Stability spectroscopy of rotons in a dipolar Bose gas

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We study the stability of a quasi-one-dimensional dipolar Bose-Einstein condensate that is perturbed by a weak lattice potential along its axis. Our numerical simulations demonstrate that systems exhibiting a roton-maxon structure destabilize readily when the lattice wavelength equals either half the roton wavelength or a low roton subharmonic. We apply perturbation theory to the Gross-Pitaevskii and Bogoliubov–de Gennes equations to illustrate the mechanisms behind the instability threshold. The features of our stability diagram may be used as a direct measurement of the roton wavelength for quasi-one-dimensional geometries.

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It is widely believed that ultracold, gaseous samples of bosonic atoms or molecules possessing sufficiently large dipole moments will exhibit internal structure reminiscent of the roton in superfluid helium [1]. The basic phenomenology of the roton, in analogy with helium, is a local minimum in the quasiparticle dispersion $\omega(k)$. The existence of such a minimum is predicted to lead to a host of attendant phenomena in these dilute gases, including structured ground-state density profiles [2–4], reduced and anisotropic critical superfluid velocity [1,5,6], enhanced sensitivity to external perturbations [7], abrupt transitions in Faraday patterns [8,9], short-wavelength immiscibility phases [10], and strongly oscillatory two-body correlations on the roton length scale [11]. Signatures of the roton in Bragg spectroscopy of trapped dipolar Bose-Einstein condensates (DBECs) have been calculated in Ref. [12]. While these many exciting predictions are in principle observable in current experiments with highly magnetic atoms [13–15], or in future experiments with electrically polar molecules [16–18], rotons remain to be seen directly in DBECs [19].

In a dipolar condensate, the roton represents a mode of finite wavelength that has an anomalously low energy—hence the minimum in $\omega(k)$. The location of this minimum is given by a momentum $k_{\text{rot}} \sim l_{\text{f}}^{-1}$, where $l_{\text{f}} = \sqrt{\hbar / m \omega_{t}}$ denotes the harmonic oscillator length of the lowest confinement of the DBEC (usually along the polarization axis). Without this confinement, a homogeneous DBEC would be energetically unstable to collapse due to the attraction between dipoles that are aligned head to tail. In the presence of this confinement, the collapse is prevented by the zero-point energy introduced by the confinement, at least up until a critical dipole moment or density. When this critical parameter is exceeded, the condensate collapses in localized “clumps” of size $\ell_{\text{rot}} \sim l_{\text{f}}$, that is, via a dynamical instability into the roton mode [20].

A low-energy roton is therefore a mode that is linked intrinsically to condensate instability. This link suggests that the DBEC may respond nontrivially as an object of conventional spectroscopy in that it would absorb and distribute energy differently from different wavelengths of an applied probe. For example, if one imposes on a DBEC a weak potential of periodicity $\lambda_L$ (via a one-dimensional (1D) lattice beam [21], for example), then one expects to trigger an instability most easily when $\lambda_L \approx \ell_{\text{rot}}$. In this Rapid Communication we verify this conjecture via mean-field simulations of a quasi-one-dimensional (Q1D) DBEC. Strikingly, we find structure in addition to this main peak, analogous to nonlinear spectroscopy of atoms or crystals in strong laser fields. Namely, we see hastened destabilization by probes with wavelengths that are integer multiples of $\lambda_{\text{rot}}$, reminiscent of “multiphoton” scattering. We also observe a similar feature at the shorter wavelength $\lambda_L = \lambda_{\text{rot}}/2$, reminiscent of resonant Raman coupling. Since the stability of a condensate is easy to assess experimentally, the observation of such structures constitutes a direct stability-spectroscopic measurement of the roton wavelength as well as an alternate signature of roton physics.

