Hybrid multi-site excitations in dipolar condensates in optical lattices

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Strong 1D lattices usually lead to unconnected two-dimensional gases. The long-range character of the dipole-dipole interactions leads to a novel scenario where non-overlapping gases at different sites may interact significantly. We show that the excitations of non-overlapping condensates in 1D optical lattices acquire a band-like character, being collectively shared by different sites. In particular, the hybridization of the modes significantly enhances the rotonization of the excitations, and may induce roton-instability. We discuss the observability of this effect in on-going experiments.

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A novel path on cold gases is currently being opened by recent experiments in which (magnetic or electric) dipole-dipole interaction (DDI) plays a significant or even dominant role. On one side the recent creation of heteronuclear molecules in the lowest ro-vibrational level of a quantum degenerate gas of polar molecules, which may possess large dipole moments (e.g. of a quantum degenerate gas of polar molecules, which may possess large dipole moments (e.g. $\sim 0.5$ Debyes for KRb [1]). On the other side, the magnetic DDI has been shown to lead to exciting novel phenomena in recent experiments in Bose-Einstein condensates (BECs) of Chromium (which has a magnetic moment $\mu = 6\mu_B$, with $\mu_B$ the Bohr magneton) [2]. Particularly interesting is the fact that the short-range interactions (SRI) may be suppressed by means of Feshbach resonances, leading to a purely dipolar gas [3]. The DDI plays also a significant role in very recent experiments on spinor Rubidium BECs, in spite of the small $\mu = 1\mu_B$, since the energy scale of the DDI becomes comparable with the (also very small) energy scale of spin-changing collisions [4]. Very recent experiments have shown as well that the DDI leads to a observable damping of Bloch oscillations in Potassium BECs in tilted optical lattices [5].

The partially attractive character of the DDI results in nontrivial stability conditions for dipolar BECs. Low-momentum instability (phonon instability) [6] results in a geometry-dependent instability against collapse in 3D traps, as recently observed experimentally [7], or soliton formation in 2D geometries [8]. Interestingly, the momentum dependence of the DDI allows for a second type of instability (roton instability) related to the appearance of a roton-like minimum in the dispersion law of elementary excitations [9]. Roton instability leads to local collapses [10] or stabilized modulated density profiles in sufficiently tight traps [11].

The long-range character of the DDI induces a nonlocal nonlinearity in dipolar BECs that resembles that encountered in plasmas [12] or nematic liquid crystals [13]. As a consequence, novel phenomena as stable 2D solitons become possible [14, 15]. This nonlocality leads to fundamentally new physics for quantum gases in optical lattices, since it induces interactions between neighboring sites. As a consequence, dipolar bosons in optical lattices are described by extended versions of the Bose-Hubbard Hamiltonian, and may present a wealth of novel phases, as supersolid [16] or Haldane-phases [18]. In addition, contrary to the case of SRI, very deep optical lattices do not lead to independent low-dimensional gases, since non-overlapping atoms at different sites interact. As a consequence nonoverlapping BECs in two-well potentials may scatter [19], pair superfluidity may appear in ladder-like lattices [20], and even filament condensation may occur [21]. The effects of the intersite DDI have been observed experimentally for the first time in very recent experiments in Florence on Bloch oscillations [6].

This Letter is devoted to the analysis of non-overlapping dipolar BECs placed at different sites of a deep two-well potential or 1D optical lattice. As mentioned above, contrary to the case of purely SRI, the deep potential does not lead to independent 2D BECs. In particular, we show that the elementary Bogoliubov excitations of disconnected BECs placed in a two-well potential couple through the DDI leading to hybrid modes which are collectively shared by both wells. Interestingly this hybridization may significantly alter the stability of the system against roton instability. We show that this effect is significantly enhanced for the case of a 1D optical lattice with multiple sites, where a band-like spectrum is induced by the inter-site DDI. We analyze in detail the stability diagram, and finish with a discussion of the experimental observability in different experiments.

