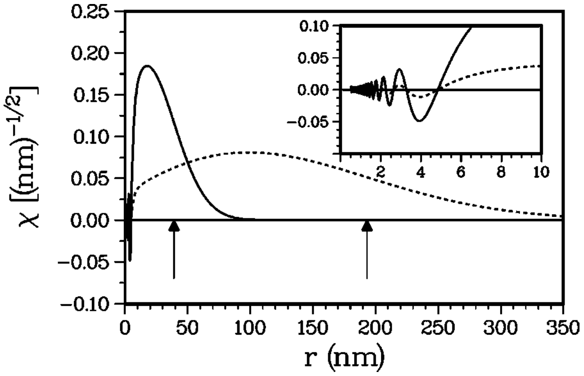

FIG. 3. The $v=0$ wave function for the relative motion of two trapped doubly polarized Cs atoms as a function of internuclear separation. The inset shows a blowup of the short-range internuclear separations. The full line corresponds to a spherical harmonic trap with $\nu=\omega/2\pi=200$ kHz, while the dotted line corresponds to a harmonic trap with a frequency of 10 kHz. The two cases describe a strongly and weakly confining trap, respectively. Here the scattering length of the interaction potential for doubly polarized Cs atoms is -37 nm. The arrows indicate the outer turning point of the eigenstates.

In other words the pseudopotential approximation is valid when $E_W/E^{\text{exact}}_{v,l=0}\approx E_W/(\hbar\omega)\gg 1$ and thus is equivalent to $2a^2/d^2\ll 1$ in terms of length scales in the problem. The scattering length of sodium is small compared to the size of the trap such that $a/d<0.36$ for frequencies up to 10 MHz. However for cesium, $|a/d|>1$ for $\nu>100$ kHz. Notice that whenever the eigenenergies of the δ-function potential are in agreement with the exact eigenenergies, these energies are given by the first-order expression of Eq. (6).

Figure 3 shows the Cs dimer radial wave function of the lowest positive-energy eigenstate for trapping frequencies of $\nu=10$ kHz and 200 kHz. The inset depicts the wave functions for small internuclear separations. For the smaller trapping frequency $|a/d|=0.30<1$ and the pseudopotential approximation for the eigenenergies is valid, while for the other trapping frequency $|a/d|=1.3$ and the approximation is incorrect.

The shape of the radial wave functions in Fig. 3 can be explained from the shape of the harmonic oscillator, regularized δ-function potential and freely scattering wave functions. The *nodeless* radial $n=0$, $\ell=0$ harmonic oscillator wave function has outer turning points of 210 nm and 50 nm for $\nu=10$ kHz and 200 kHz, respectively. These outer turning points compare well with the outer turning points of the exact wave functions as indicated by the arrows in Fig. 3. However, at small internuclear separation the exact wave functions are dramatically modified by the interaction poten-

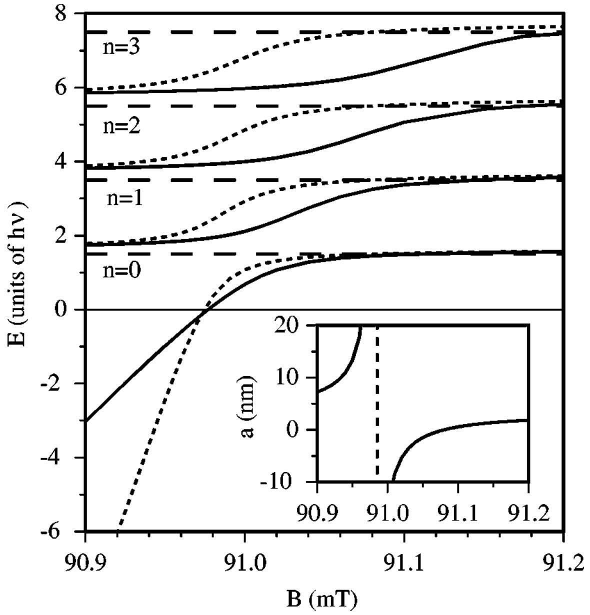

FIG. 4. The energy in the relative motion of two trapped interacting Na atoms in their lowest $|a\rangle$ hyperfine states as a function of magnetic field. The trapping frequency $\nu=\omega/2\pi$ is 1 MHz. The full lines correspond to energies obtained from exact numerical calculations. The dotted lines correspond to eigenenergies for trapped Na atoms interacting via a regularized δ-function potential with a magnetic field dependent scattering length given by the inset. This inset shows the exact scattering length for two freely scattering $|a\rangle$ states near a Feshbach resonance. The scattering length is infinite at 90.985 mT and zero at 91.08 mT. The long-dashed lines correspond to energies of the $l=0$, $n=0,1,2$, and 3 harmonic oscillator states.

tial. The wave functions have 56 nodes, which equals the number of bound states of the $a\,^3\Sigma_u$ potential. In fact inside 10 nm the interaction potential is much stronger than the trapping potential and the shape of the wave function is nearly identical to the free scattering wave function at zero collision energy.

