Inelastic collisions in ultracold gases confined by one-dimensional optical lattices

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(Received 14 October 2009; published 14 January 2010)

We present a formalism for rigorous multichannel scattering calculations of cross sections for inelastic collisions of atoms and molecules confined in one-dimensional optical lattices. We obtain analytical expressions for the mean frequency of inelastic collisions in a confined gas in the temperature regime $T \sim \hbar\omega$ and at temperatures $T \gg \hbar\omega$, where ω is the oscillation frequency of trapped particles in the confining potential. Our numerical calculations for the gaseous mixture of Li and Rb atoms show that inelastic collisions in the temperature regime $T \sim \hbar\omega$ exhibit a deviation from three-dimensional scattering. This deviation is more significant for systems with stronger confinement and larger scattering lengths. We find that the ratios of rate constants for inelastic scattering and elastic collisions are suppressed in confined gases at $T \sim \hbar\omega$, and this suppression is significant for Li-Rb collisions at $T < 40$ μK.

DOI: 10.1103/PhysRevA.81.012701 PACS number(s): 34.50.Lf, 34.50.Rk

I. INTRODUCTION

Atomic ensembles cooled to ultracold temperatures can be confined by optical forces and trapped in an optical lattice, which is a standing-wave interference pattern of counterpropagating laser beams. By providing for the variation of the depth and the geometry of confining potentials, optical lattices can be used as powerful instruments to study fundamental problems and to explore new phenomena in several areas of physics [1–4]. For example, they may allow for quantum simulations of novel condensed-matter systems [5,6] and the development of new schemes for quantum computation [7,8]. Optical lattices can also be used to produce low-dimensional quantum gases. Of particular interest here is an ultracold gas confined by a one-dimensional (1D) optical lattice, where atoms or molecules move freely in two dimensions and oscillate harmonically in the third dimension. Such gases exhibit novel quantum phase transitions and dynamics not observable in unconfined thermal ensembles of atoms [9–17]. The many-body behavior of confined gases can be manipulated by adjusting the depth of the confining potential [12,18–20] as well as the frequency of the trapping laser light. The study of collision dynamics of atoms and molecules in 1D optical lattices may lead to fundamental discoveries and new research directions [21–23]. For example, the threshold energy dependence of elastic and inelastic cross sections in an ultracold gas under strong confinement is very different from that in three dimensions (3D) [23,24], and the threshold laws for inelastic collisions can be tuned by varying the confinement strength and external magnetic fields [21]. Applying laser confinement in one direction may stabilize ultracold collision systems and allow for the study of ultracold chemistry in restricted geometries [21,25] and collisional decoherence [26]. The study of collision dynamics of atoms and molecules in 1D optical lattices may therefore have applications reaching beyond the field of cold atoms and molecules.

Petrov and Shlyapnikov have recently developed a theory of elastic collisions between atoms confined in a 1D harmonic trap [22] and studied the effect of the confinement on elastic collisions in a single-species atomic gas. They identified two regimes of scattering for confined atoms: (i) the quasi-two-dimensional (quasi-2D) regime ($T \ll \hbar\omega$) and (ii) the confinement-dominated 3D regime ($T \sim \hbar\omega$), where T is the temperature of the confined gas and ω is the oscillation frequency of particles in the confining potential. They found that the scattering wave function of ultracold atoms in the quasi-2D regime exhibits the features of a scattering wave function in a purely 2D geometry, whereas in the confinement-dominated 3D regime, the 2D character of the scattering wave function is not significant. However, the confinement may still affect the interparticle interactions to a great extent, even when $T > \hbar\omega$. In our previous communication, we extended the work of Petrov and Shlyapnikov to present a formalism for rigorous scattering calculations of probabilities for inelastic and chemically reactive collisions of atoms and molecules in the quasi-2D regime [21]. Our results showed that the elastic-to-inelastic ratio of collision cross sections is enhanced in the presence of confinement. However, the effects of confinement on the dynamics of inelastic collisions in the confinement-dominated 3D regime remain unknown.

In this article, we extend our theory for quantum calculations of inelastic cross sections in a quasi-2D geometry [21] to the confinement-dominated 3D regime and discuss in detail the effects of the confinement on inelastic collisions of atoms and molecules confined in 1D optical lattices. We present rigorous multichannel scattering calculations of inelastic collision rates in a mixture of atomic gases. We show that inelastic collisions in the confinement-dominated 3D regime deviate from 3D scattering and this deviation is more significant for systems with stronger confining potentials and larger scattering lengths. We also show that inelastic collisions in the confinement-dominated 3D regime are generally suppressed. As the temperature of the gas increases, this suppression becomes less significant. In many experiments with optical lattices, the temperature of atoms and molecules is not cold enough to reach the quasi-2D or confinement-dominated 3D regimes. Petrov and Shlyapnikov demonstrated that when the temperature of atomic ensemble is much higher than the confinement strength, the confinement modifies the dynamics of elastic collisions of atoms and molecules only through changing the density distribution along the confining axis. This result indicates that

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the effect of the confinement on binary elastic collisions of atoms vanishes above a certain temperature. Our calculations here are based on accurate interatomic interaction potentials for ^{6}Li and ^{87}Rb atoms generated by fitting experimentally measured Feshbach resonances [27,28]. The main goal of this article is to identify the temperature intervals where the effects of the confinement on binary inelastic collisions and the suppression of inelastic collisions can be observed.