In the following, we consider a BEC of particles with mass $m$ and electric dipole $d$ (the results are equally...
valid for magnetic dipoles) oriented along \( z \) by an external field, and that hence interact via a dipole-dipole potential: \( V_{2D}(\vec{r}) = d^2(1 - 3 \cos^2(\theta))/r^3 \), where \( \theta \) is the angle formed by \( \vec{r} \) with the \( z \) axis. At sufficiently low temperatures the physics of the dipolar BEC is provided by a non-local non-linear Schrödinger equation (NLSE):

\[
\frac{i\hbar}{\partial t} \Psi(\vec{r}, t) = \left[ -\frac{\hbar^2}{2m} \nabla^2 + V(\vec{r}) + g|\Psi(\vec{r}, t)|^2 \right. + \int d^3r'V_d(\vec{r} - \vec{r}')|\Psi(\vec{r}', t)|^2 \right] \Psi(\vec{r}, t),
\]

where \( g = 4\pi\hbar^2 a/m \), with \( a \) the \( s \)-wave scattering length, and \( V(\vec{r}) \) is the trap potential. In the following we use the convenient dimensionless parameter \( \beta = g_d/g \), that characterizes the strength of DDI compared to the short range interaction, where \( g_d = 8\pi\hbar^2/3 \). Note that \( \beta \) may be easily controlled experimentally by means of Feshbach resonances, as recently shown in Ref. [3].

We consider first the case of a quasi-2D homogeneous BEC confined in \( z \) by \( V(\vec{r}) = m\omega_z^2 z^2/2 \), which is sufficient strong such that \( \Psi(\vec{r}, t) = \Psi_{\perp}(\vec{r}, t)\Phi_0(z) \), where \( \Phi_0(z) = \exp(-z^2/(2l_z^2))/\pi^{1/4}l_z^{1/2} \) is the ground state of the transversal oscillator (\( l_z = \sqrt{\hbar/m\omega_z} \)). The ground state of the homogeneous 2D BEC is of the form \( \Psi_{\perp}(\vec{r}, t) = \exp(-i(\mu/h + \omega_z)t)\sqrt{n_0} \), where \( n_0 \) is the 2D density, and \( \mu \) is the 2D chemical potential. Introducing this form into the NLSE, one obtains \( \mu = (g + g_d)n_0/\sqrt{2\pi}l_z \) (the 2D condition is satisfied for \( \mu \ll \hbar\omega_z \)). Inserting a plane-wave Ansatz \( \Psi(\vec{r}, t) = (\sqrt{n_0} + u_q \exp(iq_z z - i\omega_q t))\Phi_0(z) \exp(-i(\mu/h + \omega_z)t) \) into the NLSE, and linearizing in \( u_q, v_q \), we obtain the Bogoliubov spectrum of elementary excitations:

\[
\epsilon(q) = \{E_q [E_q + 2A]\}^{1/2}
\]

where \( E_q = \hbar^2 q^2/(2m) \), \( A = \mu - (g_a n_0/\sqrt{2\pi}l_z)F(q_l z/\sqrt{2}) \) and \( F(x) = \frac{3}{\sqrt{\pi}}(x^2) \operatorname{erf}(x) x^2 \). Note that without DDI (\( \beta = 0 \)) we recover the usual Bogoliubov spectrum for a 2D BEC with purely SRI. In particular, if \( a < 0 \) and \( \beta = 0 \), \( \epsilon(q)^2 < 0 \) for \( q \to 0 \), recovering the well known phonon instability (and subsequent collapse) in homogeneous BEC with \( a < 0 \). If the dipole is sufficiently large, such that \( g + g_d > 0 \), then the DDI prevents the instability at \( q \to 0 \). However, due to the \( q \)-dependence of the DDI (given by the monotonously decreasing character of the function \( F \)), the dispersion \( \epsilon(q) \) may show for intermediate \( g_d \) values a roton-like minimum at a finite value of \( q_l z \) (Fig. 2). For sufficiently low DDI \( \epsilon(q)^2 < 0 \) at the roton-like minimum, leading to dynamical instability (roton instability). For \( \beta > \beta_{cr} \) (with \( \beta_{cr} \) dependent on the ratio \( g_a n_0/\hbar\omega_z \)) roton instability is prevented, and the 2D homogeneous BEC is stable.

