Dipolar gases in quasi one-dimensional geometries

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We analyze the physics of cold dipolar gases in quasi one-dimensional geometries, showing that the confinement-induced scattering resonances produced by the transversal trapping are crucially affected by the dipole-dipole interaction. As a consequence, the dipolar interaction may drastically change the properties of quasi-1D dipolar condensates, even for situations in which the dipolar interaction would be completely overwhelmed by the short-range interactions in a 3D environment.

Low-dimensional ultra cold gases have recently attracted a major attention. One and two-dimensional gases are created in sufficiently strong optical lattices [1], or by means of magnetic wires [2]. Low-dimensionality leads to a very rich physics, highlighted by the recently observed Berezinskii-Kosterlitz-Thouless transition in 2D gases [3], the enhanced role of thermal and quantum fluctuations in elongated gases [4], and the realization of the Tonks-Girardeau regime of 1D bosons [5].

In addition, the combination of the DDI and the dressing of rotational excitations with static and microwave fields may allow for the engineering of novel types of interaction potentials for polar molecules in 2D geometries [22].

In this Letter, we analyze the scattering properties of dipolar gases in quasi-1D geometries. By solving the corresponding scattering problem, including the short-range interaction, the DDI, and the trap potential, we obtain an effective 1D pseudopotential consisting of a contact interaction with an effective 1D coupling constant and a regularized dipolar potential. Similar as for the case without DDI we observe the appearance of a CIR, however the position of the CIR is crucially modified by the DDI. In particular, even for large values of $a$ for which in a 3D environment the short-range interaction fully dominates the DDI, the latter can dramatically modify the 1D scattering. As a consequence, the properties of the 1D gas may be crucially modified, leading to observable effects, which we discuss at the end of this Letter.

In the following, we consider a dipolar gas of particles with (electric or magnetic) dipole moment $d$ in a quasi-1D geometry along the axial $x$-direction. The transversal $yz$-confinement is given by an harmonic potential of frequency $\omega$, whereas no trapping is assumed in the $x$-direction. We are interested in the scattering of two dipolar particles under these conditions, and hence (due to the separability of the Hamiltonian) we consider the corresponding scattering problem in the relative coordinate $\vec{r}$, given by the Schrödinger equation:

$$\left[ -\frac{\hbar^2}{2\mu}\nabla^2 + \frac{1}{2}\mu\omega^2 \rho^2 + V_{sh}(\vec{r}) + V_d(\vec{r}) \right] \psi = E \psi, \quad (1)$$

where $\rho^2 = y^2 + z^2$, $\mu = m/2$ is the relative mass, $V_{sh}(\vec{r})$ is the short-range potential, and $E = \hbar \omega + \hbar^2 k^2/2\mu$, with $k$ the axial momentum. Assuming the dipoles oriented along $x$, the DDI is given by:

$$V_d(\vec{r}) = \frac{\rho^2}{r^3} \left[ 1 - \frac{3x^2}{r^2} \right] \quad (2)$$
and hence the DDI is attractive along $x$. This configuration is particularly convenient for the analysis since it maintains the cylindrical symmetry of the problem. This symmetry may be also preserved if the dipoles while forming an angle $\phi$ with the $x$-axis are rotated in the plane perpendicular to the trap axis fast enough to lead to an effective time averaged DDI \( [23] \), similar to that of Eq. (2) but in which \( d^2 \) transforms into \( \alpha d^2 \), where $\alpha$ may range between 1 ($\phi = 0$) and $-1/2$ ($\phi = \pi/2$). Note that for $\alpha < 0$ the DDI becomes repulsive along the axis.

If the system is assumed in the single-mode approximation (SMA), i.e. only the transversal ground-state is considered, the wavefunction may be split as

$$\psi_{\text{SMA}}$$

and hence the DDI becomes repulsive along the axis.

The SMA may become insufficient to describe the two-body scattering problem in a quasi-1D geometry. In particular, as discussed above, an analysis beyond the SMA \([3, 9]\) shows that for short-range interactions the scattering process in the presence of a transverse harmonic confinement potential undergoes a CIR, at which the coupling strength of the effective 1D pseudopotential diverges. For a 3D contact pseudopotential \( \frac{\hbar^2}{2a} \delta (r) \), the effective 1D coupling constant is given by \([8]\):

$$g_{1D} = \frac{2\hbar^2 a}{\mu l^2 (1 - 1.466a/l)},$$

and hence $g_{1D}$ diverges when $a \sim 0.68l$. It has been verified numerically that the shape and the position of the CIR does not depend on the details of the interatomic interaction, when the range of the interaction is much smaller than the radial confinement length \([9]\).