II. THEORY

A. Atomic mixture with 1D harmonic confinement

If a single laser field is used to confine a mixture of cold atoms, different atomic species will experience different trapping potentials. Here, we consider a cold mixture of Li and Rb atoms and denote the frequencies of the confining potentials for Li and Rb by $\omega_{\rm Li}$ and $\omega_{\rm Rb}$, respectively. Collision dynamics of the Li-Rb system in the presence of the confining laser force is determined by the following Hamiltonian (in atomic units):

$$\begin{aligned}\hat{H} = &-\frac{1}{2m_{\rm Li}}\Delta_{\rm Li} - \frac{1}{2m_{\rm Rb}}\Delta_{\rm Rb} \\ &+ \hat{V}(x_{\rm Li}, y_{\rm Li}, z_{\rm Li}, x_{\rm Rb}, y_{\rm Rb}, z_{\rm Rb}) \\ &+ \frac{1}{2}m_{\rm Li}\omega_{\rm Li}^2 z_{\rm Li}^2 + \frac{1}{2}m_{\rm Rb}\omega_{\rm Rb}^2 z_{\rm Rb}^2, \end{aligned} \tag{1}$$

where m denotes the atomic mass and $\hat{V}$ models the interatomic interaction potentials. Rewriting Eq. (1) in terms of the center-of-mass coordinates and the interatomic separation r, we obtain

$$\begin{aligned}\hat{H} = &-\frac{1}{2M}\Delta_{\rm c.m.} - \frac{1}{2\mu}\Delta_{\rm rel} + \hat{V}(r) \\ &+ \frac{1}{2}\left(m_{\rm Li}\omega_{\rm Li}^2 + m_{\rm Rb}\omega_{\rm Rb}^2\right)z_{\rm c.m.}^2 + \left(\omega_{\rm Rb}^2 - \omega_{\rm Li}^2\right)\mu z z_{\rm c.m.} \\ &+ \frac{1}{2}\left(\frac{\mu^2}{m_{\rm Li}}\omega_{\rm Li}^2 + \frac{\mu^2}{m_{\rm Rb}}\omega_{\rm Rb}^2\right)z^2, \end{aligned} \tag{2}$$

where $M = m_{\rm Li} + m_{\rm Rb}$, μ is the reduced mass of the Li-Rb collision complex, and $z_{\rm c.m.}$ and z describe the center-of-mass motion and the relative motion of particles along the z-axis, respectively.

We note that if $\omega_{\rm Li} \neq \omega_{\rm Rb}$, the center-of-mass motion and the relative motion of the collision complex are coupled by the term $(\omega_{\rm Rb}^2 - \omega_{\rm Li}^2)\mu z z_{\rm c.m.}$. If this term is significant enough, it may be possible to control the center-of-mass motion of the binary-collision complex by varying the difference between the frequencies. This can be achieved by applying an additional laser potential that would selectively modify one of the two frequencies. In our calculations, we assume that $\omega_{\rm Li} = \omega_{\rm Rb} = \omega$. As a result, the center-of-mass motion and the relative motion can be separated and the former can be omitted from the scattering problem.

B. Inelastic collisions of trapped particles in a particular oscillation state

The theory described in this article is general and applies to elastic, inelastic, and reactive collisions of ultracold atoms or molecules. We will therefore refer to the trapped particles generally as "atoms and molecules." In a tightly confined system, the strength of the harmonic potential can be described by the oscillation length $l_0 = \sqrt{\hbar/\mu\omega}$ of trapped particles. The oscillation length of the confining potential is usually much larger than the characteristic radius r_e of interatomic or intermolecular interaction potentials [29]. Therefore, at short interparticle separations $r < r_e$, the interaction between collision partners is not affected by the confining potential. The collision complex of atoms and molecules is therefore unconstrained and the collision process occurs in 3D. As a result of collisions that conserve the internal energy of the colliding particles (elastic collisions in an unconfined gas), the atoms or molecules may change their oscillation states while still remaining trapped in the harmonic potential. An inelastic collision or chemical reaction, however, releases a lot of energy and accelerates the collision products. As a result, atoms and molecules escape from the trap and are free to move in 3D, leading to trap loss. The theory of Petrov and Shlyapnikov [22] relates the scattering wave function of confined atoms in the region $r_e \ll r \ll \tilde{\Lambda}_\epsilon$ to the 3D wave function by a proportionality coefficient $\eta\varphi_\nu(0)$, where $\tilde{\Lambda}_\epsilon \sim \hbar/\sqrt{\mu(\epsilon + \hbar\omega/2)}$ is the characteristic de Broglie wavelength of the particles [22], φ_ν is the wave function for a particular oscillation state in the confining potential, and ϵ is the collision energy. In this study, we consider collision processes that induce transitions from state $(\alpha; l = 0; m_l = 0)$ (denoted hereafter by $\alpha 00$) to another state $\alpha' l' m_l'$, where l' is the rotational angular momentum of the collision complex in state α' and m_l' is the projection of l' on the quantization axis. We assume that particles are initially confined in a particular eigenstate ν of the harmonic potential and any transition $\alpha \to \alpha'$ results in loss of confinement. The indices α and α' are used to describe the internal energy as well as the chemical identity of the colliding particles (i.e., they specify the collision channels).

