ROTON-DRIVEN COLLAPSE IN A QUASI-TWO-DIMENSIONAL DIPOLAR BOSE-EINSTEIN CONDENSATE: A NUMERICAL STUDY

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Abstract. *We use the GPELab toolbox of Matlab programming language to compute ground states of a dipolar Bose-Einstein condensate confined to a quasi-two-dimensional trap, with dipoles polarized perpendicular to the plane. By scanning the dipolar interaction strength* ρ_{dd} *at fixed contact interaction* $\beta = 100$*, we identify a sequence of ground-state structures — a single density peak, a density profile with a central dip, and a ring — that precedes a collapse instability. The collapse threshold is bracketed between* $\rho_{dd} = 1.6$*, the last fully converged ground state, and* $\rho_{dd} = 1.65$*, where imaginary-time propagation fails to converge. Near this threshold, an intermediate value* ($\rho_{dd} = 1.63$) *converges only marginally, consistent with critical slowing down near an instability. Collapsed states show energy two to three orders of magnitude above the stable branch and localized density spikes at the grid scale. These results reproduce the qualitative roton-instability picture expected for dipolar condensates and provide a numerically characterized threshold for this trap and interaction geometry.*

Keywords: *Bose-Einstein condensates, Dipolar BEC, Gross-Pitaevskii equation, GPELab, Roton instability, Collapse threshold, Quasi-two-dimensional condensates, Ground states, Mean-field theory, Dipolar interaction*

Annotatsiya. *Ushbu ishda tekislikka perpendikulyar polyarizatsiyalangan dipollarga ega bo‘lgan va kvazi-ikki o‘lchamli qopqonda ushlanib turilgan dipol Bose-Eynshteyn kondensatining asosiy holatlarini hisoblash uchun Matlab dasturlash tilining GPELab paketidan foydalanildi. O‘zgarmas kontakt ta’sirlashuvida dipol ta’sirlashuvi jadalligini skanerlash orqali kollaps beqarorligidan oldin sodir bo‘ladigan asosiy holat tuzilmalarining ketma-ketligi — yagona zichlik piki, markazida botiqligi bo‘lgan zichlik profili hamda halqasimon tuzilma aniqlandi. Kollaps bo‘sag‘asi to‘liq moslashgan (konvergensiyalangan) oxirgi asosiy holatga mos keluvchi 1,6 qiymati hamda mavhum vaqt bo‘yicha tarqalish moslashmaydigan (konvergensiyalanmaydigan) qiymat oralig‘ida*

joylashgan. Ushbu bo‘sag‘a yaqinida oraliq qiymat faqat qisman moslashadi, bu esa beqarorlik yaqinidagi kritik sekinlashuv hodisasiga mos keladi. Kollapsga uchragan holatlar barqaror tarmoqqa nisbatan energiyaning ikki-uch tartibga yuqoriligini hamda panjara masshtabida lokalizatsiyalangan zichlik piklarini ko‘rsatadi. Ushbu natijalar dipol kondensatlari uchun kutilayotgan roton beqarorligining sifat manzarasini namoyon etadi va ushbu qopqon hamda ta’sirlashuv geometriyasi uchun sonli ravishda aniqlangan bo‘sag‘a qiymatini beradi.

Kalit so‘zlar: *Bose-Eynshteyn kondensati, dipol BEK, Gross-Pitaevskiy tenglamasi, GPELab, roton beqarorligi, kollaps bo‘sag‘asi, kvazi-ikki o‘lchamli kondensatlar, asosiy holat, o‘rtacha maydon nazariyasi, dipol ta’sirlashuvi*

