Collisional Aspects of Bosonic and Fermionic Dipoles in Quasi-Two-Dimensional Confining Geometries

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Fundamental aspects of ultracold collisions between identical bosonic or fermionic dipoles are studied under quasi-two-dimensional (Q2D) confinement. In the strongly dipolar regime, bosonic and fermion species are found to share important collisional properties as a result of the confining geometry, which suppresses the inelastic rates irrespective of the quantum statistics obeyed. A potential negative is that the confinement causes dipole-dipole resonances to be extremely narrow, which could make it difficult to explore Q2D dipolar gases with tunable interactions. Such properties are shown to be universal, and a simple WKB model reproduces most of our numerical results. In order to shed light on the many-body behavior of dipolar gases in Q2D we have analyzed the scattering amplitude and developed an energy-analytic form of the pseudopotentials for dipoles. For specific values of the dipolar interaction, the pseudopotential coefficient can be tuned to arbitrarily large values, indicating the possibility of realizing Q2D dipolar gases with tunable interactions.

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Extensive experimental and theoretical efforts have recently been devoted to explore the production of dipolar gases and to uncover novel quantum phases resulting from the anisotropic nature and long-range character of the dipolar interaction [1]. The recent experimental realization of a dense sample of ultracold ground-state KRb molecules [2] has opened up ways to realize several new phenomena, ranging from ultracold chemistry, condensed matter physics and quantum information [2–4]. A crucial step towards realizing such ideas is to understand the collisional properties of dipoles at ultralow temperatures. In fact, recent theoretical work has proposed a classification of ground-state molecules in terms of their chemical reactivity [5]. A number of such molecules are expected to be extremely reactive while others have energetically forbidden decay channels. Although reactive molecules are great candidates for studying chemical dynamics [2, 3], such processes limit the lifetime of the gas. The introduction of a quasi-two-dimensional confinement (Q2D) adds a new handle for controlling the physics of the problem [6], which drastically changes this scenario [7, 8] and ultimately leads to improved stability. This should in turn enable an exploration of various many-body phenomena.

In this paper, we explore the effect of Q2D confinement on collisions of bosonic and fermionic dipolar species. We have found that in the strong dipolar regime the ultracold scattering properties of Q2D dipoles do not depend on the details of the short-range interactions. The effective interactions are also characterized by calculating the Q2D pseudopotential coupling constants. Our analysis shows that at *any* finite collision energy there exists a value of the dipolar interaction at which the coupling constant diverges, a phenomenon that can be traced back to the Ramsauer-Townsend effect. Although our present analysis does not address the issues of implementing our pseudopodential formalism to the many-body problem, we believe that our findings can shed light on the possible ways of controlling the interactions in a dipolar gas.

In order to study dipolar collisions in Q2D, an adiabatic separation of the radial and angular motion is introduced. This expresses the wavefunction as $\Psi(\vec{r}) = e^{im\phi}\sum_\nu r^{-1}F_\nu(r)\Phi_\nu(r;\theta)$, where r, θ, and ϕ, are the spherical radius and angles, respectively, and m is the angular momentum projection. Here, ν is the channel index, F_ν is the ν-th radial wave function and Φ is the channel function. In the adiabatic representation, the Schrödinger equation reduces to a simple system of ordinary differential equations given (in atomic units) by,

$$\left[-\frac{1}{2\mu}\frac{d^2}{dr^2} + W_\nu(r) - E\right]F_\nu + \sum_{\nu'\neq\nu} W_{\nu\nu'}(r)F_{\nu'} = 0, \quad (1)$$

where μ is the two-body reduced mass, E is the total energy, $W_{\nu\nu'} = -\left(P_{\nu\nu'}\partial/\partial r + Q_{\nu\nu'}\right)/2\mu$, with $P_{\nu\nu'} = \langle\Phi_\nu|\partial/\partial r|\Phi_{\nu'}\rangle$ and $Q_{\nu\nu'} = \langle\Phi_\nu|\partial^2/\partial r^2|\Phi_{\nu'}\rangle$, are the nonadiabatic couplings which drive inelastic transitions, and $W_\nu = U_\nu - Q_{\nu\nu}/2\mu$ are the adiabatic potentials supporting bound and quasi-bound states. The adiabatic potentials and channel functions are obtained by solving eigenvalue equation for the angular motion:

$$\left[-\frac{1}{2\mu r^2}\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} - \frac{m^2}{\sin^2\theta}\right) + v_{sr}(r) + \frac{d_\ell}{\mu}\frac{1-3\cos^2\theta}{r^3} + \frac{r^2\cos^2\theta}{2\mu a_{ho}^4} - U_\nu(r)\right]\Phi_\nu(r;\theta) = 0, \quad (2)$$

