Control of ultraslow inelastic collisions by Feshbach resonances and quasi-one-dimensional confinement

V. A. Yurovsky
School of Chemistry, Tel Aviv University, 69978 Tel Aviv, Israel

Y. B. Band
Departments of Chemistry and Electro-Optics and The Ilse Katz Center for Nano-Science, Ben-Gurion University of the Negev, Beer-Sheva 84105, Israel

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Inelastic collisions of ultracold atoms or molecules are analyzed using very general arguments. In free space, the deactivation rate can be enhanced or suppressed together with the scattering length of the corresponding elastic collision via a Feshbach resonance, and by interference of deactivation of the closed and open channels. In reduced dimensional geometries, the deactivation rate decreases with decreasing collision energy and does not increase with resonant elastic scattering length. This has broad implications; e.g., stabilization of molecules in a strongly confining two-dimensional optical lattice, since collisional decay of excited states due to inelastic collisions is suppressed. The relation of our results to the Lieb-Liniger model for bosonic atoms is addressed.

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Feshbach resonances [1,2] have been used to control atomic interactions in trapped ultracold quantum gases by tuning a magnetic field near a diatomic molecule Feshbach resonance to convert atoms into weakly bound molecules. For fermionic atoms the molecules formed were remarkably long lived [3], whereas for bosonic atoms in a BEC [4], collisional decay of the highly excited vibrational molecular state occurs [5] and only a small fraction of molecules is observed in this case.

Here we show, using very general scattering theory arguments, that inelastic ultracold collisions in reduced dimension can be strongly suppressed. A similar effect has been predicted [6] within the exactly solvable Lieb-Liniger (LL) many-body model for indistinguishable bosons in one-dimension (1D) [7], however, other processes, such as reflection and dissociation in atom-dimer collisions and three-atom association become allowed when the integrability of the LL model is lifted [8]. The present results demonstrate that suppression of inelastic collisions is not a special effect of the integrable LL model, and occurs in all kinds of quasi-1D scattering processes, e.g., in collisions of atoms and molecules in atomic waveguides. Quasi-1D scattering occurs in a gas in the presence of a waveguide potential that tightly confines a 3D gas in two directions so the radial confinement energy $\omega_\perp$ (in units where $\hbar=1$) is much larger than the collision energy [9], as in 2D optical lattices [10], elongated atomic traps [11], and atomic integrated optics devices [12]. This suppression has broad implications, e.g., it can be used to stabilize molecules produced from bosonic atoms in tight atomic waveguides, since inelastic energy-transfer collision rates at low collision energy are significantly reduced relative to 3D rates. Suppression of inelastic scattering can also occur in collisions of other excited collision partners (e.g., in hyperfine excited atom collisions).

The theoretical framework for calculating atom-diatom scattering or even more complicated collision processes can be drawn along the lines of the Arthurs and Dalgarno model [13]. The scattering state $|\Psi\rangle$ can be expressed in terms of a sum over basis functions

$$|\Psi\rangle = \sum_j \psi_j(\mathbf{r})|\chi_j\rangle, \tag{1}$$

where $\mathbf{r}$ is the atom-diatom relative coordinate, $\psi_j(\mathbf{r})$ is the relative wave function, and $|\chi_j\rangle$ includes internal and center-of-mass degrees of freedom for channel j. The center-of-mass motion can be separated from the relative motion for free space and harmonic trap potentials considered below. We shall not require details of the collision partners since our arguments are very general (e.g., they apply to arbitrary molecule-molecule collisions).

Low-energy inelastic exoergic collisions in the presence of a Feshbach resonance can often be treated as multichannel scattering with zero-range interactions described by boundary conditions for s-wave radial wave functions $\varphi_j(r) = \frac{r}{4\pi}\int \psi_j(\mathbf{r})d\Omega_{\mathbf{r}}$. This method has been validated for multichannel scattering in free space (see Ref. [14], and references therein) and for harmonic waveguides [15]. In our case of low energy inelastic scattering resulting in deactivation of the excited state of a molecule, the boundary conditions take the form

$$\left.\frac{d\varphi_j(r)}{dr}\right|_{r=0} = \sum_{k=o,c,\{d\}} U_{jk}\varphi_k(0), \tag{2}$$

for the input channel φ_o, the closed channel φ_c, and the deactivation products having a set of output channels $\{d\}$ (see Fig. 1). This method is applicable to collisions of any type of particles when s-wave scattering is allowed. Note that collisions of broad Feshbach molecules [16] cannot be treated using the zero-range approach of Eq. (2), however, in considering atom-molecule or molecule-molecule collisions, the resonance does not coincide with the resonance in atom-atom collisions, and the molecules can be treated as zero-range objects. For example resonances in collisions of Cs_2 molecules have been observed at 12.72 and 13.15 G [17], far off the atom-atom resonance at 19.84 G.