Consider a DBEC that is tightly confined in the $\hat{y}$ and $\hat{z}$ directions by a harmonic trap of frequency $\omega_{t}$, with no trapping potential in the $\hat{x}$ direction. The dipole moments of the constituent atoms or molecules are polarized along $\hat{z}$. To this initially stable system is applied a probe in the form of an optical lattice potential

$$U(x)/\hbar\omega_{t} = s \cos^{2}\left(\frac{k_{L}}{2} x\right)$$

whose periodicity $\lambda_{L} = 2\pi/k_{L}$ and (dimensionless) lattice depth $s \equiv -\Re\{\omega(\omega_{t})\} / 2\epsilon_{0}\hbar\omega_{0}$ (assumed positive, without loss of generality) are tunable parameters. Such a potential can be realized using retroreflected or crossed off-resonant laser beams of peak intensity $I_{0}$ [21]. We take the single-mode approximation, assuming that the order parameter is a Gaussian of width $\ell_{0} = \sqrt{\hbar / m \omega_{t}}$ in the directions of tight confinement [22]. We suppose that there are $N = 2L_{\text{1D}}$ atoms spread over the periodic domain $x \in [-L, L]$, where $L_{\text{1D}}$ is the one-dimensional integrated density. Expressed in natural length ($\ell_{0}$) and energy ($\hbar\omega_{0}$) units, the Gross-Pitaevskii equation for this situation reads

$$\mu \psi(x) = -\frac{1}{2} \partial^{2}_{x} \psi(x) + U(x) \psi(x)$$

$$+ N \int dx' \psi^{*}(x') \psi(x') V(x - x') \psi(x').$$

The momentum-space form of the Q1D interaction potential is

$$V(k) = 2a_{s} + 4a_{dd} \left[ 1 - \frac{3}{\sqrt{2}} \int_{0}^{\infty} dw e^{-w^{2}/2} g \left( \sqrt{\frac{w^{2} + k^{2}}{2}} \right) \right].$$

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\[ \mu = \omega_t d \]

In both cases, the spectra clearly show three features, which are more prominent for softer rotons: (i) A weak laser drives the condensate to instability for probe periodicities near the roton wavelength, accounting for the lowest dip in Fig. 1. Indeed, the weakest laser required to destabilize the condensate has periodicity \( \lambda_\text{rot} \). We emphasize that at the threshold of stability, our simulations show that the lattice probe is not chopping the condensate into smaller, unstable pieces, but rather is weakly perturbing it. (ii) A secondary dip in stability appears when the lattice spacing is twice the roton wavelength. In terms of the analogy to optical absorption in a nonlinear medium, this situation is reminiscent of the excitation of the resonant state by absorption of two photons of half the energy required to excite the state directly. (iii) Finally, a third dip in stability is observed at half the roton wavelength. We have also observed these structures in full 3D simulations of horizontal, cigar-shaped DBECs where the roton “wavelength” is less well defined.

The origin of these features becomes clear within perturbation theory. Rigorous perturbation theory for the Gross-Pitaevskii equation was worked out in Refs. [7,24–26]. Let \( \psi^{(0)} \) and \( \mu^{(0)} \) represent the order parameter and chemical potential in the absence of the probe \( U(x) \). Expanding \( \psi = \psi^{(0)} + \psi^{(1)}, \mu = \mu^{(0)} + \mu^{(1)} \), one derives the first-order perturbation equation

\[ \mu^{(1)} \psi^{(0)} = \frac{1}{2} \nabla_x^2 \psi^{(1)}(x) + U(x) \psi^{(0)} + 2n_{1D} \int dx' \psi^{(1)}(x')V(x - x'). \tag{4} \]

Given the condition \( \langle \psi^{(1)} | \psi^{(0)} \rangle = 0 \), the solutions to (4) are easily found to be \( \mu^{(1)} = s/2 \) and

\[ \psi^{(1)}(x) = -\left( \frac{s}{2 \sqrt{2} k_L x} \right) \frac{1}{2L} \cos(k_L x). \tag{5} \]

We have introduced the Hartree-Fock energy [27] \( \epsilon(k) = k^2/2 + 2n_{1D} V(k) \). Figure 2 compares \( \epsilon(k) \) to the Bogoliubov spectra \( \omega(k) = \sqrt{k^2/2 + 2n_{1D} V(k)} \) for the two cases of DBEC considered in Fig. 1.