solved for fixed values of r and in concert with the proper bosonic and fermionic boundary conditions at $\theta = \pi/2$. In the equation above, $v_{sr}(r) = D\mathrm{sech}^2(r/r_0)$ is the short-range isotropic potential, where r_0 is the characteristic range of the interactions (similar to the van der Waals length), and the next two terms are the anisotropic dipole-dipole and Q2D confinement potentials, respectively. The dipolar interaction and confinement introduce two new important length scales into the system,

namely, the "dipole length" $d_\ell = \mu d_m^2$, where d_m is the dipole moment in a.u., and the reduced-mass oscillator length $a_{ho}^2 = \mu w_{ho}$, where w_{ho} is the harmonic trap frequency experienced by each molecule in the $\hat{z}$ direction.

In Figure 1 we show a set of adiabatic potentials obtained by solving Eq. (2) for the lowest bosonic ($m = 0$) and fermionic ($m = 1$) symmetries with even z-reflection parity. For distances $r \lesssim a_{ho}$, the adiabatic potentials are mainly controlled by the short-range interactions (v_{sr} and dipolar). As r increases the confinement becomes important and the transition between 3D and 2D physics is characterized by the series of avoided crossings along the values of the averaged confinement potential $r^2/\mu a_{ho}^4$ (see the solid curve in Fig. 1). For ultracold collisions, however, the scattering properties are mainly determined by the asymptotic forms of the adiabatic potentials which we found, for $r \gg r_{ho} = (4a_{ho}^4 d_\ell)^{1/5}$, to be given by

$$W_\nu(r) \approx E_{ho}^{(\nu)} + \frac{m^2 - 1/4}{2\mu r^2} + \frac{d_\ell}{\mu r^3}. \qquad (3)$$

Here $E_{ho}^{(\nu)} = (n_\nu + 1/2)/\mu a_{ho}^2$ is the oscillator energy level and n_ν is the principal quantum number. Notice that in contrast to the 3D case [9] the dipolar interaction at large r is repulsive $1/r^3$ for *both* bosonic and fermionic species. This fact has important consequences for the collisional properties of dipoles in Q2D, as we discuss below.

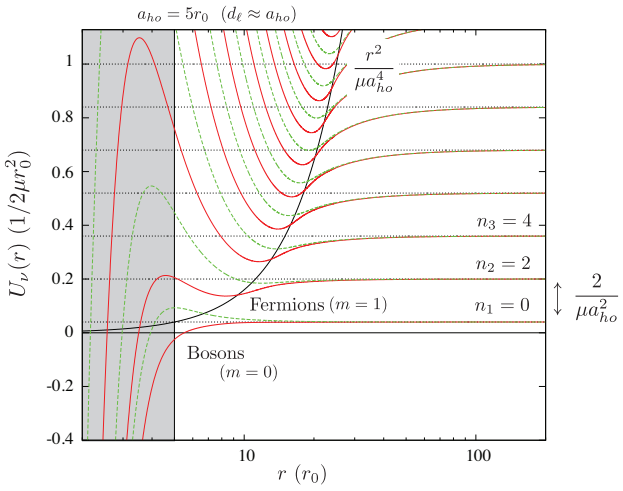

FIG. 1: (color online). Adiabatic potentials for Q2D bosonic (solid) and fermionic (dashed) dipoles (see text).

Having determined the adiabatic potentials and couplings, we calculate elastic and inelastic rates by solving Eq. (1) and matching our numerical solutions to the proper cylindrical asymptotic solutions to obtain the corresponding T-matrix and the collision rate coefficients [8],

$$\mathcal{K}_{el} = \frac{2\hbar}{\mu} \sum_{m,f} \Delta_m |T_{i\leftarrow i}^{(m)}|^2, \quad \mathcal{K}_{in} = \frac{2\hbar}{\mu} \sum_{m,f} \Delta_m |T_{f\leftarrow i}^{(m)}|^2, \qquad (4)$$

where $\Delta_m = 2 - \delta_{m,0}$ and i and f label the initial and final collision channels. Here, we study collisions from the lowest transverse mode ($n_1 = 0$ in Fig. 1) and we have added an artificial deeply bound channel (with adjustable coupling) to incorporate the effects of inelastic collisions relevant for reactive ground-state polar molecules [5].

