2-Dimensional Dipolar Scattering

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We characterize the long range dipolar scattering in 2-dimensions. We use the analytic zero energy wavefunction including the dipolar interaction; this solution yields universal dipolar scattering properties in the threshold regime. We also study the semi-classical dipolar scattering and find universal dipolar scattering for this energy regime. For both energy regimes, we discuss the validity of the universality and give physical examples of the scattering.

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Many theoretical proposals are based on dipolar gases in 2-dimensional (2D) geometries. For example, there are predictions of Wigner crystals [1], anisotropic solitons [2], and phonon instabilities [3]. Such theories show dipolar systems will lead to exotic and highly correlated quantum systems. Reduced dimensionality also offers another level of control to exert over ultracold matter. In pursuit of such quantum systems, there has been exciting experimental progress in the production of polar molecules [4, 5] and in the production of quasi-2 dimensional cold gases [6, 7]. This makes it seem that the experimental production of 2D dipolar gases is at hand. However, reduced dimensionality may not offer the semi-classical limits. In contrast to 3D, there is a diagonal s-wave dipolar interaction, and this leads to universal dipolar scattering in the threshold regime. We refer to the isotropic $m = 0$ partial wave as s-wave. For threshold scattering in 3D, it is required that $a_s \ll D$ to have universal dipolar scattering [8, 9]. This is challenging because $a_s$, the s-wave scattering length, depends sensitively on the details of the short range interaction. However, in 2D, the repulsive dipolar interaction prevents ultracold particles from reaching the short range interaction where it can acquire a non-universal phase shift. To have universal dipolar scattering we require only that the range of the short range interaction is much smaller than the dipolar length scale ($\rho_0 \ll 1$). This criteria does not rely on serendipity to be met.

In this regime, the s-wave scattering properties are derived from an analytic zero energy solution to the Schrödinger equation including the dipolar interaction. This solution shows that dipolar interaction results in an s-wave scattering length of 6.344D. We also present the Born approximation which predicts the threshold scattering for non-zero partial waves. In the large $Dk$ limit, the semi-classical universal dipolar scattering cross section can be estimated by the Eikonal approximation and scales as $\sqrt{D/k}$. These estimates offer accurate predictions of the scattering in their respective energy regimes.

To monitor the scattering we use the scattering cross section, which in 2D for distinguishable particles is $\sigma = \frac{4}{\pi} \sum_{m=0}^{\infty} \sin^2(\delta_m)$, where $\delta_m$ is the scattering phase shift for the $m^{th}$ partial wave [11, 12, 13]. For identical bosons (fermions) the sum is restricted to even (odd) $m$ and there is an additional factor of 2. Note that in 2D, $\sigma$ has units of length. We numerically solve Eq. (1) and obtain the scattering phase shift by matching $\phi_m$ to the free solution at large $\rho$: $\sqrt{k\rho} \cos(\delta_m) J_m(k \rho) - \sin(\delta_m) N_m(k \rho)$], where $J_m/N_m$ are regular Bessel functions of order $m$. An interesting fact of 2D scattering is that the s-wave, cross section diverges as $k \to 0$. To illustrate this, we solve the s-wave scattering with no dipolar
interaction and a hard wall at $\rho_0$. This yields

$$\sigma_{hw}(\rho_0) = \frac{4}{k} \sin^2(\delta_{hw}),$$

$$\tan(\delta_{hw}) = J_0(k\rho_0)/N_0(k\rho_0).$$

As $k$ goes to zero the phase shift becomes logarithmically small because $N_0 \propto \ln(k\rho_0)$; however this is not quick enough to counter the diverging $1/k$.

We have plotted the cross section for three physical systems. In Fig. 1(a) we show the cross section as a function of energy for bosonic LiK ($\sigma_b$), fermionic RbK ($\sigma_f$), and distinguishable scattering between LiK-RbK ($\sigma_d$). We have used $D = 5.29 \times 10^{-3}$ cm ($10^2 a_0$); this value of $D$ can easily be achieved for each system and is discussed below. Note the divergence of the cross sections containing s-wave contributions, and the Wigner suppression of $\sigma_f$. In fig. 1(b) we show the dimensionless quantity $k\sigma$ as a function of $Dk$. $k\sigma$ is proportional to the scattering rate, and $(Dk)^2$ is twice the ratio of the kinetic energy and the dipolar energy of the system, $2E/(d^2/D^3)$. The symbols are the data from (a), but the energy range has been extended to show the low energy trend of the scattering.

In fig. 1(b) we also show three analytic methods to estimate the scattering cross section: Born Approximation (solid blue line), threshold s-wave scattering (black triangles), and semi-classical (solid green line); each of these estimates is detailed below.