In the following we analyze the effects of the dipolar interaction in the CIR by considering the scattering process beyond the SMA. We solve the 3D scattering (simplified by the cylindrical symmetry of the problem) numerically. For simplicity, we consider a simplified model for the short range potential, namely a finite-depth potential well: $V_{sh} = -V_0 \theta (r_0 - r)$, for which the 3D scattering length $a$ is analytically known $a = r_0 \left[ 1 - \tan(\sqrt{m^2 V_0/\hbar^2}) / \sqrt{m^2 V_0/\hbar^2} \right]$ \([23]\). $r_0$ denotes the range of the interactions, which is kept small compared to the radial confinement length $l$ (in the calculations below we use $r_0 = 0.1l$). In the following we assume that for the DDI considered the system is sufficiently far away from shape resonances, and hence we maintain the analytical value of $a$ obtained in absence of the DDI. The 3D dipolar interaction is considered of the form $\frac{\alpha d^2}{r^3} \left[ 1 - \frac{3r^2}{r^2 + L^2} \right] \theta (r - r_0)$, where we have imposed a cut-off at short distances to avoid divergences. This cut-off is physically justified since at short distances the short-range potential dominates.

To evaluate the effective 1D coupling constant $g_{1D}$ we solve the 3D Schrödinger equation \([2]\) for a momentum $k = 0$. Employing the cylindrical symmetry of the problem, we consider a 2D numerical grid for the radial and axial coordinates, choosing the maximal radial value such that the wave function vanishes at the border, whereas the axial box has a length $L > > l \gg l_d >> r_0$. Note that the latter restricts our calculation to sufficiently small values of dipole moments to satisfy the 1D condition $l > l_d$. In order to increase the precision near the scattering center, we employ a non-uniform grid $\eta (i) = \text{sech}(\Delta_\eta i)$, where $\eta = \rho, x$, and $\Delta_\eta$ are properly chosen. Since only the even parity wave function contributes to the low-energy scattering problem, we impose the boundary condition $\delta \phi (0, \rho) = 0$. For $L > l_d$, the wave function can be written in a product form:

$$\psi (x, \rho) = f(x) \phi_0 (\rho).$$

Imposing at $x = L$ the logarithmic derivative $\frac{df}{dx}$ in a fully 1D calculation, we evolve
the 1D wavefunction from $x = L$ to $x = 0$ using $V_{1D}(x)$. From the logarithmic derivative of the 1D wavefunction at $x = 0$ we obtain $g_{1D}$.

Fig. 1 shows the value of $g_{1D}$ for different dipolar strengths $d^2/l^3\hbar\omega$, as a function of the 3D scattering length. For vanishing dipole moment, our numerical results are in good agreement with the analytical results of Ref. [8]. For sufficiently large values of $a$, the effective coupling constant approaches an asymptotic universal negative value $-\frac{1.376}{\mu l}$. The DDI significantly modifies the behavior of $g_{1D}$ as a function of $a$. With growing $d$ the position of the CIR shifts towards larger positive values of $a$. At some particular value of the dipole strength ($d^2/l^3 \sim 0.3\hbar\omega$), the position of the CIR is displaced towards $a = +\infty$, and as a consequence the CIR disappears and $g_{1D}$ monotonically increases with $a$. Further increasing $|d|$ shifts the CIR to negative values of $a$. When increasing $d$ even further the CIR is found again for $a > 0$, scanning again all values of $a$ until $+\infty$ and back from $-\infty$ to 0, and so on in a cyclic way.

Note that in SMA a sufficiently large repulsive DDI on the $x$-axis would lead eventually to a shielding of the short-range potential, and $g_{1D}$ would become an universal function of $d$. However, in the calculations presented in this paper we consider the case in which $l \gg l_d$. Therefore the anisotropy of the DDI becomes important, and the relative wavefunction can surround the repulsive axial barrier, and explore the short-range part of the potential.

Note that in a 3D environment when $|a|$ is sufficiently large the DDI becomes irrelevant compared to the short-range interactions. Remarkably, this apparently intuitively obvious fact is not what occurs in a waveguide geometry. Fig. 2 shows the asymptotic value of $g_{1D}$ for large $|a|$, which interestingly, due to the DDI can approach a positive value, i.e. the gas acquires a repulsive character. This qualitatively differs from the behavior for $d = 0$, for which the effective 1D contact interactions acquire for sufficiently large $|a|$ an universal attractive character [8]. Hence, even if the short-range interactions fully dominate the physics in a 3D geometry, the DDI can dramatically change the properties of the dipolar gas in quasi-1D geometries, eventually changing the sign of $g_{1D}$. The prediction of this remarkable property introduced by the DDI (which should be experimentally observable for quasi-1D dipolar gases at a Feshbach resonance) can be considered the main result of this Letter.

