Quantum State Control via Trap-Induced Shape Resonance in Ultracold Atomic Collisions

René Stock* and Ivan H. Deutsch

Department of Physics and Astronomy, University of New Mexico, Albuquerque, New Mexico 87131, USA

Eric L. Bolda

Atomic Physics Division, NIST, Gaithersburg, Maryland 20899-8423, USA

We investigate controlled collisions between trapped but separated ultracold atoms. The interaction between atoms is treated self-consistently using an energy-dependent delta-function pseudopotential model, whose validity we establish. At a critical separation, a "trap-induced shape resonance" between molecular bound states and a vibrational eigenstate of the trap can occur. This resonance leads to an avoided crossing in the eigenspectrum as a function of separation. We investigate how this new resonance can be employed for quantum control.

The ability to arbitrarily manipulate the quantum state of a many-body ensemble represents the ultimate control of a physical system. This task has steadily advanced in atomic-molecular-optical systems with tremendous progress in cooling and trapping technology. This has led to the creation of Bose-Einstein condensates and Fermi degenerate gases, and the explorations of new forms of matter and mesoscopic quantum states previously accessible only in condensed matter systems [1]. The addition of engineered traps, such as optical lattices [2] and other optical [3] and magnetic [4] microtraps, provides a new knob with which to control the quantum state. A dramatic example of many-body control in lattices was demonstrated through the observation of a superfluid to Mott insulator quantum phase transition and the collapse and revival of the mean field coherence [5].

The standard approach to modeling and designing coherent states of matter, such as occur in a quantum phase transition, has its foundations in condensed matter theory, where one considers solutions to the entire many-body Hamiltonian. An alternative viewpoint arises from a fundamental theorem of quantum information theory [6]: an *arbitrary* state of a many-body system can be reached entirely through operations on single bodies and pairwise interactions. This provides a direct approach to engineering mesoscopic states through the application of a "quantum circuit" [7]. Moreover, one requires only a *single* two-body interaction (e.g., CPHASE or CNOT gate) that entangles the "particles" to contribute to a universal set of quantum logic gates.

In the context of ultracold neutral atoms, whereas manipulating the quantum state of an individual atom is a very mature technique, arbitrary unitary mapping of a two-atom system has not yet been achieved. Neutrals, by their very nature, do not strongly couple to anything. This may be an advantage for avoiding noise, but it implies that the two-body interaction will generally require close overlap of the atomic wave packets. By bringing two atoms within the same well of a tightly confining microtrap, one can achieve this strong coupling while remaining in the electronic ground state. Proposals for two-atom control in such a geometry have been considered using ground state *s*-wave collisions [8], Feshbach resonances [9], and laser induced Raman transitions [10]. At such close range, the atoms lose their individual identities and instead must be described as a molecular dimer which generally does not respect the atomic symmetries. This constrains the possible encodings of quantum information such that two-body logic gates can be performed within a well-defined "logical basis." This constraint can be overcome by placing the particles in distinguishable locations where the atomic quantum numbers are conserved asymptotically. Under typical conditions, such separated atoms would generally encounter very weak interactions. The coupling between atoms can be dramatically increased, however, when a resonance of the two-body system is excited, resulting in long-range interactions. An example of this is induced electric dipole-dipole interactions associated with excited electronic states [11,12].

In this Letter, we describe the physics at the foundation of these protocols by considering ultracold collisions between trapped but *separated* atoms. Our studies show that the trapping potential can lead to new resonances not found in free space. Unlike standard atomic collisions, here the relative motion of the atoms is quantized by the trap, making its description intrinsic to the process. Resonances can then occur between eigenstates of the trap and molecular bound states, allowing us to overcome the generally very weak interactions associated with the van der Waals potential. These "trap induced shape resonances" (TISR) can be substantial but are not accounted for within perturbation theory, which was applied in previous proposals for quantum logic via cold collisions [8]. The TISR provides a new tool for molecular dimer control (e.g., the production of cold molecules) and the design of two-atom quantum logic gates.

Our model system consists of two trapped and separated atoms that interact through the molecular potential V_{int}, described by a Hamiltonian,

$$\hat{H} = \frac{\hat{\mathbf{p}}_1^2}{2m} + V_t\left(\mathbf{r}_1 + \frac{\Delta \mathbf{z}}{2}\right) + \frac{\hat{\mathbf{p}}_2^2}{2m} + V_t\left(\mathbf{r}_2 - \frac{\Delta \mathbf{z}}{2}\right)$$
$$+ V_{int}(\mathbf{r}_1 - \mathbf{r}_2), \qquad (1)$$

where Δz is the separation of the traps (chosen in the z direction). The trapping potential V_t for the two atoms could be, for example, the state-dependent trap of a three-dimensional optical lattice potential. In this system, Δz can be continuously controlled by the angle between the polarization vectors of the counterpropagating laser beams [2,13]. We assume atoms are well localized near a potential minimum that is approximated as isotropic and harmonic with frequency ω. The two-atom Hamiltonian then separates into one for the center-of-mass moving in an isotropic harmonic potential, and one for relative coordinate dynamics governed by

$$\hat{H}_{rel} = \frac{\hat{\mathbf{p}}_{rel}^2}{2\mu} + \frac{1}{2}\mu\omega^2|\mathbf{r} - \Delta \mathbf{z}|^2 + V_{int}(\mathbf{r}). \qquad (2)$$