To obtain the threshold scattering properties of the 2D dipolar problem, we use an analytic zero energy ($k = 0$) solution to Eq. (1):

$$\phi^0_0(\tilde{\rho}) = 2\sqrt{\tilde{\rho}} \left[ K_{2m} \left( \sqrt{8/\tilde{\rho}} \right) + CI_{2m} \left( \sqrt{8/\tilde{\rho}} \right) \right]$$

where $K_{2m}/I_{2m}$ are modified Bessel functions. $C$ is determined by the boundary condition: $\phi^0_0(\rho_0) = 0$. Considering the s-wave case in the limit of small $\rho_0$, $C$ becomes small and is proportional to $e^{-2\sqrt{8/D}}$. In this limit $\phi^0_0(\tilde{\rho}) = 2\sqrt{\tilde{\rho}}K_{2m} \left( \sqrt{8/\tilde{\rho}} \right)$ and this wavefunction is plotted in Fig. 2 as a solid black line. We have also plotted $\phi_0$ (blue x) for $Dk = 5 \times 10^{-3}$, and it agrees well with $\phi^0_0$ at small $\rho/D$, as is shown by the inset.

To exploit the analytic solution, we find the form of the free solution, $\phi^0_0$, which is analogous to the zero energy 3D wavefunction: $\psi^0_D(r) = r - a_s$, which has the property: $\psi^0_D(a_s) = 0$. In 2D the scattering length is defined as where zero energy free solution is zero: $\phi^0_0 = \sqrt{\tilde{\rho}} \ln(\tilde{\rho}/\tilde{a_s})$ [14]. To extract the s-wave scattering length, we take the large $\tilde{\rho}$ limit of $\phi^0_0$ and find:

$$\phi^0_0 \to \sqrt{\tilde{\rho}} \left[ -2\gamma - \ln(2) + \ln(\tilde{\rho}) \right] = \sqrt{\tilde{\rho}} \ln(\tilde{\rho}/\tilde{a_s})$$

$$\tilde{a_s} = \frac{a_s}{D} \equiv e^{2\gamma+\ln(2)} \times 6.344.$$  

where $\gamma \sim 0.577...$ is Euler’s constant. Note $\phi^0_0$ in the large $\tilde{\rho}$ limit is the zero energy free solution, and the free solution is plotted in Fig. 2 as red squares. The inset shows the wavefunctions near the origin. The threshold cross section for 2D dipolar scattering can be approximated by the cross section of a hard wall at $a_s$, i.e.
\[ \phi_0^f(a_s) = 0: \]
\[ \sigma_{th} = \sigma_{hw}(a_s). \]  
\[ (5) \]

This is a remarkable result in both its simplicity and accuracy. In Fig. 3(a) we have plotted \( k\sigma_f \) (black +), \( k\sigma_h \) (red squares), \( k\sigma_{hw} \) (black triangle) for both the bosons and distinguishable case, and \( k\sigma_{SC} \) (solid green line) as a function of \( Dk \). From this figure we see Eq. (5) reproduces the scattering well in the threshold regime when \( Dk < 10^{-2} \).

To predict the threshold scattering of non-zero partial waves we use the Born Approximation (BA) \([11,12]\), and find
\[ \sigma_{fBA} = \frac{4}{k} \frac{(Dk)^2}{(m^2 - 1/4)^2}. \]  
\[ (6) \]

This offers a very good estimate of the non-zero partial waves scattering cross sections. For identical fermions, the BA gives \( k\sigma_f^{BA} \sim 29(Dk)^2 \). We have plotted the BA (blue solid line) in Fig. 3(b) for \( k\sigma_f \) (blue circles). In the small \( Dk \) limit, the BA reproduces the \( k\sigma_f \) well. In Fig. 3(a), we see that the fermionic cross section \( \sigma_f \) is Wigner suppressed, as expected \([13]\). This is in contrast to 3D where all non-zero partial wave become energy independent as energy goes to zero \([10]\). The analytic solution presented by Ref. \([16]\) produces the results in Eq. (6) when applied to 2D.

To estimate the transition out of the threshold regime for \( m = 1 \), we can also equate the centrifugal and dipolar terms and find the energy of that length scale to be roughly \( Dk \sim 0.3 \). This is a reasonable estimate of when the scattering leaves the threshold regime, and is seen in Fig. 3(b). The transition from the threshold regime does require higher energy collisions. \( D \) can be larger, which activates more partial waves.