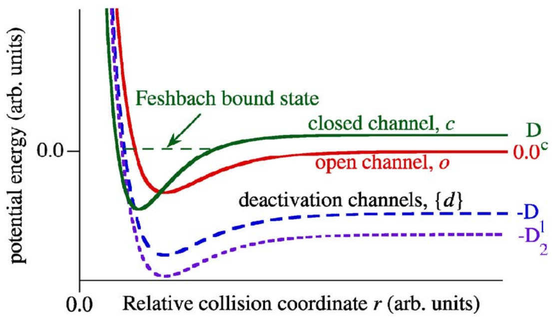

FIG. 1. (Color online) Schematic description of channel potentials for free space scattering.

When the coupling of the input channel to the other channels vanishes, Eq. (2) reduces to the Bethe-Peierls boundary condition [14], and $U_{00}=-1/a_{\mathrm{bg}}$, where a_{bg} is the nonresonant background elastic scattering length. Outside the interaction region, $\psi_o(\mathbf{r})$ satisfies the Schrödinger equation

$$-\frac{1}{2m}\nabla^2\psi_o(\mathbf{r})+V_{\mathrm{conf}}(\mathbf{r})\psi_o(\mathbf{r})=E\psi_o(\mathbf{r}), \tag{3}$$

where V_{conf} is the confining harmonic waveguide trapping potential, E is the collision energy, and m is the reduced mass of the colliding particles. Moreover, the radial wave functions φ_c and φ_d satisfy the Schrödinger equations

$$-\frac{1}{2m}\frac{d^2\varphi_{c,d}}{dr^2}\pm D_{c,d}\varphi_{c,d}(r)=E\varphi_{c,d}(r), \tag{4}$$

where D_c is the asymptotic value of the closed channel potential, D_d is the deactivation energy for channel d (see Fig. 1), and we assumed that $V_{\mathrm{conf}}\ll D_{c,d}$. Equations (4) can be solved to obtain

$$\varphi_c(r)=\varphi_c(0)\exp[-\sqrt{2m(D_c-E)}r], \tag{5}$$

$$\varphi_d(r)=\varphi_d(0)\exp(ip_d r), \tag{6}$$

where $p_d=\sqrt{2m(E+D_d)}$. The closed channel has an attractive potential ($U_{cc}<0$) and a single bound state with energy $E_{\mathrm{Fesh}}=D_c-U_{cc}^2/(2m)$.

Substitution of Eqs. (5) and (6) into Eq. (2) leads to the following boundary condition:

$$\left.\frac{d\varphi_o(r)}{dr}\right|_{r=0}=-\frac{1}{a_{\mathrm{eff}}}\varphi_o(0). \tag{7}$$

Here the length a_{eff} has an imaginary part due to coupling to the deactivation channels. The deactivation energies typically substantially exceed all interaction energies. Therefore only the contributions of zero and first orders in $|U_{jk}|/p_d$ need be retained, and a_{eff} can be expressed as

$$a_{\mathrm{eff}}=a_{\mathrm{bg}}\frac{E_\delta-i\Gamma_c}{E_\delta+\mu\Delta-i\Gamma}, \tag{8}$$

with widths

$$\Gamma=\sum_{\{d\}}\frac{1}{p_d}\left[\frac{|U_{dc}|^2\mu\Delta}{a_{\mathrm{bg}}|U_{oc}|^2}+2\mu\Delta\,\mathrm{Re}\left(\frac{U_{od}U_{dc}}{U_{oc}}\right)-a_{\mathrm{bg}}|U_{do}|^2E_\delta\right],$$

$$\Gamma_c=\frac{\mu\Delta}{a_{\mathrm{bg}}|U_{oc}|^2}\sum_{\{d\}}\frac{1}{p_d}|U_{cd}|^2.$$