The probability of inelastic or chemically reactive collisions in 3D scattering is described by the elements $S_{\alpha'\leftarrow\alpha}$ of the scattering S-matrix [30]. For $r > r_e$, different collision channels are uncoupled, and we can treat the confined and unconfined collision channels separately. We express the s-wave component of the wave function for the confined channel α in a particular oscillation state ν at $r_e \ll r \ll \tilde{\Lambda}_\epsilon$ as a regular single-channel wave function in 3D multiplied by $\eta\varphi_\nu(0)$:

$$\psi_\alpha^\nu(r) = \frac{i\eta\varphi_\nu(0)}{2k_\alpha r}\left[e^{-ik_\alpha r} - S_{\alpha\leftarrow\alpha}e^{ik_\alpha r}\right]\phi_\alpha, \tag{3}$$

where k_α is the wave number of the collision complex, ϕ_α is the eigenfunction of the Hamiltonian at $r = \infty$, and $S_{\alpha\leftarrow\alpha}$ is the S-matrix element for elastic scattering in 3D. Repeating the derivation of Petrov and Shlyapnikov [22] and using Eq. (3), we obtain the following expression for η in terms of the S-matrix element:

$$\eta = \frac{\sqrt{4\pi}}{\frac{(1-S_{\alpha\leftarrow\alpha})\mathbf{w}(\epsilon/2\hbar\omega)}{ik_\alpha l_0} + \sqrt{\pi}(1 + S_{\alpha\leftarrow\alpha})}, \tag{4}$$

where $\mathbf{w}(\epsilon/2\hbar\omega)$ is a complex function [22]. This expression is more general than Eq. (17) in Ref. [22] because it is valid also in the temperature regime where the s-wave cross section cannot be represented by the square of the energy-independent

scattering length. Note that the expression for η in our previous communication [21] should be multiplied by $\sqrt{4\pi}$ and all cross sections for inelastic collisions reported in communication [21] should be multiplied by the factor 4π. This error does not modify any of the conclusions of Ref. [21].

In the region of $r_e \ll r \ll \tilde{\Lambda}_\epsilon$, the wave function given by Eq. (3) for channel α and oscillation state ν can be generally written as

$$\psi^{\nu}_{\alpha 00} = \frac{\upsilon_\alpha^{-\frac{1}{2}} r^{-1}}{\sqrt{4\pi}} \left[\mathscr{A}^{\nu}_{\alpha 00} e^{-ik_\alpha r} - \mathscr{B}^{\nu}_{\alpha 00} e^{ik_\alpha r} \right] \phi_\alpha, \tag{5}$$

where $\mathscr{A}^{\nu}_{\alpha 00}$ and $\mathscr{B}^{\nu}_{\alpha 00}$ are the amplitudes of the incoming and outgoing scattering waves, and υ_α is a normalization constant [31]. For $r_e \ll r \ll \tilde{\Lambda}_\epsilon$, $\mathscr{A}^{\nu}_{\alpha 00}$ can be written as $\chi_\nu A_{\alpha 00}$, where $A_{\alpha 00}$ is the amplitude of the incoming scattering wave for s-wave collisions in 3D. By comparing the coefficient in front of the term $e^{-ik_\alpha r}$ in Eq. (3) with that in Eq. (5) and using the conventional form $A_{\alpha 00} = i\sqrt{\pi}/k_\alpha$ [30], we obtain the coefficient

$$\chi_\nu = -\frac{i\sqrt{\pi}\eta\varphi_\nu(0)}{k_\alpha A_{\alpha 00}} = \eta\varphi_\nu(0). \tag{6}$$

The confinement thus modifies the amplitude of the incoming scattering wave in the 3D collision region $r_e \ll r \ll \tilde{\Lambda}_\epsilon$. Because the asymptotic motion of the collision products after a reactive or inelastic process is unconstrained, a combination of the exponential functions and 3D spherical harmonics should be used to describe the wave function in the outgoing collision channels:

$$\psi^{\nu}_{\alpha' l' m'_l} = -\upsilon_{\alpha'}^{-\frac{1}{2}} r^{-1} \mathscr{B}^{\nu}_{\alpha' l' m'_l} e^{i(k_{\alpha'} r - l'\pi/2)} \phi_{\alpha'} Y_{l' m'_l}(\hat{r}). \tag{7}$$

The 3D wave function after a collision ψ_{out} is related to the 3D wave function before the collision ψ_{in} by the S-matrix operator $\psi_{\text{out}} = \hat{S}\psi_{\text{in}}$. Therefore, the amplitudes of the outgoing scattering waves $\mathscr{B}^{\nu}_{\alpha' l' m'_l}$ are related to the amplitude of the incoming wave $\mathscr{A}^{\nu}_{\alpha 00}$ by the S-matrix elements

$$\mathscr{B}^{\nu}_{\alpha' l' m'_l} = S_{\alpha' l' m'_l \leftarrow \alpha 00} \mathscr{A}^{\nu}_{\alpha 00}. \tag{8}$$

Because the colliding particles are initially prepared only in the internal state α, the scattered part of the wave function in the inelastic channels is given by

$$\psi^{\nu}_{\text{sc(inel)}} = -\sum_{\alpha' \neq \alpha} \sum_{l'} \sum_{m'_l} \upsilon_{\alpha'}^{-\frac{1}{2}} r^{-1} S_{\alpha' l' m'_l \leftarrow \alpha 00} \chi_\nu \times \frac{i\sqrt{\pi}}{k_\alpha} e^{i(k_{\alpha'} r - l'\pi/2)} \phi_{\alpha'} Y_{l' m'_l}(\hat{r}). \tag{9}$$