In general, a calculation of elastic and inelastic rates in the strong dipolar regime, $kd_\ell \gg 1$, where $k^2 = 2\mu(E - E_{ho}^{(0)})$, requires the inclusion of a large number of partial waves in Eq. (4). Here, however, we have found that the rates in this regime assume a universal form, allowing for a simple WKB model for the phase-shifts that tremendously economizes the calculations. We compare our numerical results for the elastic rates for $m = 0$ and 1 with the WKB model in order to demonstrate this universality and present the calculation for the total rates [Eq. (4)] for values of m up to 200 using our WKB result. The topology of the adiabatic potentials (Fig. 1) allows us to directly apply the WKB phase-shift formula derived in Ref. [10]. Here, however, we write the phase-shift as a sum of two terms,

$$\delta_m(k) = \delta_m^{lr}(k) + \delta_m^{sr}(k), \qquad (5)$$

where $\delta_m^{lr} = \int_{r_m^c}^{\infty} [K_m(r) - k]\, dr + \frac{\pi}{2} m - k r_m^c$ is the long-range phase-shift, r_m^c being the classical turning point [11], and $\delta_m^{sr} = \tan^{-1}[\frac{1}{4} e^{-2\gamma_m} \tan \Phi_m^{sr}]$ is the short-range phase-shift. Here $K_m(r) = [k^2 - (2d_\ell + m^2 r)/r^3]^{1/2}$, $e^{-2\gamma_m} = \exp[-2 \int_{r_{ho}}^{r_m^c} |K_m(r)| dr]$. In our formulation, the only non-universal part of the phase-shift comes from δ_m^{sr} through the phase Φ_m^{sr} accumulated for $r < r_{ho}$. We have determined, however, that for $kd_\ell \gg 1$, the phase δ_m^{sr} is exponentially small [$\gamma_m \propto (d_\ell/a_{ho})^{2/5}$], due to the $1/r^3$ barrier in the entrance channel [Eq. (3)], except in an extremely narrow region near a dipole-dipole resonance [12]. As a result the scattering problem becomes universal, depending *only* on the long-range physics encapsulated in $\delta_m^{lr} \equiv \delta_m^{lr}(k, d_\ell)$. The fact that, in Q2D, dipole-dipole resonances are extremely narrow, seems likely to make the exploration of Q2D dipolar gases with tunable interactions prohibitively difficult. However, as we will show later, tunability is still possible, although instead due to the physics of the Ramsauer-Townsend effect.

Figure 2 demonstrates some of these points through our numerical calculations (for $m = 0$ and 1) and WKB results for the partial rates $\mathcal{K}_{el}^m = (8\hbar/\mu)\Delta_m \sin^2 \delta_m(k)$ and $\mathcal{K}_{in}^m$ for $a_{ho}/r_0 = 5$ and $k = 0.071/r_0$ (vertical lines in Fig. 2). Figs. 2 (a) and (d) compare our numerical results for $m = 0$ and $m = 1$ (thick dashed lines) with the WKB results from Eq. (5) (thin dot-dashed lines). Extremely good agreement is found for $kd_\ell > 1$, but for $kd_\ell < 1$, this agreement deteriorates and dipole-dipole resonances [12] becomes visible. In fact, throughout the entire range of values of d_ℓ there exist dipole-dipole resonances, but as we mentioned above, they are extremely narrow and only become visible in the inelastic rates [Figs. 2 (b) and (e)]. Interestingly, all partial rates oscillate as d_ℓ increases, as a result of the Ramsauer-Townsend effect. Evidently,