Here, $\Delta=a_{\mathrm{bg}}|U_{cc}||U_{oc}|^2/(\mu m)$ is the resonance strength, μ is the difference of the magnetic moments in the closed and open channels, and

$$E_\delta=\frac{|U_{cc}|}{m}\left[\sqrt{U_{cc}^2+2m(E_{\mathrm{Fesh}}-E)}-|U_{cc}|\right] \tag{9}$$

is an effective detuning. For a tightly bound closed-channel state, or when the detuning of the collision energy from the Feshbach energy is small, $|E_{\mathrm{Fesh}}-E|\ll U_{cc}^2/m$, then $E_\delta\approx E_{\mathrm{Fesh}}-E$. In this case, neglecting deactivation, one can approximate a_{eff} by the real effective energy-dependent length [19]

$$a_{\mathrm{eff}}(E)\approx a_{\mathrm{bg}}\left[1+\frac{\mu\Delta}{E-\mu(B-B_0)}\right], \tag{10}$$

where $B-B_0\equiv\Delta+E_{\mathrm{Fesh}}/\mu$ is the detuning of the external magnetic field B from its resonant value B_0.

The deactivation cross section can be expressed as

$$\sigma=4\pi\sum_d\varphi_d^*\frac{1}{im}\frac{d}{dr}\varphi_d=\frac{4\pi S}{m}|\varphi_o(0)|^2, \tag{11}$$

where φ_o corresponds to the input channel wave function normalized to unit incident flux density, and the factor

$$S=\sum_{\{d\}}\frac{1}{p_d}\left|U_{do}-\frac{U_{dc}\mu\Delta}{a_{\mathrm{bg}}U_{oc}(E_\delta-i\Gamma_c)}\right|^2 \tag{12}$$

accounts for interference of deactivation of the closed and open channel states.

First, we consider collisions in free space ($V_{\mathrm{conf}}=0$). The proper solution of Eq. (3) has the form

$$\psi_o(\mathbf{r})=\sqrt{\frac{m}{p_0}}\left[\exp(i\mathbf{p}_0\cdot\mathbf{r})-\frac{1}{a_{\mathrm{eff}}^{-1}+ip_0}\frac{1}{r}\exp(ip_0r)\right], \tag{13}$$

where the collision momentum is $p_0=\sqrt{2mE}$. For low-energy collisions such that $a_{\mathrm{bg}}p_0\ll 1$, we find

$$\varphi_o(0)=-(m/p_0)^{1/2}a_{\mathrm{eff}}. \tag{14}$$

The deactivation cross section $\sigma_{\mathrm{free}}=4\pi S|a_{\mathrm{eff}}|^2/p_0$ diverges at low collision energies, while the deactivation rate coefficient

$$K_{\mathrm{free}}=\frac{p_0}{m}\sigma_{\mathrm{free}}\approx\frac{4\pi S}{m}|a_{\mathrm{eff}}|^2 \tag{15}$$

has a finite limit proportional to $|a_{\mathrm{eff}}|^2$. Deactivation can be suppressed near $E_\delta=0$, where a_{eff} is close to zero, and enhanced near resonance of a_{eff} at $E_\delta=-\mu\Delta$, such that

$$\frac{4\pi}{m}\sum_{\{d\}}\frac{1}{p_d}\left|\frac{U_{dc}}{U_{oc}}\right|^2 \leqslant K_{\text{free}} \leqslant \frac{4\pi S}{m}\left[\frac{a_{\text{bg}}\mu\Delta}{\Gamma(E_\delta=-\mu\Delta)}\right]^2. \tag{16}$$

Under certain conditions it can also be suppressed due to interference in the factor S.

Consider now collisions in a harmonic waveguide potential $V_{\text{conf}}=m\omega_\perp^2 r_\perp^2/2$, where $\omega_\perp$ and $r_\perp$ are the transverse frequency and coordinate, respectively. This problem has been analyzed in Refs. [9,15] for a single-channel Huang pseudopotential, which is equivalent to the Bethe-Peierls boundary condition. (See also Ref. [18] for finite-range potentials.) The case of a multichannel δ-function interaction has been considered in Ref. [19] using a renormalization procedure. Equations 17 and 19 in Ref. [19] express the proper solution of Eq. (3) in terms of the transverse Hamiltonian eigenfunctions $|n0\rangle$ with zero angular momentum projection on the waveguide axis z,

$$\psi_o(\mathbf{r}) = a_\perp\sqrt{\frac{\pi m}{p_0}}\Bigg[\exp(ip_0 z)|00\rangle - \frac{1}{2}ma_\perp T_{\text{conf}}(p_0)\sum_{n=0}^{\infty}\frac{\exp(ip_n|z|)|n0\rangle}{\sqrt{n-(p_0a_\perp/2)^2}}\Bigg]. \tag{17}$$