The scattering amplitudes for inelastic collisions are defined as follows:

$$\psi^{\nu}_{\text{sc(inel)}} = \sum_{\alpha' \neq \alpha} \upsilon_{\alpha'}^{-\frac{1}{2}} f^{\nu}_{\alpha' \leftarrow \alpha} \left(\frac{e^{ik_{\alpha' r}}}{r} \right) \phi_{\alpha'}. \tag{10}$$

Comparing Eq. (9) with Eq. (10), we obtain the inelastic scattering amplitude

$$f^{\nu}_{\alpha' \leftarrow \alpha} = -\sum_{l'} \sum_{m'_l} S_{\alpha' l' m'_l \leftarrow \alpha 00} \chi_\nu \left(\frac{i\sqrt{\pi}}{i^{l'} k_\alpha} \right) Y_{l' m'_l}(\hat{r}), \tag{11}$$

which yields the integral cross section for inelastic or reactive scattering of atoms and molecules originally confined in a particular oscillation state ν:

$$\sigma^{\nu}_{\alpha' \leftarrow \alpha} = \sum_{l'} \sum_{m'_l} \frac{\pi}{k_\alpha^2} |\eta|^2 \varphi_\nu^2(0) |S_{\alpha' l' m'_l \leftarrow \alpha 00}|^2, \tag{12}$$

where η is given by Eq. (4) and $\varphi_\nu(0) = \frac{(\nu-1)!!}{\sqrt{\nu!}} (\pi l_0^2)^{-1/4}$.

C. Collision frequency for ultracold mixture in 1D trap

The mean collision frequency Ω is usually used to describe kinetic properties of atoms and molecules in a thermal gas. For a single-species system, Ω is given by

$$\Omega = \widetilde{n}\langle\alpha\rangle, \tag{13}$$

where $\widetilde{n}$ is the density of atoms and α is the collision rate constant. For a two-component gaseous mixture, Ω is related to the density of both species and has the following expression:

$$\Omega = \frac{n_{\text{A}} n_{\text{B}}}{n_{\text{A}} + n_{\text{B}}} \langle\alpha\rangle = n\langle\alpha\rangle, \tag{14}$$

where $n = n_{\text{A}} n_{\text{B}}/(n_{\text{A}} + n_{\text{B}})$, and n_{A} and n_{B} are the densities of species A and B, respectively.

At the temperature $T \geqslant \hbar\omega$, atoms and molecules in 1D optical lattices populate a manifold of states ν in the confining potential, where the distribution of the particles obeys the Boltzmann law. We can obtain the mean frequency for inelastic collisions by averaging inelastic cross sections over a Maxwell-Boltzmann velocity distribution and the oscillation states:

$$\Omega_{\text{inel}} = n \left\langle v \sum_{l'} \sum_{m'_l} |\eta|^2 \varphi_\nu^2(0) \frac{\pi}{k_\alpha^2} |S_{\alpha' l' m'_l \leftarrow \alpha 00}|^2 \right\rangle, \tag{15}$$

where v is the velocity of particles. During the collision process, the distance between two particles along the z-axis is much smaller than l_0 ($z \ll l_0$). Therefore, the contribution of the scattering amplitude from the part of the wave function corresponding to odd eigenstates of the harmonic potential is negligible. The mean collision frequency is thus an average over even values of ν [22]. Our numerical calculations show that the dependence of $|\eta|^2$ on the energy ϵ is no longer significant at $T \geqslant \hbar\omega$. We can therefore take $|\eta|^2$ out from the mean value [cf. Eq. (15)]. Note that Eq. (12) can be rewritten in terms of the proportionality coefficient and 3D cross sections $\sigma^{\text{3D}}_{\alpha' \leftarrow \alpha}$: $\sigma^{\nu}_{\alpha' \leftarrow \alpha} = |\eta|^2 \varphi_\nu^2(0) \sigma^{\text{3D}}_{\alpha' \leftarrow \alpha}$. In order to get an analytical expression for Ω_{inel}, we expand $\sigma^{\text{3D}}_{\alpha' \leftarrow \alpha}$ as $\sigma^{\text{3D}}_{\alpha' \leftarrow \alpha} = -4\pi \text{Im}(a)/k + \beta$ [32]. Here, a is the zero-temperature scattering length for ultracold particles in state α and β is a fitting constant. The values of a and β are obtained from rigorous multichannel scattering calculations. The analytical expression for the mean frequency of inelastic collisions at $T \geqslant \hbar\omega$ is thus given by

$$\Omega_{\text{inel}} = \frac{n}{2} |\eta|^2 \left[-\frac{4\pi\hbar \text{Im}(a)}{\mu} + \beta \left(\frac{8 k_{\text{B}} T}{\pi \mu} \right)^{\frac{1}{2}} \right] \times \frac{1}{\sqrt{\pi} l_0} \tanh^{\frac{1}{2}} \left(\frac{\hbar\omega}{k_{\text{B}} T} \right). \tag{16}$$