The reduced mass $\mu = m/2$ moves under the combined effects of a harmonic trap centered at $\Delta \mathbf{z}$ and a central interatomic potential (Fig. 1).

The harmonic trap is characterized by $z_0 = (\hbar/\mu\omega)^{1/2}$, the width of the trap ground wave function, while the interatomic potential has a much shorter range x_0; for ground state van der Waals interaction $V_{int}(r) = -C_6/r^6$ at large interatomic separation, $x_0 = (2\mu C_6/\hbar^2)^{1/4}/2$ [14]. Since for alkali atoms in typical optical lattices $x_0 \ll z_0$, distortion of the interatomic potential due to the harmonic trap can be neglected. Furthermore, for the ultracold collisions under consideration here, s-wave scattering dominates the collision. Under these conditions, the interatomic interaction $V_{int}(\mathbf{r})$ can be replaced by a zero-range effective-scattering length pseudopotential [15–17]

$$\hat{V}_{eff}(\mathbf{r}, E_K) = \frac{2\pi\hbar^2}{\mu} a_{eff}(E_K)\delta(\mathbf{r})\frac{\partial}{\partial r} r. \qquad (3)$$

Here $E_K = (\hbar k)^2/(2\mu)$ is the kinetic energy of relative motion for two atoms in an asymptotic scattering state with momentum $\hbar k$. It determines an "energy-dependent
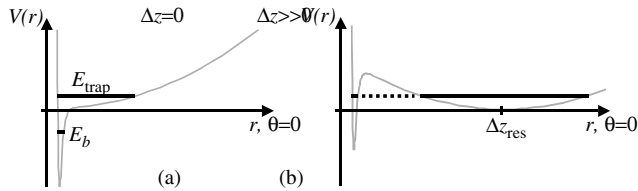

FIG. 1. Sum of the harmonic trapping potential and chemical binding potential (gray line) in the relative coordinate r for zero trap separation (a) and larger trap separation $\Delta z \gg z_0$ (b). The molecular bound state at E_b and trap eigenstate at E_{trap} can become resonant at a critical separation Δz_{res}.

scattering length,"

$$a_{eff}(E_K) = -\frac{\tan\delta_0(E_K)}{k}, \qquad (4)$$

where $\delta_0(E_K)$ is the s-wave collisional phase shift. However, unlike in a traditional collision where the two atoms are asymptotically free, in this system the atoms are trapped. The eigenvalues of the system must thus be solved *self-consistently* [16]. To this end, the eigenspectrum of the system is first calculated as a function of the (energy-independent) scattering length. Second, the effective-scattering length is calculated as a function of kinetic energy E_K for two *untrapped* atoms. The self-consistent energy eigenvalues are then found numerically as the simultaneous solutions of these functions. This method has been shown to yield the correct scattering behavior and energy spectrum for two atoms in a tight harmonic trap [16] for $z_0 \gg x_0$.

Full characterization of the interatomic potential by a pseudopotential requires not only accurately reproducing the scattering behavior but also the molecular bound state spectrum. This is particularly important for the TISR described below. We accomplish this by analytic continuation of the effective-scattering length Eq. (4) to *negative* kinetic energies $E_K = -\hbar^2\kappa^2/(2\mu)$ according to $a_{eff}(E_K) = -\tanh\iota\delta_0(E_K)/\kappa$, with real and positive κ. The self-consistent solutions for these negative energies then accurately reproduce the entire s-wave bound state spectrum as can be easily understood as follows. Suppose there is a bound state of the actual potential V_{int} at $E_b = -(\hbar\kappa_b)^2/(2\mu)$. The corresponding pole of the S matrix implies that $\tanh\iota\delta_0(E_b) \to 1$, and, hence, $a_{eff}(E_b) = 1/\kappa_b$. Now, a pseudopotential with scattering length $a > 0$ possesses exactly one bound state at $E_\delta = -\hbar^2/(2\mu a^2)$. By setting $a = a_{eff}(E_b)$, we recover the exact bound state, $E_\delta = E_b$. Note that without a self-consistent solution one cannot choose a pseudopotential which simultaneously matches the scattering length and last bound state of the true potential. Moreover, although the pseudopotential can have no more that one bound state, this self-consistent solution via the energy-dependent scattering length captures exactly *all* of the s-wave bound states, since they are obtained from $a_{eff}(E_K)$ and therefore the S matrix.