The Hartree-Fock spectrum of a soft-roton DBEC possesses a shallow minimum at \( k \approx k_{\text{rot}} \), and this minimal energy approaches zero as the roton softens. The effect of this low-lying mode is to strongly perturb the ground state, as suggested by (5). Indeed, a modest perturbation \( \delta \psi \) becomes amplified in the density by a factor \( s/\delta(k_{\text{eq}}) \). The \( m \)th order of perturbation
theory additionally introduces density modulations of the general form \( n_{\text{ID}}^{(m)}(x) \sim \frac{\alpha}{\epsilon(k_L)} \cos(mk_Lx) \). That is, the roton can be driven by overtones of the fundamental wave number of the lattice, when \( mk_L \approx k_{\text{rot}} \), or \( \lambda_L \approx mk_{\text{rot}} \). The stability minimum corresponding to \( m = 2 \) can be seen in Fig. 1. Even away from one of these resonant conditions, the probe laser introduces density modulations that manifest themselves in a mean-field potential \( U_{\text{mf}}(x) = N \int dx' \langle \psi(x') \rangle^2 V(x - x') \), which combines with the probe field itself to make a combined potential

\[
U_c(x) = U(x) - \mu + U_{\text{mf}}(x) = \frac{s}{\epsilon k^2_L} \cos(k_L x) + O(s^2).
\]

Thus again, whatever influence the periodic probe potential has on propagation of the excited states in the condensate, this effect is amplified for probes in the vicinity of the roton (or a subharmonic thereof, as a higher-order effect).

There remains the task of explaining the feature in the stability spectrum at \( \lambda_L \approx \lambda_{\text{rot}}/2 \). This cannot be done by considering the ground state only. Rather, it is necessary to explore how the spectrum of excited states is modified by the combined potential energy \( U_c(x) \). The Bogoliubov–de Gennes (BdG) equations describing the excitations can be written compactly as

\[
\left( H_0 - \mu + C + X - X \right) \mathbf{u} = E \mathbf{u},
\]

where \( H_0 = -\frac{\hbar^2}{2m} \nabla^2 + U(x) \) is the free-particle Hamiltonian, \( C \hat{X}(x) = U_{\text{mf}}(x) \hat{X}(x) \) describes direct interactions with the mean field, and \( \hat{X}(x) = N \int dx' \langle \psi(x') \rangle^2 V(x - x') \) is an integral operator describing exchange interactions. The functions \( u_k(x) \) and \( v_k(x) \) define the usual Bogoliubov transformation of the quantum fluctuation field operator \( \delta \hat{\Psi} = \sum_j [\hat{a}_j \mu_j + \hat{a}^\dagger_j \nu_j^*] \), and they allow one to write the nontrivial part of the grand canonical Hamiltonian in approximate diagonal form as \( \hat{H} - \mu \hat{N} \approx \sum_k E_k \hat{a}^\dagger_k \hat{a}_k \). In the absence of the perturbation, Eq. (7) is easily solved using complex exponentials parametrized by momentum \( k \), yielding the unperturbed energies \( E_k^{(0)} = \omega(k) \). The perturbation (1) separates modes of definite parity, so we write the unperturbed modes in a basis of cosine and sine functions:

\[
u_{k_L}^{(0)}(x) = v_k \cos(k_Lx)/\sqrt{L}, \quad u_{k_L}^{(0)}(x) = u_k \sin(k_Lx)/\sqrt{L}, \]

\[
u_{-k_L}^{(0)}(x) = v_k \sin(k_Lx)/\sqrt{L}, \quad u_{-k_L}^{(0)}(x) = u_k \cos(k_Lx)/\sqrt{L}.
\]