It might be interesting to analyze the high-temperature limit of Eq. (16). In order to do this, we express $\Omega_{\rm inel}$ in terms of the axial momentum $\vec{k}$ as follows:

$$\Omega_{\rm inel} = \sum_{\nu} n \iint_{-\infty}^{+\infty} \frac{\hbar^2}{2\pi\mu k_{\rm B}T} \left(v\sigma^{\nu}_{\alpha'\leftarrow\alpha}\right) A e^{-\epsilon/k_{\rm B}T} d^2\vec{k}. \quad (17)$$

where $A = 1 - \exp(-\hbar\omega/k_{\rm B}T)$ is the normalization factor. Because our expression for inelastic cross sections of atoms and molecules under confinement is written in terms of 3D S-matrix elements, we need to average the rate constant over the 3D momentum $k = (k_x^2 + k_y^2 + k_z^2)^{1/2}$. When the temperature of atoms and molecules in 1D optical lattices is much higher than the confinement strength, i.e., $T \gg \hbar\omega$, $\varphi_\nu^2(0) \approx (\frac{1}{\pi l_0^2})^{\frac{1}{2}}(\frac{2}{\pi\nu})^{\frac{1}{2}}$, we can replace the summation over ν with an integral. Converting the integration over ν to an integration over $\vec{k}_z$, using the relation $k_z^2 = 2\nu/l_0^2$, and integrating out the angular part of the axial momentum, we obtain the following expression for the inelastic collision frequency:

$$\Omega_{\rm inel}^{T\gg\hbar\omega} = n \int_0^{+\infty} \frac{\hbar^2}{4\pi^2\mu k_{\rm B}T} (v\sigma_{\rm 3D})|\eta|^2 \times A \exp\left(-\frac{\hbar^2k^2}{2\mu k_{\rm B}T}\right) 4\pi k^2 dk, \quad (18)$$

which yields

$$\Omega_{\rm inel}^{T\gg\hbar\omega} = 2nA|\eta|^2 \left[-\frac{{\rm Im}(a)}{\mu}\sqrt{2\pi\mu k_{\rm B}T} + \frac{\beta k_{\rm B}T}{\pi\hbar}\right]. \quad (19)$$

At temperatures $T \gg \hbar\omega$, $|\eta| \sim 1$ and Eq. (18) coincides with the expression for the average 3D rate constant multiplied by the density distribution in a 1D optical lattice, which is given by

$$\Omega_{\rm 3D} = \frac{1}{N}\int n_{\rm B_A}(z)\langle v\sigma_{\rm inel}^{\rm 3D}\rangle n_{\rm B_B}(z) dx dy dz. \quad (20)$$

Here, N is the total number of particles in the trap, and

$$n_{\rm B_{A(B)}}(z) = \frac{n_{\rm A(B)}}{\sqrt{\pi R_{\rm A(B)}^2}} e^{-z^2/R_{\rm A(B)}^2} \quad (21)$$

is the classical Boltzmann density profile along the z-axis for particles in a harmonic potential with $R_{\rm A(B)}^2 = 2k_{\rm B}T m_{\rm A(B)}^{-1}\omega^{-2}$. That Eq. (18) coincides with Eq. (20) at high temperatures is consistent with the results for elastic collisions of atoms under confinement [22]. It indicates that at high temperatures, the confinement modifies the dynamics of a confined quantum gas only through changing the density distribution of atoms and molecules in a 1D optical lattice.

III. NUMERICAL RESULTS

The experimental realization of ultracold atomic and molecular ensembles confined in optical lattices has been achieved by many research groups [9–17]. The study of kinetic properties of quantum gases in restricted geometries is therefore of significant interest to researchers of ultracold atoms and molecules. Here, we present the results of rigorous multichannel calculations of collision frequencies for inelastic collisions and the inelastic-to-elastic ratios of collision rate constants for Li and Rb atoms confined in 1D optical lattices. Our study focusses on the collision dynamics of confined atoms in the confinement-dominated 3D regime, where $T \sim \hbar\omega$, and at temperatures $T \gg \hbar\omega$. Based on calculations using accurate interatomic interaction potentials [27], our results demonstrate the effect of the confining potential on inelastic collisions of Li and Rb atoms in 1D optical lattices and provide guidance for future experiments as to when this effect is significant and can be observed experimentally.

Equation (12) gives an expression for the cross sections for inelastic or reactive scattering of atoms and molecules initially confined in a particular oscillation state ν. However, this expression, derived in terms of the 3D S-matrix elements, cannot be used to obtain a general analytical formula for inelastic collision frequencies in the confinement-dominated 3D regime. For our calculations, we rewrite Eq. (12) as the product of a proportionality coefficient and the 3D inelastic cross section. The latter can be represented as a series expansion in relative momentum of the colliding particles [32]. This allows us to obtain the analytical expressions for the mean frequency of inelastic collisions at temperatures $T > \hbar\omega$. Our numerical calculations show that at a collision energy of 10^{-3} cm^{-1} and a magnetic field of 200 G, the cross section for s-wave inelastic collisions of Li in the state $|f = \frac{1}{2}, m_f = -\frac{1}{2}\rangle_{^6{\rm Li}}$ with Rb in the state $|f = 1, m_f = 0\rangle_{^{87}{\rm Rb}}$ is 5.35 bohr^2. The notation $|fm_f\rangle$ is used to label different energy states of Rb and Li atoms, where f and m_f refer to the total atomic spin and its projection, respectively [27]. The s-wave cross section is 50 times larger than the cross section for p-wave inelastic collisions 0.114 bohr^2. Therefore, p-wave scattering of Li and Rb can be neglected for $T < 10^{-3}$ K. The s-wave scattering cross section at collision energies corresponding to $T < 10^{-3}$ K obtained from our numerical calculations can be well approximated by the two leading terms in the momentum expansion: $\sigma_{\rm inel}^{\rm 3D} = -4\pi{\rm Im}(a)/k + \beta$ [32]. The reader should be cautioned that this expansion may not be valid for inelastic cross sections near Feshbach resonances. Instead, the Breit–Wigner expression should be used to fit the cross sections near a resonance.