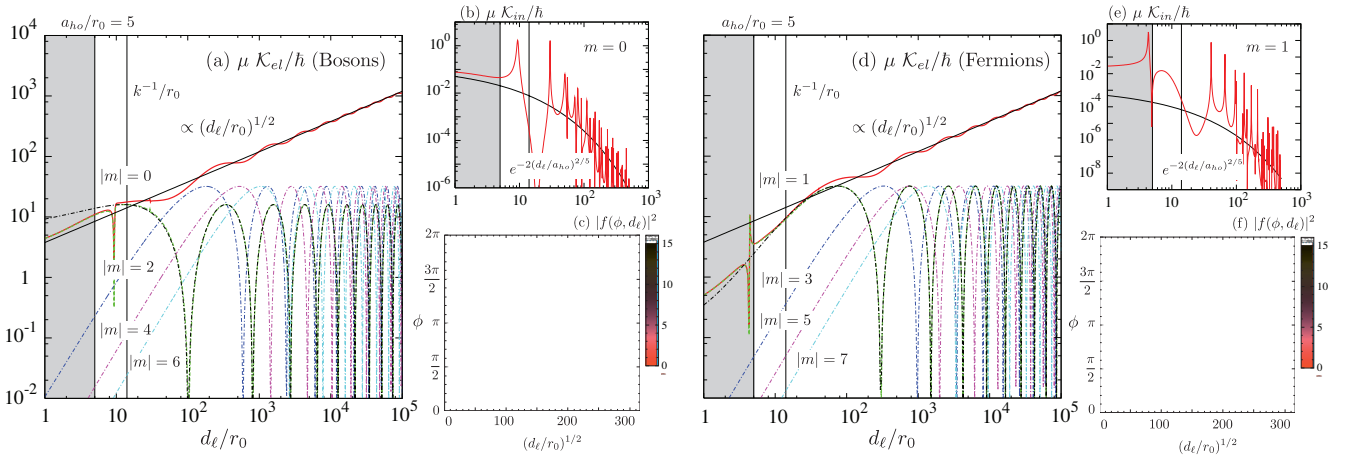

FIG. 2: (color online). Elastic and inelastic rates for bosonic, (a) and (b), and fermionic, (d) and (e), dipoles as a function of d_ℓ for $a_{ho} = 5r_0$ and $k = 0.071r_0^{-1}$. In the strongly dipolar regime, $kd_\ell \gg 1$, the elastic rates approaches to their semi-classical expectation [7] [solid straight line in (a) and (d)] and the inelastic rates are strongly suppressed [(b) and (e)]. (c) and (f) shows the scattering amplitude displaying anisotropy effects (see text).

the total rates will not display actual zeros since the partial rates are out of phase. Nevertheless, the total rates, shown in Figs. 2 (a) and (d) as solid lines, oscillate around the semi-classical result of Ref. [7] (solid straight line). Still, such oscillations are universal and reflect the Ramsauer-Townsend effect. Figures 2 (b) and (e) also show another dramatic effect due to the Q2D confinement. The inelastic rates for *both* bosonic and fermionic dipoles are suppressed as $\exp[-2(d_\ell/a_{ho})^{2/5}]$ for values of d_ℓ beyond a_{ho}, in agreement with Ref. [7]. This result emphasizes the importance of the confinement in allowing for the realization of stable ultracold dipolar gases, irrespective of their quantum statistics.

Figures 2 (c) and (f) shows other properties of dipolar scattering through plots of the scattering amplitude versus the azimuthal angle, ϕ, and d_ℓ. As one can see, the dipolar scattering is by itself anisotropic. For both bosonic and fermionic dipoles [Figs. 2 (c) and (d)], the preferential outgoing scattering flux occurs around $\phi = 0$, π, and 2π. Therefore, two dipoles tend to scatter in such a way that they can either completely repel or else simply "ignore" each other. Nevertheless, our results also show that there exist other specific directions in which dipoles can scatter. These are indicated by the less intense "fringes" between the maximum values of the scattering amplitude. From a more general perspective, the properties of the scattering amplitude could prove useful in many-body theories of dipolar gases [13].

Another way to analyze the many-body behavior is through the pseudopotentials for Q2D dipoles [14, 15]. However, pseudopotentials for dipoles (both in 3D and Q2D) suffer from a number of still-unresolved problems in the limit $k \to 0$, and thus their applicability in many-body contexts has remained questionable. Here, we propose a modified version of Q2D potentials

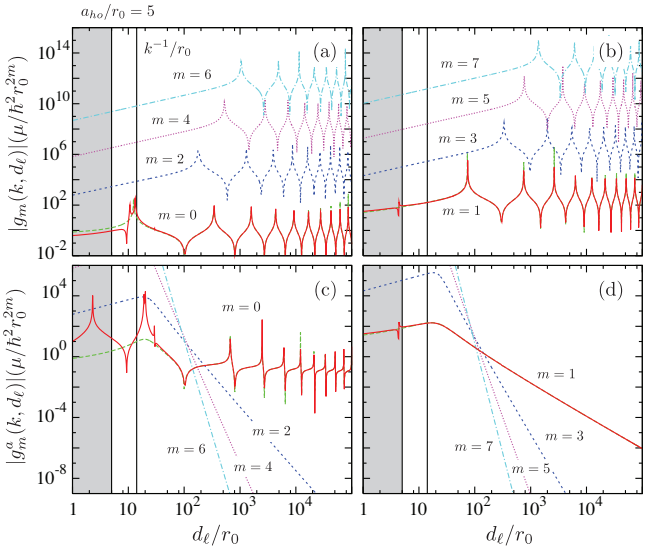

FIG. 3: (color online). (a) Q2D coupling constant, g_m, and (b) its equivalent energy-analytic form, g_m^a. Figure shows interesting "resonant" behavior related to the Ramsauer-Townsend (see text).