In the following we show that \( \beta_{cr} \) is significantly modified in the presence of other neighboring quasi-2D dipolar BECs. We consider the case of an optical lattice along \( z \) (Fig. 1) described by a potential \( V(\vec{r}) = sF(x)\sin^2(\pi z/\Delta) \), where \( \Delta \) is the intersite spacing, and \( s \) provides the lattice depth in units of the recoil energy \( E_r = \hbar^2/2m\Delta^2 \). As in the previous discussion we consider no trapping on the \( xy \)-plane (we discuss the potentially important role of the harmonic confinement on the \( xy \)-plane at the end of this Letter). At each lattice node \( V(\vec{r}) \) may be approximated by an effective harmonic oscillator potential \( V_{eff}(z) \), with effective oscillator length \( l_z \approx \Delta s^{-1/4}/\pi \). The lattice is considered strong enough so that we can assume that there is no spatial overlap between wavefunctions in different lattice sites, and hence we may neglect any hopping. We assume the DDI small enough to neglect pairing [20] or filamentation [21].

We start our discussion on inter-site effects with the two-well case. This simplified scenario already captures many features of the effect discussed. In addition, two-well potentials may be experimentally realized and are currently of considerable interest [22, 23]. The quasi-2D BEC in the \( i \)-th layer is given by the extended NLSE:

\[
\frac{i\hbar}{\partial t} \Psi_i(\vec{r}, t) = \left[ -\frac{\hbar^2}{2m} \nabla^2 + V_{eff}(z) + g|\Psi_i(\vec{r}, t)|^2 \right. + \int \sum_j d^3r'V_d(\vec{r} - \vec{r}')|\Psi_j(\vec{r}', t)|^2 \right] \Psi(\vec{r}, t),
\]

where for a two-well potential, \( i, j = 1, 2 \). Note that, crucially, the DDI couples now the \( i \)-th layer to the \( j \)-th one. Similar to the single-site discussion, we consider a strong \( z \)-confinement at each site, and hence we may employ a quasi-2D Ansatz \( \Psi_i(\vec{r}) = \Psi_{\perp,i}(\vec{r}, t)\Phi_0(z - z_i) \), where \( \Phi_0(z) \) has the form discussed above, and \( z_i \) is the position of the \( i \)-th lattice node. The ground-state of the condensates at the two layers in given by the Ansatz \( \Psi_{\perp,i}(\vec{r}, t) = \sqrt{n_0}\exp(-i(\mu/h + \omega_z)t) \), where we consider the same 2D density \( n_0 \) at both sites. Introducing this Ansatz into the NLSE [3] we obtain the 2D chemical potential \( \mu = \mu + \lambda(\Delta) \), with \( \mu \) the chemical potential of an individual well and \( \lambda(\Delta) = (g_a n_0/\sqrt{2\pi}l_z)e^{-\Delta^2/\pi l_z^2} \).

As above we are interested in the elementary excitation of these systems. For \( \Delta \to \infty \) the Bogoliubov modes at each site are independent and described by the single-
site expression \(\hat{\Psi}(\vec{r}, t) = (\sqrt{n_0} + u_{q_i} \exp(i\vec{q}_i \cdot \vec{r} - i\epsilon t/\hbar) - v_{q_i} \exp(-i\vec{q}_i \cdot \vec{r} - i\epsilon t/\hbar))\hat{\Phi}_0(z) \exp(-i(\tilde{\mu}/\hbar + \omega_z)t)\) into the NLSE (5), and linearize in \(u_{q_i}, v_{q_i}\). In this way we obtain four coupled Bogoliubov-de Gennes equations for \(\{u_{1,2}, v_{1,2}\}\), which may be diagonalized to obtain the Bogoliubov modes:

\[
e_{\pm}(q) = \{E_q[(E_q + 2A \pm C(\Delta))]^{1/2},
\]

where

\[
C(\Delta) = \lambda(\Delta) - \frac{g d n_0}{\sqrt{2\pi} l_z} \tilde{F} \left( \frac{q l_z}{\sqrt{2}}, \frac{\Delta}{\sqrt{2}\pi l_z} \right),
\]

with \(\tilde{F}(x, y) = \frac{3v_x}{4} \sum_{\alpha = \pm 1} e^{-2\alpha xy} \mathrm{erfc}(x - \alpha y)\).

Note that for \(\Delta \to \infty\), \(C(\Delta) = 0\) and we recover two degenerate independent modes. For finite \(\Delta\) the modes at the two wells hybridize, and two different branches appear for each \(q\), one stiffer than the modes for \(\Delta \to \infty\), and the other softer. The latter is particularly interesting, since the soft mode is more prone to rotonization (Fig. 3).

Interestingly, under proper conditions, two parallel non-overlapping BECs may become roton-unstable even if they were stable separately. As a consequence, a larger \(\beta_{cr}\) is necessary to stabilize the two-well system.

The hybridization (and consequent destabilization) in two-well potentials becomes even more pronounced for the case of dipolar BECs at \(N_s > 2\) sites of a 1D optical lattice, since a site \(i\) couples with all its neighbors \(j\) (of course with decreasing strength for growing \(|i - j|\)). For simplicity of our analysis we consider the case in which all lattice sites present the same 2D density \(n_0\). In that case, one may easily generalize the two-site analysis to the multi-site case, to reach a set of coupled Bogoliubov-de Gennes equation for \(f_{q_i} = u_{q_i} + v_{q_i}\):

\[
\epsilon^2 f_{q_i} = E_q(E_q + 2A)f_{q_i} + 2E_q \sum_{j \neq i} C(\Delta|i - j|)f_{q_j}.
\]

Figure 3: Dispersion law (in units of \(E_0 = \hbar/m\Delta^2\)) for a single site (dashed) and for two wells (solid) for \(\beta = -1.2, \Delta = 0.53\) \(\mu m\), \(s = 13.3, a = -2\) \(nm\), and \(n_0/\sqrt{2\pi} l_z = 10^{14}/\text{cm}^3\).

After diagonalizing the matrix of coefficients at the rhs of Eqs. (4), we obtain numerically the corresponding band-like set of \(N_s\) elementary excitations (Fig. 4). Note that the band-like spectrum has an upper phonon-like boundary which for large \(N_s\) has an approximate sound velocity \(c_s \simeq \sqrt{(A + \sum_n C(\Delta|m|))/m}\). The lower mode of the \(N_s\) manifold becomes significantly softer than the individual modes for independent sites. As a consequence the roton instability extends to larger \(\beta_{cr}\) when \(N_s\) increases, until saturating for a sufficiently large \(N_s\) (due to the decreasing DDI for increasing distance between sites).

Figure 4: Band-like dispersion (in units of \(E_0 = \hbar/m\Delta^2\)) for \(N_s = 40\) and \(\beta = -2.44\). Other parameters are as in Fig. 3.

We indicate the dispersion law for \(N_s = 1\).

Fig. 5 summarizes our results on the stability as a function of \(\beta\) (we recall that \(g < 0\)). As mentioned above if \(g + g_d < 0\) (\(|\beta| < 1\)) the system is unstable against phonon instability. For \(1 < |\beta| < |\beta_{cr}(N_s)|\) the system is unstable against roton instability. \(|\beta_{cr}|\) increases when \(N_s\) grows until saturating for sufficiently large \(N_s\). For \(|\beta| > |\beta_{cr}(N_s)|\) the quasi-2D BECs are stable.