Here $a_\perp=(m\omega_\perp)^{-1/2}$ is the transverse harmonic oscillator length, $p_n=\sqrt{2m[E-(2n+1)\omega_\perp]}$ is the longitudinal channel momentum,

$$T_{\text{conf}}(p_0) = \frac{2}{ma_\perp}\left[\frac{a_\perp}{a_{\text{eff}}}+\zeta\left(\frac{1}{2},-\left(\frac{a_\perp p_0}{2}\right)^2\right)\right]^{-1} \tag{18}$$

is the transition matrix, and $\zeta(\nu,\alpha)$ is the Hurwitz zeta function [15]. The wave function (17) is normalized so the average incident flux density per waveguide area $\pi a_\perp^2$ is unity. The sum in Eq. (17) diverges as $r\to 0$. The divergent part can be evaluated as $a_\perp/r$ [15]. This leads to $\varphi_o(0)=-\frac{1}{2}ma_\perp^2\sqrt{m/p_0}T_{\text{conf}}(p_0)$, and to the deactivation rate coefficient $K_{\text{conf}}=\pi m a_\perp^4|T_{\text{conf}}|^2 S$.

For weak confinement, $a_\perp p_0 \gg 1$, approximation (49) in Ref. [19] leads again to Eq. (13) for the wave function and to Eq. (15) for the deactivation rate. For strong confinement, i.e., when $a_\perp p_0 \ll 1$, approximation (41) in Ref. [19] leads to

$$T_{\text{conf}}(p_0) \approx -i\frac{p_0}{m}\left(1+\frac{i}{2}Ca_\perp p_0 - i\frac{a_\perp^2 p_0}{2a_{\text{eff}}}\right)^{-1}, \tag{19}$$

where $C\approx 1.4603$. At low collision energies, or at large a_{eff}, where $p_0 \ll |a_{\text{eff}}|/a_\perp^2$, the wave function at the origin, $\varphi_o(0)\approx\frac{i}{2}a_\perp^2\sqrt{mp_0}$, is much less than the corresponding value of $\varphi_o(0)$ in free space (14). Thus confinement prevents the particles from occupying the same position. A similar effect is responsible for fermionization of 1D bosons with strong interactions [9]. Under these conditions the deactivation rate, $K_{\text{conf}}\approx a_\perp^4 p_0^2/(4|a_{\text{eff}}|^2)K_{\text{free}}$, can be substantially suppressed by confinement.

This conclusion is graphically demonstrated in Fig. 2 under conditions when a_{eff} is expressed by Eq. (10). It shows resonances in the deactivation rate at $E_\delta=-\mu\Delta$ for

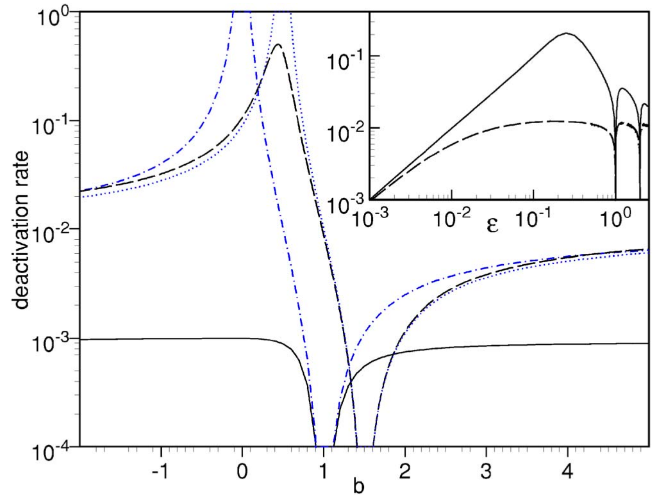

FIG. 2. (Color online) Scaled deactivation rate coefficient $\frac{Km}{4\pi S a_\perp^2}$ as a function of scaled magnetic field detuning $b=\mu(B-B_0)/(2\omega_\perp)-\frac{1}{2}$ and collision energy $\varepsilon=E/(2\omega_\perp)-\frac{1}{2}$, calculated for $a_{\text{bg}}=0.1a_\perp$ and $\mu\Delta=2\omega_\perp$. In the confined geometry, the solid and dashed curves correspond to $\varepsilon=10^{-3}$ and $\varepsilon=0.5$, respectively, whereas the free space results are given by the dot-dashed and dotted curves, respectively. The inset shows the deactivation rate versus ε in confined geometry for $b=0$ (solid curve) and $b=100$ (dashed curve).