With this model, we calculate the energy spectrum of Eq. (2) for two trapped but separated atoms. First, consider the spectrum for a given scattering length. We represent the Hamiltonian for arbitrary Δz in the basis corresponding to the solutions with $\Delta z = 0$ and a *fixed* scattering length a (i.e., not the self-consistent solution). This basis, derived by Busch *et al.* [18], consists of 3D-harmonic-oscillator-like solutions. The pseudopotential couples only s waves, resulting in irregular $l = 0$ radial waves with singularities at the origin. These solutions also include the pseudopotential bound state at negative energy. The $l \geq 1$ wave functions are the regular 3D-harmonic oscillator wave functions. The trap potential,

proportional to $|\mathbf{r} - \Delta\mathbf{z}|^2 = r^2 - \Delta z\, r\cos\theta + \Delta z^2$, is axially symmetric and dipolar, thereby preserving the magnetic quantum number of relative motion and coupling the partial waves l to $l \pm 1$. The Hamiltonian is diagonalized in this basis at each trap separation Δz. The resulting energy spectrum for two atoms is shown in Fig. 2 for both positive and negative scattering lengths, $a = +0.5z_0$ and $a = -0.5z_0$, as a function of Δz. The results of first-order perturbation theory are also shown for comparison. For $\Delta z \gg z_0$, we recover the expected unperturbed 3D harmonic oscillator eigenenergies. As the separation between traps is decreased, perturbation theory predicts a negative ($a < 0$) or positive ($a > 0$) energy shift to the ground state. The expected behavior is seen for $a = -0.5z_0$, but an unexpected solution is seen for $a = +0.5z_0$.

The results for the positive scattering length are explained as follows. For large positive a, there is a molecular bound state close to dissociation. As Δz is increased, the interatomic potential, located at very small internuclear distances, is pushed up in energy by $\mu\omega^2\Delta z^2/2$ due to the parabolic trapping potential in Eq. (2). That is, in order for the separated atoms to collide, they must overcome the potential barrier created by the trap (see Fig. 1). When the molecular bound state becomes resonant with the lowest trap eigenstate, an avoided crossing occurs in the energy spectrum (see Fig. 2). As the separation is increased even further, the molecular bound state becomes resonant with higher-lying trap states and more avoided crossings occur. This is a new "shape resonance" for s-wave collisions in which the trap barrier plays the role of the centrifugal barrier in a standard free-space shape resonance for higher partial waves. Analogous, Feshbach-like, "confinement induced resonances" have recently been predicted for 1D and 2D trapped Bose gases and for delocalized states in 3D-optical lattices [16,19].

The separation at which the lowest resonance occurs, Δz_{res}, is easily estimated by equating the sum of molecular binding energy and trapping potential at the origin, $E_b + \mu\omega^2\Delta z^2/2$, to the vibrational ground state energy of the oscillator, $3\hbar\omega/2$, yield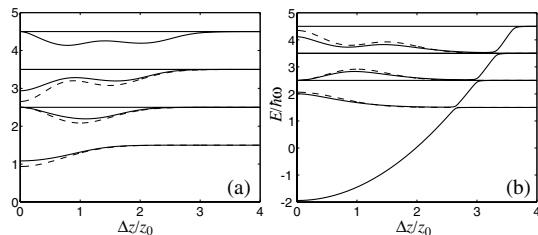ing $\Delta z_{\mathrm{res}}/z_0 = \sqrt{3 + z_0^2/a^2}$. The location and gap of the avoided crossing depends strongly on the molecular binding energy. For a deeply bound state, but still positive scattering length, corresponding to $0 < a \ll z_0$, the resonance occurs at much larger separations and with an exponentially small energy gap. This corresponds to the small probability for the atoms to tunnel from the trap into the chemical binding potential. Using a standard variational approach [20] based on symmetric and antisymmetric combinations of the $\Delta z = 0$ bound state [18] and the trap ground state, we find that for $0 < a < 0.2z_0$ the gap is smaller than $10^{-4}\hbar\omega$. For $a \gg z_0$ the energy gap asymptotes to a large value, $\Delta E_{\mathrm{max}} = 0.5640\hbar\omega$. The shape resonance can therefore be easily observed for large positive scattering lengths, where the bound state would be close to dissociation. This can be achieved in tight traps, where the scattering length is on the order of z_0 and the energy gap approaches a significant fraction of $\hbar\omega$ (see Fig. 3). For example, in an optical lattice of ^{133}Cs atoms the large scattering lengths of $280a_0$ to $2400a_0$ are comparable to typical trap sizes in an optical lattice, corresponding to a modest Lamb-Dicke parameter $\eta = k_L z_0 = 0.1$. A substantial TISR will result.