The nodeless $v=0$, $\ell=0$ wave function χ of the regularized δ-function potential has a nonvanishing value at $r=0$. Remnants of this behavior can be observed in the exact radial wave function for the weak 10-kHz harmonic trap by noting the nearly linear $C(r-a)$ fit between 10 nm and 70 nm. In other words, the exact wave function seems to extrapolate to a node at $r=-a$, in the same way that the pseudopotential wave functions extrapolate to $r=-a$. On the other hand, for the exact wave function for $\nu=200$ kHz no $r-a$ behavior can be distinguished, since the δ-function approximation has failed.

VI. TRAPPING NEAR A Na FESHBACH RESONANCE

The *s*-wave Hamiltonian for two interacting sodium atoms in their $|a\rangle$ hyperfine state involves five coupled channels (see Sec. II). A Feshbach resonance occurs at $B=91.0$ mT where the $|aa\rangle$ scattering length near the resonance is presented in the inset of Fig. 4. This scattering length is parametrized by [3,16,19]

$$a=a_{bg}\left(1+\frac{\Delta_{bg}}{B-B_{res}}\right) \tag{8}$$

with $B_{res}=90.98$ mT, $\Delta_{bg}=0.10$ mT, and $a_{bg}=3.38$ nm.

Confining two $|a\rangle$ state atoms in a spherically harmonic potential leads to a multichannel eigenvalue problem. Numerically the five coupled Schrödinger equations are discretized using a DVR. Although the size of the resulting eigenvalue problem is five times larger than that encountered in Sec. V, it remains sufficiently small that iterative eigenvalue solvers are not needed.

Figure 4 shows the results of the exact calculation as a function of magnetic field for a fixed trapping frequency ν of 1 MHz. The zero energy is at the $|aa\rangle$ dissociation limit in the absence of the trapping potential. Negative energies correspond to "real" bound states and positive energies correspond to trapped states. Clearly for increasing B a real bound state turns into a trapped state, shifts the energy of the trapped states up by approximately one $\hbar\omega$, and creates a picture of avoided crossings. This is the Feshbach resonance.

The figure also shows the eigenenergies when a (single-channel) regularized δ function replaces the exact five-channel potential, such that the strength of the δ function is related to the exact scattering length of a $|aa\rangle$ collision. For positive scattering length the regularized δ function potential has a bound state that crosses zero energy when the scattering length is infinite. Consequently as B increases the bound state turns into a trapped state and again a picture of avoided crossings is created. The magnetic field behavior of the bound state, however, is much stronger than for the exact calculation.

The exact and approximate positive eigenenergies are in agreement on both sides of the resonance as is expected when one realizes that the scattering length is small compared to a d of 29.7 nm for the $\nu=1$ MHz harmonic trap. Consequently these energies are also close to the radial harmonic oscillator energies $E_n/\hbar\omega=3/2+2n$ for $n=0,1,2$, and 3. Large differences between the exact and approximate eigenenergies occur only near the resonance when the scattering length is on the order of, or larger than, d.

VII. PHASE SHIFT OF QUANTUM GATES

The energies that were calculated in the previous sections can be used to calculate the entanglement or phase shift of a quantum gate. If the trapping potentials are initially nonoverlapping and both atoms are in the lowest trap state, their energy is $3\hbar\omega$. The wells are then brought together. For overlapping wells the total energy of the lowest state is $3/2\hbar\omega+E_{0,0}^{\text{exact}}$. After a time Δt the wells are separated and a reasonable estimate of the additional phase that the *interacting* atom pair accumulates after a time Δt is

$$\Delta\delta(t)=(E_{0,0}^{\text{exact}}-3/2\hbar\omega)\Delta t/\hbar. \tag{9}$$

Notice that it is implicitly assumed that overlapping of the wells has been achieved in an adiabatic fashion and the time to overlap is short compared to Δt. Whenever the scattering length is small compared to the size of the trapping potential,

E^{exact} can be replaced with the corresponding eigenenergy from the regularized δ-function potential yielding for $v=0$,

$$\Delta\delta(t)=\frac{2}{\sqrt{\pi}}\frac{a}{d}\omega\Delta t=4\pi\frac{\hbar}{2\mu}a\bar{n}\Delta t \tag{10}$$

to first order in a/d, and $\bar{n}$ is defined by $1/(\pi^{3/2}d^3)$. Note that the quantity $\bar{n}$ can be interpreted as the mean density defined by the average value of the local density $n(\vec{x})=|\Psi_{1p}(\vec{x})|^2$ of the lowest unit-normalized three-dimensional harmonic-oscillator wave function Ψ_{1p} for an isolated atom; that is,

$$\bar{n}=\int d^3x\Psi^*_{1p}(\vec{x})|\Psi_{1p}(\vec{x})|^2\Psi_{1p}(\vec{x}). \tag{11}$$

The latter part of Eq. (10) is provided to show the connection to mean-field descriptions of Bose condensates [6] and collisional frequency shifts for atomic clocks [30], althought here there are only two particles.