Petrov and Shlyapnikov showed that elastic collisions of atoms in a tightly confined cold gas deviate from regular 3D collision behavior in the confinement-dominated 3D regime [22]. Here, we study the effect of the confinement on inelastic collisions of atoms in this regime. Our results are consistent with their observation. Figure 1 shows the quantities Ω/n and $\Omega_{\rm 3D}/n$ for s-wave inelastic collisions of ^{6}Li and ^{87}Rb atoms in the states $|f = \frac{1}{2}, m_f = -\frac{1}{2}\rangle_{^6{\rm Li}} \otimes |f = 1, m_f = 0\rangle_{^{87}{\rm Rb}}$ in 1D optical lattices as functions of the temperature of the atomic ensemble for two different confining potentials with $l_0 =$ 600 bohr and $l_0 = 1000$ bohr. The calculation is for a magnetic field of 200 G, which yields the scattering length $|a| = 13.58$ bohr. The S-matrix elements were computed as described in Ref. [30]. We find a substantial deviation of the scattering cross sections for inelastic collisions in the confinement-dominated 3D regime from the 3D cross sections. This deviation is more significant for stronger confinement. As the temperature of the atoms increases, the effect of the confinement becomes less significant and the mean collision frequency of the atomic ensemble gradually merges to that

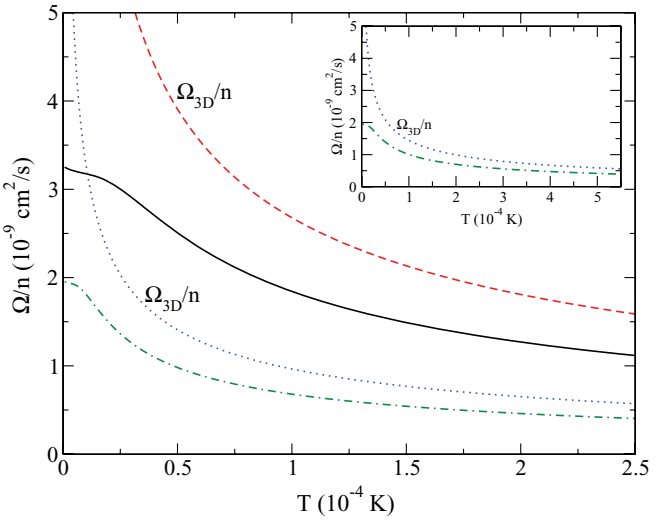

FIG. 1. (Color online) The quantities Ω/n and Ω_{3D}/n for s-wave inelastic collisions of ^{6}Li and ^{87}Rb atoms confined in 1D optical lattices as functions of the temperature of the atomic ensemble for the confining potential with $l_0 = 600$ bohr (solid and dashed curves, respectively) and $l_0 = 1000$ bohr (dot-dashed and dotted curves, respectively). The inset shows the merging of Ω/n and Ω_{3D}/n at $T \gg \hbar\omega$ for the confining potential with $l_0 = 1000$ bohr. The initial atomic states are $|f = \frac{1}{2}, m_f = -\frac{1}{2}\rangle_{^6\mathrm{Li}}$ and $|f = 1, m_f = 0\rangle_{^{87}\mathrm{Rb}}$. The magnetic field $B = 200$ G ($|a| = 13.58$ bohr).

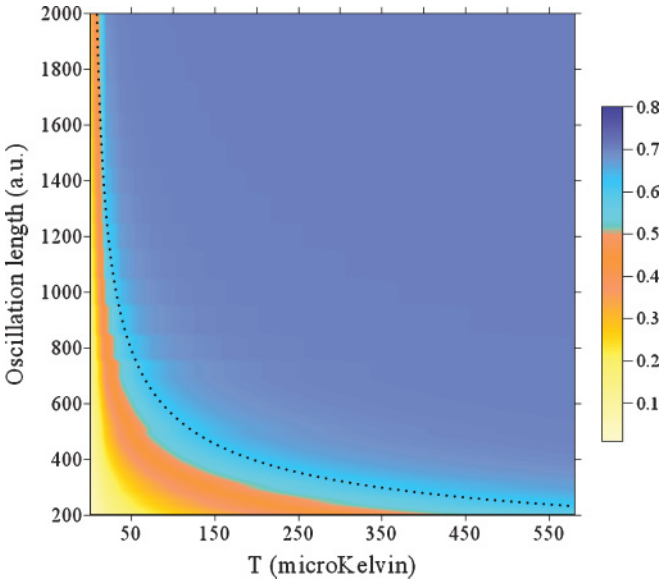

FIG. 2. (Color online) The ratio Ω/Ω_{3D} for s-wave inelastic collisions of ^{6}Li and ^{87}Rb atoms confined in 1D optical lattices as functions of the temperature of the atomic ensemble and the confining potentials. The dotted curve shows the locus of points where $T = \hbar\omega$. The initial hyperfine atomic states are $|f = \frac{1}{2}, m_f = -\frac{1}{2}\rangle_{^6\mathrm{Li}}$ and $|f = 1, m_f = 0\rangle_{^{87}\mathrm{Rb}}$. The magnetic field $B = 200$ G ($|a| = 13.58$ bohr).

in the 3D regime, as shown in the inset of Fig. 1. However, this merging is slow, which is consistent with the previous observation of the effect of laser confinement on inelastic collisions induced by perturbative weak interactions [22].