The value of \(q_{rot}\) when the roton becomes unstable is of particular importance. Fig. 6 shows a typical variation of \(q_{rot}\Delta\) at the curve \(\beta = \beta_{cr}(N_s)\) as a function of \(N_s\). Note that \(q_{rot}\) at \(\beta_{cr}\) shows a maximum for small \(N_s\). For small \(N_s\), \(\beta_{cr}\) (and hence the on-site repulsive DDI) increases significantly, and hence the value of \(q_{rot}\) at \(\beta_{cr}\) increases. For larger \(N_s\) \(\beta_{cr}\) tends to saturate, as mentioned above, and the repulsive on-site DDI remains approximately constant along the curve \(\beta_{cr}(N_s)\). As a consequence, the increase in \(N_s\) just increases the attractive contribution of the DDI of neighboring sites, and the
DDI becomes less effective in compensating the attractive on-site SRI. As a result of that, $q_{rot}$ decreases until saturating at a value lower than that for a single site.

Typical experiments work with an harmonic $xy$-trapping (of frequency $\omega_{xy}$). Although we have assumed homogeneous quasi-2D gases, we may estimate the effect of the $xy$-trapping by considering an effective cut-off at low momenta $q_{cut} \approx 1/l_{xy}$, where $l_{xy} = \sqrt{\hbar/m\omega_{xy}}$ is the harmonic oscillator length characterizing the $xy$-trap. In a good approximation we may consider that all features occurring at momenta $q < q_{cut}$ are suppressed by the trap. As a consequence one expects that the $xy$ confinement suppresses roton instability for frequencies $\omega_{xy} > \omega_{cut}$. For typical densities $10^{14}$cm$^{-3}$, and typical intersite separation $\Delta = 0.53\mu$m, we estimate for $^{52}$Cr that for a single site $\beta_{cr}$ is achieved at a scattering length $a \simeq -31a_0$, and that for this case $\omega_{cut} \simeq 66$Hz. For the same case but $N_s = 4$ (which is the maximum of the corresponding $q_{rot}$ curve), $\beta_{cr}$ is achieved for $a \simeq -24a_0$, and $\omega_{cut} \simeq 160$Hz. For the latter case an instability rate of $\Gamma^{-1} \simeq 5$ms is expected for $a = -24.5a_0$. For $^{39}$K, the numbers are more restrictive (due to the lower magnetic moment). For $N_s = 25$ (maximum of the $q_{rot}$ curve), $\beta_{cr}$ is achieved for $a \simeq -0.52a_0$, and $\omega_{cut} \simeq 4$Hz. For this case, one expects $\Gamma^{-1} \simeq 180$ms at $a = -0.53a_0$.

Note that the fact that $q_{rot}$ shows a maximum may have interesting consequences in experiments, since this suggest that for some intermediate trapping frequencies the instability may be just present for a given window of values of $N_s$. Note also that the previous discussion just refers to the destabilization when the roton touches zero. For even larger values of $|a|$, a larger region of $q$ may become unstable. However if the $xy$-trap just allows for the resolution of the upper boundary of the unstable region and not the lower one, roton and phonon instability may become experimentally indistinguishable.

Summarizing, the nonlocal character of the DDI leads to a novel scenario where non-overlapping gases at different sites interact significantly. Contrary to the case of pure SRI, the DDI leads to the hybridization of the excitations at different sites, which acquire a collective band-like character. In particular, the hybridization of the modes leads to a significant enhancement of the rotonization of the excitations, and may induce roton-instability for values of the SRI at which a single site is stable. Finally, we have discussed the experimental requirements for the observation of the roton instability.

Note: After the completion of this work we became aware of a similar analysis by Wang and Demler [24], in which roton-softening due to intersite interactions is discussed in the context of recent experiments in Florence [3]. Although we consider that roton softening plays no significant role in the damping observed in Ref. [1] due to the $xy$-confinement, a weaker $\omega_{xy}$ (along the lines discussed above) could allow for the instability discussed by Wang and Demler, and by us in this manuscript. However, a more careful quantitative analysis is necessary, taking into account both the $xy$-trapping, and the $z$-trapping, which we plan to investigate in a further work.

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