which eliminates the non-analyticity of the pseudopotentials in the limit $k \to 0$. Our approach consists in determining the pseudopotentials with respect to the energy analytic radial 2D solutions in the spirit of generalized quantum defect theory [16]. In the present case this amounts to replacing the usual regular and irregular Bessel solutions by a new pair that are both entire analytic functions of energy: $F_m^a = (kb)^{-m} J_m(kr)$ and $G_m^a = (kb)^m [Y_m(kr) - \frac{2}{\pi} \ln(kb) J_m(kr)]$, where J_m and Y_m are the usual Bessel functions and b is an appropriate length scale which, based on our numerical calculations, is set to $b = d_\ell$. From this analysis, and following [14],

we obtain the energy-analytic pseudopotentials as,

$$\hat{v}_m^a(r) \overset{r\to 0}{\equiv} g_m^a(k) \times \delta(r)\hat{R}_m^a(r), \tag{6}$$

where g_m^a is the energy analytic coupling constant and $\hat{R}_m^a$ is the regularization operator given, respectively, by

$$g_m^a = -\frac{\hbar^2}{2\mu}\frac{2}{\pi}\frac{(m!)^2}{(2m)!}(2d_\ell)^{2m}\tan\delta_m^a(k), \tag{7}$$

$$\hat{R}_0^a = \ln(\frac{r}{2d_\ell\beta_0})^2\frac{d}{dr}\left[\frac{-1}{\ln(\frac{r}{2d_\ell\beta_0})}\right], \tag{8}$$

$$\hat{R}_m^a = \frac{1}{r^{m+1}}\frac{d^{2m}}{dr^{2m}}r^m\left[1-\frac{2(kr)^{2m}\ln(\frac{r}{2d_\ell\beta_m})}{2^{2m}m!(m-1)!}\right]^{-1}. \tag{9}$$

In the equations above, $\beta_m = e^{-\gamma+\sum_{p=1}^{m}p^{-1}}$, where $\gamma \approx 0.577$ is the Euler constant and δ_m^a is the energy analytic phase-shift, which relates to the physical phase-shift by

$$\tan\delta_m^a(k) = \frac{\tan\delta_m(k)/(kd_\ell)^{2m}}{1-\frac{2}{\pi}(kd_\ell)^{2m}\ln(kd_\ell)\tan\delta_m(k)}. \tag{10}$$

Note that our form of the pseudopotential has an explicit dependence on the dipole length d_ℓ while most of the k dependence comes through $\tan\delta_m^a$. In fact, for $m = 0$ our pseudopotential becomes energy *independent* in the $kd_\ell \ll 1$ regime. These properties appear to be absent from previous analyses of Q2D pseudopotentials but they appear to be desirable for many-body calculations. In Figure 3 we show the contrast between using the usual form of the pseudopotentials and the energy-analytic form [Eqs. (6)-(9)]. Figures 3 (a) and (b) shows our results for the physical coupling constant g_m [obtained by replacing d_ℓ by $1/k$ and δ_m^a by δ_m in Eq. (7)] for the same set of parameters chosen in Fig. 2. As one can see, g_m increases for large m $\tan\delta_m/k^{2m} \propto 1/k^{2m-1}$ $(m \neq 0)$, while g_m^a [Figs. 3 (c) and (d)] decreases for $kd_\ell \gg 1$. This indicates that our form of the pseudopotential might be more suitable in the strongly dipolar regime. Apart from the above considerations, we note that for every m, g_m diverges at particular values of d_ℓ [15]. These divergences are related to the Ramsauer-Townsend effect and do *not* correspond to a zero-energy bound state. If these "resonances" persist in a many-body context it can indicate that the Q2D dipolar gas could undergo a transition to a strongly correlated regime where the interactions can be tuned from repulsive $(g_m > 0)$ to attractive $(g_m < 0)$ almost at will by varying the external electric field. Moreover, the positions of the poles in g_m, according to our model, should be universal in the regime $kd_\ell \gg 1$. However, since the positions of resonant features depend on k they might be smeared out in a quantum gas. But they could be observable in a collision between two clouds at a definite relative momentum [17]. Now, the fact that the poles in g_m^a are visible only for $m = 0$ emphasizes the necessity of extending the many-body analysis in the energy-analytic framework, a task beyond the scope of our present investigation.

In summary, we have studied scattering properties of bosonic and fermionic dipoles under Q2D confinement. Both species display universal behavior, which significantly improves the prospects of creating a stable gas of Q2D dipoles. We have also computed two-body parameters, such as the scattering amplitude and coupling constants, which can be important for many-body treatments of strongly interacting dipolar gases.

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