A criterion for the usefulness of this collisional phase shift for a quantum gate is defined as the time it takes to create π phase difference. For the δ-function potential we find

$$\Delta t=\frac{\pi^{3/2}}{2}\frac{d}{a}\frac{1}{\omega}. \tag{12}$$

Hence, since we assumed that $d/a\gg 1$, the time interval Δt is much larger than the classical oscillation time, $2\pi/\omega$, in a harmonic oscillator potential. For Cs and for Na near a Feshbach resonance the scattering length can become sufficiently large that $d/a\approx 1$ and Eq. (12) can only be used as a qualitative guide to the required interaction time. More exact calculations using Eq. (9) are then required.

For some implementation of quantum gates the phase shift is not the whole story. So far we have assumed that each atom is in a single spin state. However, for a quantum gate each atom can be in atomic eigenstates $|\alpha\rangle$ and $|\beta\rangle$ and hence the two-atom state vector in a linear superposition of product states $|\mu\nu\rangle$, where $\mu(\nu)=\alpha$, or β. The pair wave function is then

$$c_{\alpha\alpha}|\alpha\alpha\rangle+c_{\alpha\beta}|\alpha\beta\rangle+c_{\beta\alpha}|\beta\alpha\rangle+c_{\beta\beta}|\beta\beta\rangle, \tag{13}$$

where the coefficients c are arbitrary. Such linear superposition is called an entanglement when the state vector cannot be written as a product of atomic states or a linear superposition of atomic states. The interaction potential and hence the energy shift will be different for each state $|\alpha\beta\rangle$. As a result each term of Eq. (13) obtains a different phase shift when the trapping potentials are brought together. Hence two atoms can be entangled and for the effectiveness of the gate the relative phase shift is then crucial. If the energy shift for each $|\alpha\beta\rangle$ pair can be calculated via a δ-function pseudopotential, this then implies that the time it takes to accumulate a π phase difference is inversely proportional to the difference in scattering lengths.

VIII. COLLISIONAL DECOHERENCE

The preceding section described the effects of elastic scattering on the eigenstates of two tightly confined atoms. Two-body collisions typically introduce inelastic processes as well [16,20,22–24]. The loss or collisional decoherence will reduce the quality of a quantum gate.

For ultracold ground-state alkali-metal atom collisions, several inelastic processes exist. These processes lead to the conversion of internal hyperfine energy into excess kinetic energy, which is significantly larger than the typical depths of optical or magnetic trapping potentials. Consequently after the transition both atoms are lost from the confinement. The exception is the collision between two $|a\rangle$ state atoms, as no energetically lower two-body states exist. Other atoms are necessary to cause loss processes in those circumstances. Three-body recombination is such a process [16,19].

Two ''weak'' two-body inelastic processes are due to the spin-spin dipole [22] and second-order spin-orbit interactions [31] that cause coupling between s and d partial waves and determine the collisional lifetime of two doubly polarized alkali-metal atoms. The two processes dominate for those transitions where the sum of the atomic projections, $m_\alpha+m_\beta$, is not conserved. Typical rate coefficients are on the order of $K_{dip}=10^{-15}$ cm^3/s for the lighter alkalis and $K_{dip}=5\times10^{-12}$ cm$^3/s$ for cesium [32].

A strong loss channel is due to the spin-exchange mechanism. This process conserves $m_\alpha+m_\beta$ and is a consequence of the splitting between the $X\,{}^1\Sigma_g$ and $a\,{}^3\Sigma_u$ potentials inside $r\approx1.5$ nm, where the depth of these ABO potentials is much larger than the confinement energies. Typical loss rate coefficients are on the order of $K_{se}=10^{-11}$ cm$^3/s$ to 10^{-10} cm^3/s. An exception is the spin-exchange loss rate coefficients for ^{87}Rb where, due to the near identity of all observable scattering lengths, values on the order of a few times 10^{-14} cm^3/s are observed [21,20].