collision energies comparable to $\omega_\perp$ and in free space, as well as deactivation suppression near $E_\delta=0$. At low collision energies, when

$$p_0 \ll |a_{\text{bg}}|/a_\perp^2, \tag{20}$$

deactivation under confinement does not have resonances and can be strongly suppressed even compared to the nonresonant process in free space. Suppression appears also at $E=(2k+1)\omega_\perp$, where excitations of transverse waveguide modes become open, leading to jumps in the elastic scattering amplitude [19,20].

The above results are obtained for a system composed of two arbitrary particles interacting via s-wave scattering. A suppression of inelastic collision has been predicted in Ref. [6] for a many-body system of 1D indistinguishable bosons using the LL model [7]. However, as we shall see below, the suppression is mostly a two-body interaction effect even in this model.

Consider first the two-body scattering process with particle momenta p_1 and p_2. The two-body correlation function with the particles at the same position

$$g_2^{(2)}(p_1,p_2) = |\Psi^{(2)}_{p_1p_2}(0,0)|^2 = \frac{2}{L^2}\frac{(p_1-p_2)^2}{(p_1-p_2)^2+4m^2U_a^2} \tag{21}$$

is the probability to find two particles at the same place. Here $\Psi^{(2)}_{p_1p_2}(z_2,z_1)$ is the LL wave function [7] with unit norm in interval $[0,L]$ $(L\to\infty)$, and $U_a\approx 2a_{\text{bg}}[ma_\perp^2(1-Ca_{\text{bg}}/a_\perp)]^{-1}$ is the interaction strength [9]. Equation (21) already describes qualitatively the behavior of g_2 when the ratio of the interaction to collision energies is large, as obtained in Ref. [6], $g_2 \sim (p_1 - p_2)^2/U_a^2$.

In the N-body case, the two-body correlation function $g_2^{(N)}$ can be estimated as a sum of $g_2^{(2)}$ over all pairs of the colliding particles with the quasimomenta p_j and $p_{j'}$,

$$g_2^{(N)} \approx \sum_{j<j'} g_2^{(2)}(p_j,p_{j'}) \approx \frac{L^2}{2} \int dp_1 dp_2 f(p_1) f(p_2) g_2^{(2)}(p_1,p_2), \tag{22}$$

where the values of the quasimomenta p_j are determined by boundary conditions and the summation is replaced by integration with the quasimomentum distribution functions $f(p)$ [7]. The system properties are determined by the dimensionless parameter $\gamma = 2mU_a/\rho$, where $\rho = N/L$ is the linear particle density. Approximate analytical expressions for $f(p)$ in the ground state have been obtained in Ref. [7] for two regimes. In the mean-field one, where $\gamma \ll 1$, substitution of $f(p) \approx \pi^{-1}\gamma^{-1/2}\sqrt{1-p^2/(4\rho^2\gamma)}$ into Eq. (22) leads to $g_2^{(N)} \approx \rho^2$, in full agreement with the results of Ref. [6]. In the Tonks-Girardeau regime, $\gamma \gg 1$, where $f(p) \approx 1/(2\pi)$ for $|p| < \pi\rho$ and $f(p) = 0$ otherwise, Eq. (22) leads to $g_2^{(N)} \approx 2\pi^2\rho^2/(3\gamma^2)$. This value is half the exact value determined in Ref. [6]. The difference is due to the highly-correlated behavior of the Tonks-Girardeau gas, while Eq. (22) includes only an average with independent quasimomentum distributions of the two particles. However, this expression describes the correct behavior of $g_2^{(N)}$ as $\gamma \to \infty$, leading to suppression of all kinds of collision phenomena under tight confinement when $mU_a/\rho \gg 1$ [this condition has the same meaning as Eq. (20)].

In summary, inelastic collision rates in free space are proportional to $|a_{\text{eff}}|^2$, show resonances and dips and are capped by Eq. (16). Interference can suppress the inelastic rate. In quasi-1D scattering at low collision energies [see Eq. (20)], inelastic collisions do not have resonances and are suppressed. This effect appears in collisions of any type of atoms or molecules interacting via s waves, and is not an effect of the integrability of the 1D Bose gas LL model, unlike suppression of other processes in 1D (see Ref. [8]).

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