The BA breaks down when \( Dk \) becomes large and we enter into the semi-classical regime. In this limit the scattering is no longer dominated by a single partial wave, and to understand the scattering in the semi-classical limit one must obtain the total cross section. To do this, we estimate the scattering amplitude with the 2D Eikonal approximation \([13]\):
\[ f_{eik} = \frac{-ik}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} db \cos(\kappa b) \left[ e^{i\kappa b} \sin(\delta_{eik}) \right], \]

where the phase is
\[ \delta_{eik} = \frac{1}{\kappa} \int_{0}^{\infty} \rho \, dp \, \frac{|U(0)|}{\sqrt{\rho^2 - b^2}}, \]

and \( b \) is the impact parameter. For the dipolar interaction \( U(\rho) = 2D/\rho^3 \), the phase shift is \( -Dk/(b\kappa)^2 \). Using the optical theorem, \( \sigma = \sqrt{8\pi}/k\text{Im}[f(0)] \) \([12]\), we find the total semi-classical cross section to be
\[ \sigma_{SC} = \frac{4}{k} \sqrt{\pi Dk}. \]  
\[ (7) \]

To illustrate the universal behavior of the scattering, in Fig. 3(b) we plot \( k\sigma_d \) (red squares), \( k\sigma_f \) (black +), \( k\sigma_d \) (blue circles), and analytic estimate from Eq. (5): \( k\sigma_{SC} \) (green solid line) as a function of \( Dk \). At large \( Dk \), \( k\sigma \) clearly shows the semi-classical \( \sqrt{Dk} \) scaling. \( k\sigma_h \) and \( k\sigma_f \) oscillate out of phase about \( k\sigma_d \). Fig. 3(b) shows that the semi-classical approximation offers a very good estimate of the scattering when \( Dk > 1 \).

We have characterized the long range scattering as a function of \( Dk \) in the \( \rho_0 \ll 1 \) limit. This ensured that deviations from universal behavior due to the short range interaction were negligible. But this leads to an important question: when can the scattering be impacted by the short range interaction? We have surveyed this question and have found that for \( \rho_0 \) less than 0.1 the short range plays little to no role in the scattering, even for \( Dk \ll 1 \). When \( \rho_0 \) exceeds this value, then the short range can resonantly impact the scattering and spoil the universal threshold scattering. Once \( \rho_0 > 1 \), the scattering cannot be characterized by dipolar scattering alone, and knowledge of the short range is required. A more thorough treatment of the short range impact on 2D dipolar scattering will be presented in the future.

An aim of this work is to facilitate estimates of the cross section for 2D dipolar scattering. This can be done with Fig. 4. In (a) we have plotted \( k^{-1} \) as a function of energy for for LiH (black solid line), KLi (red squares), RbK (green dashed line), and RbCs (blue circles). With this and the value of \( D \) one can readily determine the
scattering character and estimate a value of the scattering cross section.

To estimate $D$, we use Fig. 4(b) where we have plotted $D/D_0$ as a function of electric field. $D_0$ is the length scale obtained by using the bare dipole moment, $d^2 m/\hbar^2$. For the $^1\Sigma$ molecules [4, 5], the polarization of the molecules depends on the strength of the external electric field ($\mathcal{E}$) in relation to the rotation energy of the molecules; therefore, the field can be characterized by $B/d_0$. Fig. 4(b) shows $D/D_0$ which depends on the induced dipole moment squared ($d^2$) as a function of electric field over $B/d_0$. Note that the $D$ is only a fraction of this length. A few examples are:

| $D_0/10^{-5}$ (cm) | RbCs | RbK | KLi | LiH | LiCs |
|----------------------|------|-----|-----|-----|-----|
| $\mathcal{E}_0$ (kV/cm) | 0.8  | 3.9 | 4.2 | 74  | 0.5 |

Many others are given in Ref. [2]. For mixtures, such as LiK-RbK, we need to determine the induced dipole moment of each molecule at a particular field: $D = d_i d_m r_p/\hbar^2$. To offer a concrete example, consider fermionic RbK at $1\mu K$, where $k^{-1} \sim 5 \times 10^{-6}$ cm. In Fig. 1(a) we used $D = 5.29 \times 10^{-6}$, this requires $\mathcal{E} \sim 1.25\mathcal{E}_0 = 4.96kV/cm$. Then $Dk \sim 1$, and we use the semi-classical estimate and find $\sigma \sim 4\sqrt{D/\hbar}$, which is quiet close to the numerical value in Fig. 1(a).

In conclusion, we have characterized the long range 2D dipolar scattering and have offered several means to estimate the scattering cross section. In the universal threshold regime we have found an analytic solution to the interacting 2D radial Schrödinger equation. From this solution, we have extracted the scattering length for 2D dipolar scattering: $a_s = 6.344D$. Additionally we have explored the semi-classical universal scattering, and the results are that the scattering cross section scales as $\sqrt{D/\hbar}$, from Eq. 7. This regime can be reached by not only increasing temperature, but also by increasing $D$. The strong dipolar interaction activates many partial waves to scattering and the scattering can be semi-classical even at ultracold temperatures. An important application of this work will be the use of $a_s$ in many body theories to correctly account for the dipolar interaction [18, 19, 20]. Future work will explore the scenario where $d \cdot \tilde{\rho} \neq 0$ and the inclusion of transverse confinement in the scattering.

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