Inelastic rate coefficients have a Wigner threshold law that is independent of the collision energy in the limit of zero kinetic energy. If we then assume that the effect of the confining potential on the inelastic transition is negligible and consequently that the atom loss at each point in the trap is proportional to the square of the local density $n(\vec{x})$, the time for collisional decoherence is on the order of

$$\tau=\frac{1}{K\bar{n}}, \tag{14}$$

where $\bar{n}$ is the mean density as defined in Sec. VII. For our purposes a quantitative definition of the collisional decoherence time is not necessary.

The ratio of the time scale for collisional decoherence to the time scale to accumulate up a π phase shift introduces a criterion for the feasibility of a quantum gate. That is, for best performance this ratio

$$F=\frac{\tau}{\Delta t}=\frac{2\hbar}{\mu}\frac{a}{K}=\frac{a}{a_{\text{inel}}} \tag{15}$$

must be much larger than one. Here we used Eq. (12), the definition of the mean density $\overline{n}$, and introduced the inelastic scattering length $a_{\rm inel} = \mu K/(2\hbar)$. The quantity F is independent of the mean density and hence independent of the confining potential.

The value of the ratio F is dramatically different for the ''weak'' two-body inelastic processes and the strong two-body spin-exchange mechanism. For example, for doubly polarized Na the inelastic rate coefficient is $K_{dip} \approx 10^{-15}$ cm^3/s and hence $a_{\rm inel} = 10^{-4}$ nm. Here we used $a_{\rm inel}(\text{nm}) = 0.394 m(\text{amu}) K(10^{-10}\ \text{cm}^3/\text{s})$, where the atomic mass is in atomic mass units and K is in units of 10^{-10} cm^3/s. The small value for $a_{\rm inel}$ implies that $F = 10^4$ and makes a quantum gate feasible. On the other hand, for the spin-exchange loss mechanism we have for sodium $a_{\rm inel} \approx 1$ nm and thus $F \approx 1$. In fact any quantum gate that suffers from a large spin-exchange decoherence seems impractical.

IX. CONCLUSIONS

We have investigated the effects of the atom-atom interactions on two ultracold and confined alkali-metal atoms. The confinement is due to external optical fields such as optical lattices. For simplicity we have approximated the confining potential by a spherically symmetric harmonic potential. The interaction between the atoms is given in terms of the exact short-range potentials due to chemical binding interactions.

We have numerically calculated the bound states of the radial Schrödinger equation for two doubly polarized sodium atoms, two doubly polarized cesium atoms, and two sodium atoms in the lowest hyperfine state near a magnetic-field-induced collisional Feshbach resonance. The eigenenergies just above the dissociation limit of the atom-atom interaction correspond to those populated by trapped ultracold atoms. These energies were compared to the eigen energies obtained for a regularized-delta-function pseudo potential which reproduces the ultra-cold scattering length of two freely scattering atoms.

For two doubly polarized sodium atoms the two approaches are in excellent agreement while for two doubly polarized cesium atoms the pseudopotential breaks down. The breakdown occurs when the scattering length of Cs is on the order of or large compared to the extent of the trapping potential. We also showed that for Na in the lowest hyperfine state a magnetic-field-induced Feshbach resonance leads to a similar breakdown of the pseudopotential as the scattering length of two freely scattering atoms is infinite at resonance.

Finally we estimated the interaction-induced entanglement and collisional decoherence of the two atoms. Entanglement can in principle be used to build a computational gate of a quantum computer. We find that the necessary time scale δt for the operation of a quantum gate is proportional to the trap oscillation period times d/a. The latter ratio is proportional to the extent of the lowest harmonic oscillator state and the scattering length or differences of scattering lengths depending on the implementation of the quantum gate. Consequently for doubly polarized Na the entanglement must be built up over tens to hundreds of oscillation periods, while for Cs and for Na near a Feshbach resonance a few oscillation periods should be sufficient.

We find that the time scale for collisional decoherence due to inelastic collisions is on the order of $1/(K\overline{n})$, where K is the inelastic rate constant and $\overline{n}$ the mean density. Consequently the ratio of the decoherence time and δt is independent of the trapping frequency. Moreover, this ratio is very favorable, i.e., $\gg 1$, for collisional relaxation due to the magnetic spin-spin dipole and second-order spin-orbit interactions for all alkali-metal gases except atomic cesium. Collisional relaxation due to the spin-exchange mechanism, however, is with the exception of ^{87}Rb unacceptably large.

A quantitative calculation of the interaction-induced entanglement will have to address the far more complex calculation of the energy shifts of not perfectly overlapping and inharmonic traps. Moreover such calculations have to indicate whether bringing together individually trapped atoms can be done adiabatically. A breakdown of adiabaticity could lead to decoherence of a quantum gate. We hope to address some of these issues in future publications.

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