Аннотация. *С использованием GPELab выполнен расчет основных состояний дипольного конденсата Бозе — Эйнштейна, находящегося в квазидвумерной ловушке с диполями, поляризованными перпендикулярно плоскости. Путем сканирования интенсивности дипольного взаимодействия при фиксированном контактном взаимодействии выявлена последовательность структур основного состояния — единичный пик плотности, профиль плотности с минимумом в центре и кольцевая структура, предшествующая неустойчивости коллапса. Порог коллапса заключен между значением 1,6, соответствующим последнему полностью сошедшемуся основному состоянию, и значением, при котором распространение во мнимом времени теряет сходимость. Вблизи этого порога промежуточное значение демонстрирует лишь частичную сходимость, что согласуется с эффектом критического замедления вблизи неустойчивости. Коллапсировавшие состояния характеризуются энергией на два-три порядка выше устойчивой ветви и локализованными пиками плотности на масштабе расчетной сетки. Полученные результаты воспроизводят качественную картину ротонной неустойчивости, ожидаемую для дипольных конденсатов, и обеспечивают численно определенный порог для данной геометрии ловушки и взаимодействия.*

Ключевые слова: *Конденсат Бозе — Эйнштейна, уравнение Гросса — Питаевского, GPELab, ротонная неустойчивость, порог коллапса, квазидвумерные конденсаты, основное состояние, теория среднего поля, дипольное взаимодействие*

1. Introduction

Bose-Einstein condensates (BECs) with dipolar interactions differ from condensates with only short-range contact interactions in one essential respect: the dipole-dipole interaction is long-ranged and anisotropic, attractive along the polarization axis and repulsive in the perpendicular plane. This anisotropy gives dipolar condensates a richer excitation spectrum than a purely contact-interacting gas, including a roton-like minimum in the dispersion relation at finite momentum, first predicted theoretically for dipolar BECs by Santos, Shlyapnikov and Lewenstein, and by Ronen, Bortolotti and Blume for the quasi-two-dimensional geometry considered here. When the roton minimum touches zero energy, the condensate becomes unstable against the spontaneous growth of density modulations at the corresponding wavelength, which can lead to pattern formation or outright collapse depending on the trap geometry and interaction strengths involved.

This instability has been studied extensively for three-dimensional dipolar condensates, most notably in the dysprosium and erbium experiments that established the existence of self-bound droplets and supersolid states stabilized against collapse by beyond-mean-field corrections. The quasi-two-dimensional case, in which the condensate is tightly confined along the polarization axis, is a simpler and computationally cheaper setting in which the same roton mechanism operates, and it remains a useful testbed for characterizing collapse thresholds before considering the additional physics of quantum fluctuations that stabilize droplets in three dimensions.

In this work we numerically characterize the ground-state structure and collapse threshold of a quasi-2D dipolar condensate as a function of the dipolar interaction strength, using the mean-field Gross-Pitaevskii equation (GPE) and the open-source GPELab toolbox. We do not include beyond-mean-field corrections, so the collapsed states we identify are mean-field instabilities rather than stabilized droplets; this is consistent with the scope of a first numerical characterization. Our aim is to confirm the qualitative sequence of ground-state structures predicted by roton-instability theory, and provide a numerically resolved collapse threshold for a specific, reproducible set of trap and interaction parameters.

2. Theoretical Background

2.1 The dipolar Gross-Pitaevskii equation

The mean-field wavefunction $\psi(r,t)$ of a dipolar BEC obeys the Gross-Pitaevskii equation

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V_{trap}(r) + \beta|\psi|^2 + \Phi_{dd}(r,t)\right]\psi = i\hbar\frac{\partial\psi}{\partial t}$$

2.2 Quasi-2D reduction

When the condensate is tightly confined along the polarization axis (taken as z) with harmonic-oscillator length ℓ_z much smaller than the in-plane extent, the wavefunction factorizes as $\psi(\boldsymbol{r}) \approx \varphi(x,y)\,\chi(z)$, with χ the ground state of the $z-$confinement. Integrating out the z-dependence yields an effective 2D GPE for $\varphi(x,y)$ with a nonlocal in-plane interaction whose Fourier transform is

$K(q) = 2 - 3\sqrt{\pi}\,q\,e^{q^2}erfc(q)$,

where $q = \frac{|\boldsymbol{q}|\ell_z}{\sqrt{2}}$ is the dimensionless in-plane momentum (Ronen, Bortolotti & Blume, Phys. Rev. Lett. 98, 030406, 2007). This kernel is repulsive at long wavelength ($K \to 2$ as $q \to 0$) and attractive at short wavelength ($K \to -1$ as $q \to \infty$), which is the origin of the roton minimum in the excitation spectrum: at intermediate q the net interaction can locally favor density modulation. This is exactly the kernel implemented in GPELab's DipoleDipole2d function, with the overall strength set by a dimensionless parameter we refer to as ρ_{dd}.