To obtain a more accurate spectrum in the case of trapped alkali atoms, we must account for the energy dependence of the scattering length in the self-consistent model described above. As a test case, we consider the simplest possible interatomic potential—a step-potential of radius R and depth V_0 with a single s-wave bound state. The s-wave phase shift is given explicitly by $\delta_0(E_K, V_0) = \arctan[k\tan(qR)/q] - kR$, where $q = \sqrt{2\mu(E_K + V_0)/\hbar^2}$ [20]. The energy-dependent scattering length is evaluated using Eq. (4) as a function of E_K. The relative kinetic energy of the colliding atoms is given by the total energy eigenvalue E minus the trap potential at the origin.

FIG. 2. Energy spectra as a function of separation Δz between traps for a negative (a) or positive (b) fixed scattering length a. The results of perturbation theory are shown as dashed lines. For $a > 0$, one sees the parabolic energy shift of the molecular bound state due to the harmonic trapping potential and the avoided crossings associated with the TISR.
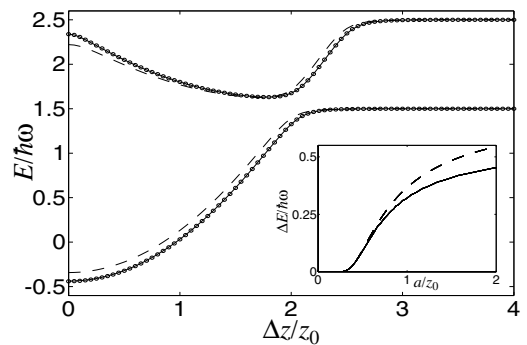

FIG. 3. Comparison between the energy spectrum of the test step potential and that of the pseudopotential approximation. The two lowest energy curves are shown for the step potential (solid line), the pseudopotential with an energy-dependent scattering length a_{eff} (circles), and constant a (dashed line). The inset shows the energy gap ΔE for these two lowest levels at resonance as a function of scattering length a calculated from energy spectra at the different scattering lengths. A variational estimate of the energy gap is shown as the dashed line.

Figure 3 shows the self-consistent energy spectrum as a function of well separation Δz. These approximate eigenvalues are compared with the exact solution for the step potential ($V_0 = 36.79\hbar\omega$ and $R = 0.2z_0$) plus harmonic potential, calculated numerically. We accomplish this by expanding the total Hamiltonian in isotropic 3D-harmonic oscillator wave functions and diagonalizing the matrix. Figure 3 also shows a plot of the constant scattering length approximation, using the zero-energy scattering length $a = a_{\text{eff}}(0)$. As expected, this approximation fails to capture the correct bound state energy and therefore the correct location of the shape resonance. In contrast, the self-consistent solution using the energy-dependent pseudopotential shows excellent agreement with the exact calculation, even for a well that was chosen to have a fairly long range, $R = 0.2z_0$. The agreement breaks down only when the range of the potential becomes on the order of trap size, $R > 0.5z_0$.

Having confirmed the validity of the self-consistent pseudopotential model, we can use the calculated energy spectrum to design two-atom quantum logic gates. The use of ultracold collisions was initially considered by Jaksch et al. [8] in the nonresonant case, using perturbation theory. Our analysis shows that in principle, for positive scattering lengths, resonances will occur at some atomic separation, and perturbation theory will break down. The resulting avoided crossing in the energy spectrum must be properly accounted for. This is particularly true for atoms with very large scattering lengths, such as ^{133}Cs. The TISR opens the door to new protocols for entangling two-atom logic gates with separated atoms. For example, a 2π Rabi oscillation between the trapped atoms and an auxiliary molecular bound state leads to a phase shift of -1 on the two-atom state. If the acquired phase shift occurs only for one logical encoding of the atoms, the resulting unitary transformation is the so-called "CPHASE" two-qubit logic gate [6]. An optimal regime for operation of this protocol is where $z_0 \ll a$. In this regime the energy gap (Fig. 3 inset) asymptotes to its maximum value, minimizing the dependence of the cooperative phase shift on the precise value of the trap width z_0, and, hence, reducing errors due to trap-laser intensity fluctuations.

More generally, beyond quantum logic, the TISR provides a new avenue for spectroscopy and coherent control of ultracold molecular dimers. Like magnetic Feshbach resonances, these shape resonances can provide new ultrahigh precision spectroscopic data on the molecular potential [21], and the production of cold molecules tunable by the trap parameters. A complete characterization of these protocols requires a generalization of our model, including the full spin-dependent nature of the collision process via the hyperfine and exchange interactions. We plan to address this in future work using multichannel Born-Oppenheimer potentials approximated by energy-dependent pseudopotentials.

*Electronic address: restock@info.phys.unm.edu
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