The merging of Ω/n to Ω_{3D}/n at high temperatures indicates that the effect of confinement on binary inelastic collisions of atoms is not significant for certain combinations of the confining potential strength and temperature. In order to explore in detail the effect of confinement on inelastic collisions, we plot in Fig. 2 the ratios Ω/Ω_{3D} for s-wave inelastic collisions of ^{6}Li and ^{87}Rb atoms as functions of the confining potential strength and the temperature of the atomic ensemble. The dotted curve shows the locus of points where $T = \hbar\omega$. This graph demonstrates that the effect of the confinement on binary inelastic collisions is significant at temperatures $T \leqslant \hbar\omega$. We find a critical temperature of about 20 μK, below which a significant difference between Ω and Ω_{3D} for inelastic collisions can be observed for harmonic potentials with different strengths. In the presence of the confining potential with $l_0 < 800$ bohr, one can observe an effect of the confinement on inelastic collisions at temperatures greater than 20 μK. For a tight confinement with $l_0 < 300$ a.u., the effect of the laser field on inelastic scattering is significant at temperatures as high as 250 μK. We also notice that the increase of the ratio Ω/Ω_{3D} is very slow in the region of high temperatures (i.e., $T > 100$ μK) and large oscillation lengths (i.e., $l_0 > 600$ bohr), which is consistent with the observation in Fig. 1.

In the experiments with optical lattices, one can control collision dynamics of atoms and molecules by varying the scattering length of the system in addition to modifying the strength of the confining potential and the temperature of the atomic ensemble. Figure 3 shows the quantities Ω/n and Ω_{3D}/n for s-wave inelastic collisions of ^{6}Li and ^{87}Rb atoms confined in 1D optical lattices as functions of temperature for two values of the scattering length. The calculations were performed with the values of the magnetic field fixed at 200 G ($|a| = 13.58$ bohr) and 1104.9 G ($|a| = 1708.26$ bohr). The confinement has a more significant effect on inelastic collisions of atoms with larger scattering length, which can be used as an additional tool to control the dynamics of inelastic collisions in a confined gas. Here, the calculations for $|a| = 1708.26$ bohr are performed at collision energies below 10^{-5} K because inelastic cross sections of ^{6}Li and ^{87}Rb atoms near Feshbach resonances can be approximated by the momentum expansion only in this temperature region. In the presence of a weak confinement (e.g., $l_0 = 5000$ bohr), atoms and molecules are still in the confinement-dominated 3D regime at these low temperatures.

In our previous communication, we demonstrated that the elastic-to-inelastic ratio of cross sections for collisions of atoms and molecules confined in a quasi-2D geometry is dramatically enhanced. The present calculations show that this trend can also be observed for atoms in the confinement-dominated 3D regime. Figure 4 displays the ratios of the mean collision rate constants for s-wave inelastic and elastic collisions of ^{6}Li and ^{87}Rb atoms in an unconfined gas and in a gas confined by 1D optical lattices with different confinement strengths. We find that inelastic collisions are suppressed more significantly than elastic collisions in the confinement-dominated 3D regime. The suppression is more significant for stronger confinement. Figure 4 shows that the inelastic-to-elastic ratio for the 3D uniform gas decreases dramatically as the temperature of the gas increases, whereas the ratios for the confined gas slightly increase with increasing

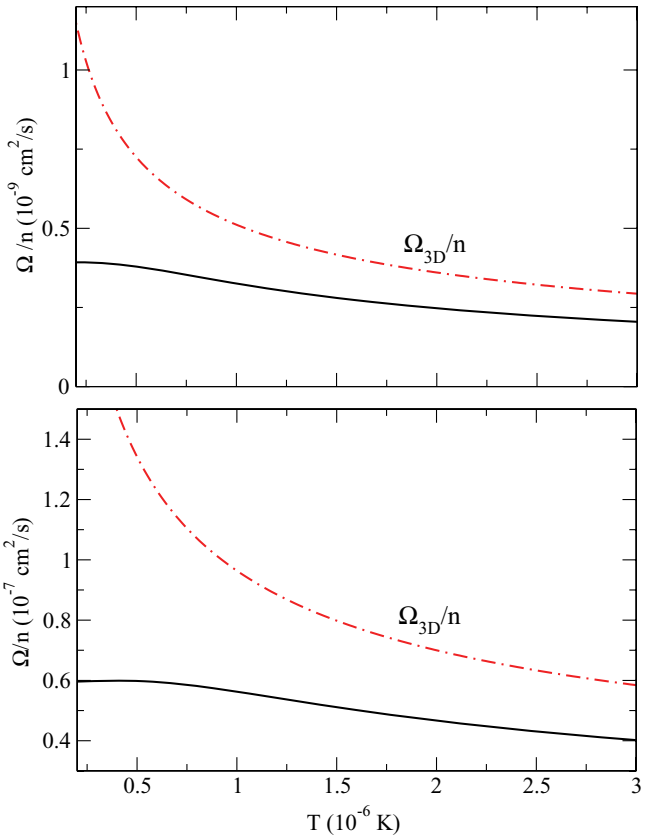

FIG. 3. (Color online) The quantities Ω/n and Ω_{3D}/n for s-wave inelastic collisions of ^{6}Li and ^{87}Rb atoms confined in 1D optical lattices as functions of the temperature of the atomic ensemble for a small scattering length $|a| = 13.58$ bohr (solid and dot-dashed curves in upper panel, respectively) and for a large scattering length $|a| = 1708.26$ bohr (solid and dot-dashed curves in lower panel, respectively). The initial atomic states are $|f = \frac{1}{2}, m_f = -\frac{1}{2}\rangle_{^6\mathrm{Li}}$ and $|f = 1, m_f = 0\rangle_{^{87}\mathrm{Rb}}$. The oscillation length of the trap $l_0 = 5000$ bohr.

temperature. These results indicate that confined systems may be more stable than a 3D unconfined gas against inelastic collisional losses in the presence of strong laser-field potential and at low temperatures. Our results suggest that it may be possible to observe significant suppression of inelastic collisions in a tightly confined gas at temperatures below 40 μK.