The amplitudes \( u_k \) and \( v_k \) are defined by \( u_k = \sqrt{\frac{\omega^2/4 - \alpha^2}{2\omega(k)}} + \frac{1}{2} \) and \( v_k = -\text{sgn}[V(k)] \sqrt{\frac{k_L^2 + \alpha^2 V(k)}{2\omega(k)}} \) for \( k > 0 \) [28]. A system destabilizes when at least one of the excitation energies \( E_k \) vanishes.

Assuming an initially stable condensate, the influence of \( U_c(x) \) on the excited states can also be approximated in perturbation theory. A perturbation theory for the BdG equations was developed rigorously in Refs. [25,26,29] in the phase-density representation. Since we are chiefly concerned with first-order mode destabilization, we develop a tractable perturbation theory that paints a physical picture of mode softening and naturally encompasses the degeneracy of the roton spectrum. After expanding \( E_k, u_k(x), \) and \( v_k(x) \) in perturbation series, and then substituting into Eq (7), we derive the first-order perturbation equation for the corrections \( E_k^{(1)}, u_k^{(1)}(x), \) and \( v_k^{(1)}(x) \):

\[
\begin{align*}
\omega(k) + \frac{1}{2} \hbar^2 \partial^2 - X^{(0)} & \sim -X^{(0)} - \omega(k) + \frac{1}{2} \hbar^2 \partial^2 - X^{(0)} \left( u_k^{(1)} \right) \\
& = \left( U_c^{(1)} + X^{(1)} \right) X^{(1)} \left( u_k^{(0)} \right) - E_k^{(1)} \left( u_k^{(1)} \right) \left( v_k^{(1)} \right) \sin(k_Lx),
\end{align*}
\]

where \( X^{(0)} \) is the zeroth-order exchange integral operator, \( U_c^{(1)}(x) \) is the first-order combined potential given by Eq. (6), and \( X^{(1)}(x) = \int dx' \chi(x')^2 V(x - x') \) is the first-order exchange integral operator. We can isolate the energy shift \( E_k^{(1)} \) on the right-hand side by taking advantage of the fact that the left-hand side vanishes whenever it is acted on by the operator \( \int dx u_k^{(0)} v_k^{(0)} \) for any \( \omega(k') = \omega(k) \). Degenerate perturbation theory is, in situations exhibiting a roton-maxon excitation spectrum, generally necessary for a complete understanding of all first-order effects; however, we will see that only certain sets of degenerate modes actually mix, due to selection rules. To simplify our notation, we denote the hermitian matrix on the right-hand side of (8) by \( \mathcal{A} \).

It turns out that the matrix elements of \( \mathcal{A} \) vanish in most instances, simplifying our analysis. First, the sine modes completely decouple from the cosine modes as anticipated. Moreover, the matrix element of \( \mathcal{A} \) between any modes \( (u_k, v_k) \) and \( (u_{k'}, v_{k'}) \) vanishes unless the mode-matching condition \( |k' \pm k| = k_L \) is satisfied. This follows from reasons of orthogonality, since all matrix elements are evaluated by integrating products of three sine or cosine functions. Satisfying both the mode-matching condition and the degeneracy condition \( \omega(k') = \omega(k) \) severely limits the number of nonzero matrix elements determining the modes (or degenerate mode mixtures) that shift at first order.

The significance of the mode matching is illustrated schematically in Fig. 3. For any given perturbation probe with wave number \( k_L \), a standing matter wave of the associated wavelength is established, defining the combined potential \( U_c(x) \) (upper panel). Against this backdrop, in the lower two panels, are shown the density fluctuations \( \langle \delta \hat{\rho}(x,t) \rangle \) and the cosine and sine density modulations for \( k = k_L/2 \).
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