2.3 Expected phenomenology

As ρ_{dd} increases relative to the contact strength β, the roton minimum is expected to deepen and move toward zero energy. Before the minimum reaches zero, the ground state can still be found by direct energy minimization, but its density profile is expected to depart from the simple Thomas-Fermi shape, developing structure at the roton wavelength (rings, or in more strongly modulated regimes, arrays of droplets). Once the minimum reaches and crosses zero, no stable ground state exists at that wavelength and the mean-field theory predicts collapse: the density profile has no minimum-energy configuration and imaginary-time propagation, which follows the local energy gradient, fails to converge. This is the phenomenology we test numerically below.

3. Methods

3.1 Numerical approach

We solved the quasi-2D dipolar GPE using GPELab (Antoine & Duboscq, Comput. Phys. Commun. 185, 2014; 193, 2015), a MATLAB toolbox implementing pseudospectral methods for the GPE, including a built-in FFT-based evaluation of the dipolar convolution term via the kernel $K(q)$ above. Ground states were computed with GPELab's backward-Euler pseudospectral scheme (BESP), which

propagates the GPE in imaginary time with renormalization at each step, converging to the lowest-energy state consistent with the given atom number.

3.2 Parameters

- Domain: $[-10, 10] \times [-10, 10]$ (dimensionless units)
- Grid: 257×257 points
- Trap: isotropic 2D harmonic potential, $V(x, y) = \frac{1}{2}(x^2 + y^2)$
- Contact interaction strength: $\beta = 100$ (fixed throughout)
- Dipolar interaction strength: ρ_{dd} , varied from 0.5 to 2.0
- Convergence criterion: relative change in the wavefunction (MaxNorm) below 10^{-6} between successive iterations

3.3 Procedure

For each value of ρ_{dd}, we computed the ground state by imaginary-time propagation to convergence, or until it became clear that the run was diverging (energy and chemical potential growing without bound over hundreds of iterations, with the stopping criterion not decreasing). We recorded the converged (or terminal) peak density, its location, the total energy, the chemical potential, and the wall-clock time to convergence or termination. Peak density was computed as $max|\varphi(x, y)|^2$, not the density at the trap center, since the two coincide only for centrally-peaked profiles; this distinction becomes important once the density develops a ring structure (Section 3.4 below).

4. Results

4.1 Ground-state evolution with dipolar strength

For weak dipolar strength ($\rho_{dd} = 0.5$ and 1.2) the ground state is a smooth, single-peaked, radially symmetric cloud with peak density 0.057 and 0.052 respectively, and energy close to 3.95– 3.97. As ρ_{dd} increases, the density at the trap center is progressively depleted. At $\rho_{dd} = 1.5$ the profile shows a central dip (origin density 0.037 against a peak of 0.058), and at $\rho_{dd} = 1.6$ the state is a well-defined ring with peak density 0.066, origin density 0.025, and energy 4.23. This redistribution of density into an annulus is consistent with the roton mechanism described in Section 2.3.

4.2 Onset of collapse

Beyond $\rho_{dd} = 1.6$, imaginary-time propagation no longer converges.