IV. SUMMARY

We have presented a formalism for rigorous multichannel scattering calculations of cross sections for inelastic collisions of atoms and molecules confined in 1D optical lattices. The theory provides expressions for inelastic and reactive scattering cross sections in terms of the S-matrix elements for collisions in 3D and the laser confinement parameters. These expressions are general and valid even in the temperature regime where the cross section for s-wave elastic scattering is energy dependent and the cross section for s-wave inelastic scattering is no longer inversely proportional to the collision velocity. Petrov and Shlyapnikov have developed a formalism based on perturbation theory to study inelastic collisions

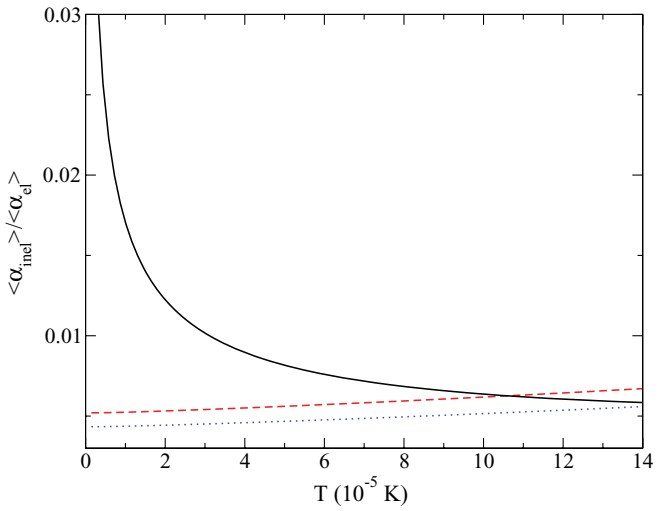

FIG. 4. (Color online) Inelastic-to-elastic ratios of the mean collision rate constants for s-wave scattering of ^{6}Li and ^{87}Rb atoms in a 3D uniform gas (solid curve) and a gas confined in 1D optical lattices with $l_0 = 600$ bohr (dotted curve) and $l_0 = 500$ bohr (dashed curve) as functions of the temperature of the atomic ensemble. The initial hyperfine atomic states are $|f = \frac{1}{2}, m_f = -\frac{1}{2}\rangle_{^6\mathrm{Li}}$ and $|f = 1, m_f = 0\rangle_{^{87}\mathrm{Rb}}$. The magnetic field $B = 200$ G ($|a| = 13.58$ bohr).

induced by weak interatomic interactions (such as the magnetic dipole-dipole interaction in collisions of alkali metal atoms) [22]. Our derivations and calculations are consistent with their results. Schmelcher and coworkers have recently developed a theory to describe collision-induced transitions of confined atoms and molecules between different oscillation states in a harmonic trap [25,33,34]. Our theory generalizes the results of Ref. [22] and can be used in conjunction with the theory in Refs. [25,33,34] for a complete description of the kinetics of ultracold gases in optical lattices. Direct numerical integration of the Schrödinger equation to obtain the probability of inelastic and reactive collisions of molecules in the presence of laser fields is prohibitively difficult. Our theory presented here makes the analysis of reactive collisions of atoms and molecules in confined geometries feasible.

We have obtained analytical expressions for the mean frequency of inelastic collisions in a confined gas in the confinement-dominated 3D regime, where $T \sim \hbar\omega$, and at temperatures $T \gg \hbar\omega$. Using these expressions, we carried out rigorous multi-channel scattering calculations of inelastic collision rates in a gaseous mixture of Li and Rb atoms. We demonstrated that inelastic collisions in the confinement-dominated 3D regime exhibit a deviation from 3D scattering, and that this deviation is more significant for systems with stronger confining potentials and larger scattering lengths. As the temperature of the atomic ensemble increases, the effect of the confinement on binary inelastic collisions becomes vanishingly small. Our calculations suggest combinations of the confining potential strength and temperature for which the effect of the confinement on binary inelastic collisions is significant. We also find a critical temperature of about 20 μK, below which the confinement with different strengths can influence inelastic collisions of confined atoms to a great extent. In addition, our results show that inelastic collisions

are suppressed more significantly than elastic collisions in the confinement-dominated 3D regime. The suppression is more significant for stronger confinement, and our results suggest that it may be possible to observe significant suppression of inelastic collisions in a tightly confined gas at temperatures below 40 μK. The calculations presented in this article are based on accurate interatomic interaction potentials and our results therefore provide guidance for future experiments.

The results presented in this article should be of significant immediate interest to researchers of ultracold atoms and molecules since it is currently feasible to create atomic and molecular systems confined in 1D optical lattices. Our work may also stimulate new experimental studies as the suppression of inelastic processes may allow for the creation of ultracold atoms in quantum states that are unstable in the usual experiments. In addition, our work suggests new research directions for the study of ultracold chemistry in the temperature regime where chemical reactions can be influenced by varying the strength and shape of the laser-field potential.

ACKNOWLEDGMENTS

I would like to thank Roman Krems, Kirk Madison, and Xuan Li for useful discussions. This work is supported by NSERC of Canada.

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