Once the pseudopotential is known, one writes down the many-body Hamiltonian for quasi-1D dipolar bosons

$$H = \int dx \Psi^\dagger(x) \left[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + \frac{1}{2} g_{1D} \Psi^\dagger(x) \Psi(x) \right] \Psi(x) + \int dx dx' \Psi^\dagger(x) \Psi^\dagger(x') \frac{V_{1D}(|x - x'|)}{2} \Psi(x) \Psi(x')$$

where $\Psi(x) \ (\Psi^\dagger(x))$ is the creation (annihilation) operator of bosons at $x$. At the CIR a Tonks gas with additional DDI would lead to a super-Tonks gas, with Luttinger parameter $K < 1$ [20]. For small values of $|g_{1D}|$, and although strictly condensation is prevented in 1D, a finite-

![FIG. 1: $g_{1D}$ in units of $\hbar^2/\mu l$ as a function of $a/l$ for various values of $d^2/l^3\hbar\omega$ for (a) $a = -1/2$ (repulsive dipoles), and (b) $a = 1$ (attractive dipoles). The bold line represents the analytical results of Ref. [8].](image1.png)

![FIG. 2: $g_{1D}$ in units of $\hbar^2/\mu l$ as a function of $d^2$ in units of $\hbar^3\omega$ for a fixed 3D scattering length $a = 10.1 l$, for $a = -1/2$ (dotted line) and $a = 1$ (solid line).](image2.png)

![FIG. 3: Quasi particle excitation energy $E(k)$ in units of $\hbar\omega$ as a function of $k l$ for $2m d^2/l^3 = 0.5 \hbar\omega$, for $ng_{1D}/\hbar\omega = -0.4$ (solid), $-0.43$ (dashed), and $-0.447$ (dotted-dashed).](image3.png)
size system at a sufficiently low temperature allows for a quasi-condensate\(^{27}\). This quasi-1D dipolar BEC may present a remarkable physics, as it becomes clear from an analysis of the dispersion law \(E(k)\) for axial excitations of momentum \(k\) on top of an homogeneous quasi-1D BEC:

\[
E(k) = \sqrt{\epsilon(k) \left[ \epsilon(k) + 2 \left( g_{1D} - \tilde{V}_{1d}(k) \right) \right] n} \tag{8}
\]

where \(\epsilon(k) = \hbar^2 k^2 / 2m\), \(\tilde{V}_{1d}(k) = \frac{4\pi a^2}{m} \left| 1 - \sigma e^{\sigma \Gamma(0, \sigma)} \right|\) is the Fourier transform of \(V_{1d}(x)\), with \(\sigma = k^2 l^2 / 4\). Note that \(\left| \tilde{V}_{1d}(k) \right|\) monotonically decreases with \(k\), with \(\left| \tilde{V}_{1d}(0) \right| = 4|\alpha|d^2 / l^2\). Hence, phonon stability demands \(g_{1D} > V_{1D}(0)\), since otherwise the homogeneous quasi-1D BEC becomes unstable against the formation of bright solitons. However, even for \(g_{1D} > V_{1D}(0)\), the homogeneous BEC can become eventually unstable. This occurs when \(g_{1D} < 0\), and \(\alpha < 0\) (repulsive DDI along the axis). In that case the function \(g_{1D} - \tilde{V}_{1d}(k)\) changes its sign for a sufficiently large \(k\), leading to the possibility of achieving a roton (see Fig. 3) in the spectrum at intermediate values of \(k\)\(^{28,29,30}\). When \(g_{1D}\) increases, the roton becomes deeper, and for a critical \(g_{1D} = g_c\), the roton minimum reaches zero energy at a finite momentum \(k_c\), leading to an instability of the homogeneous quasi-1D BEC. For \(\alpha = -1/2\), and a given \(d, k_c\) may be obtained from the equation \(1 + \sigma_c e^{\sigma_c \Gamma(0, \sigma_c)} = 1 + l^2 \hbar \omega / (4d^2 n)\), where \(\sigma_c = k^2 l^2 / 4\), whereas \(-2g_{1D} n / \hbar \omega = (1 - \sigma_c + \sigma_c^2 e^{\sigma_c \Gamma(0, \sigma_c)}) / (1 - (1 + \sigma_c) e^{\sigma_c \Gamma(0, \sigma_c)})\).

In summary, the DDI may play a crucial role in the physics of quasi-1D condensates, even for situations for which the short range interactions overwhelm the DDI in a 3D environment. The properties of the quasi-1D dipolar BEC crucially depend on the value of \(g_{1D}\), which in turn will depend in a non-trivial way on the dipole and dipole-orientation due to the dipole-induced modification of the CIR. In particular, the DDI may change the sign of \(g_{1D}\) for a large 3D scattering length, changing completely the physics of the quasi-1D dipolar condensates. For polar molecules the dipole strength may be modified by controlling the orienting electric field, and the DDI can be scanned from zero to large values. The combination of this control and the modification of the induced CIR, should allow to scan close to the CIR all physics ranging from an homogeneous stable quasi-condensate, a bright-solitonic solution, a BEC with (eventually unstable) roton minimum, and even a super-Tonks regime.

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