ρ_{dd}	Peak density	Energy	Profile	Converged
0.5	0.0566	3.951	Single peak	Yes
1.2	0.0524	3.973	Single peak	Yes
1.5	0.0576	4.059	Central dip	Yes

1.6	0.0658	4.226	Ring	Yes
1.63	≈0.08	4.387	Square-like ring	Marginal (criterion 1.6×10^{-4})
1.65	—	—	—	No
1.7	≈28	≈880	Localized spikes	No
1.8	≈47	≈1300–1950	Localized spike	No
2.0	≈45	≈1500	Localized spike	No

At $\rho_{dd} = 1.7$ and above, the energy grows by two to three orders of magnitude, the stopping criterion remains of order 1–10, and the density concentrates into one or a few grid-scale spikes with peak values 500–800 times the stable-branch values. The rms radii along x and y also become unequal in these runs (e.g. 0.98 vs. 1.45 at $\rho_{dd} = 1.8$), reflecting the loss of radial symmetry during collapse. Runtimes rise sharply, from 30–100 s for converged runs to 290–2300 s for diverging ones.

The critical strength lies between $\rho_{dd} = 1.6$, the last fully converged state, and $\rho_{dd} = 1.65$, where the solver fails. The intermediate value $\rho_{dd} = 1.63$ converged only marginally after 1425 iterations the stopping criterion remained about 150 times above tolerance, though the energy stayed finite — consistent with critical slowing down near the instability. We report the critical value as $\rho_{dd}^{c} \approx 1.6–1.65$ for $\beta = 100$.

5. Discussion

The sequence we observe — single peak, central dip, ring, marginal/distorted ring, collapse is qualitatively consistent with the roton-instability picture for quasi-2D dipolar condensates. The appearance of a ring rather than an immediate collapse is expected: before the roton minimum crosses zero, the interaction landscape favors a finite-wavelength density redistribution rather than complete instability, and a ring is the natural circularly-symmetric realization of that redistribution in an isotropically trapped condensate. The slow convergence we observe at $\rho_{dd} = 1.63$, together with the qualitative change in profile shape (from a smooth ring to a more structured, square-like ring), is consistent with the system approaching a bifurcation point, where the energy landscape becomes shallow along the unstable direction.

Several limitations should be kept in mind when interpreting these results.

First, our identification of collapse is numerical: we equate non-convergence of imaginary-time propagation, together with unbounded growth of energy and density, with a genuine physical collapse instability. This is a standard and

reasonable diagnostic, but it is not the same as demonstrating collapse dynamics directly; a real-time simulation starting from a near-threshold state (e.g. ρ_{dd}= 1.63 or 1.65) would provide a more direct dynamical confirmation and would allow us to characterize the collapse timescale as a function of distance from threshold, which is a natural extension of this work.

Second, all results reported here are for a single value of the contact interaction strength, $\beta = 100$. The dipolar collapse threshold is expected to depend on the ratio of dipolar to contact interaction strength rather than on ρ_{dd}alone, so the value $\rho_{dd}^{c} \approx 1.6–1.65$ should be understood as specific to β = 100 and this trap geometry, not as a universal threshold. A scan over several β values, even a small one, would let us characterize how the threshold scales with the interaction ratio and would substantially strengthen the generality of the result.

Finally, this study uses the mean-field GPE without beyond-mean-field (Lee-Huang-Yang type) corrections. In three-dimensional dipolar condensates, such corrections are known to arrest the mean-field collapse and stabilize self-bound droplets and supersolid states at higher densities. The collapse we characterize here should therefore be understood as a pure mean-field instability, relevant to the regime where these corrections are small or absent, rather than as a prediction that a real quasi-2D dipolar gas necessarily destroys itself at this threshold.

6. Conclusion

We have numerically characterized the ground-state structure of a quasi-2D dipolar Bose-Einstein condensate as a function of dipolar interaction strength, using the GPELab toolbox. As the dipolar strength increases at fixed contact interaction ($\beta = 100$), the ground state evolves from a single density peak to a ring-shaped profile, consistent with the roton-instability mechanism expected for this geometry, before collapsing at a threshold we bracket between ρ_{dd} = 1.6 and 1.65. Collapsed states show energy two to three orders of magnitude above the stable branch and highly localized density spikes. These results provide a concrete, reproducible numerical benchmark for the collapse threshold in this system and identify clear directions for further work: real-time collapse dynamics near threshold, a scan over contact interaction strength to establish scaling of the threshold, and a grid-resolution study to confirm the divergent character of the collapsed states.

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