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ZAMONAVIY TA'LIMDA ISLOHOTLAR VA TEXNIK TAFAKKUR

ilmiy jurnali

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“ZAMONAVIY TA'LIMDA ISLOHOTLAR VA TEXNIK TAFAKKUR”

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RING-TO-DROPLET TRANSITION IN A TWO-DIMENSIONAL DIPOLAR BOSE–EINSTEIN CONDENSATE: A GROUND-STATE SCAN WITH GPELAB

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Abstract. We use the ready-made simulation model of the MATLAB toolbox GPELab to compute ground states of a two-dimensional dipolar Bose–Einstein condensate (BEC) while the dipolar strength BetaDipole is varied from 5 to 10 at fixed contact strength $\text{Beta} = 3000$. Ground states are obtained by imaginary-time propagation with the BESP scheme. For $\text{BetaDipole} = 5$ and 6 the ground state is a rotationally symmetric set of concentric rings. A hexagonal lattice of density droplets appears between $\text{BetaDipole} = 6.1$ and 6.2, first as a core of about 19 droplets





surrounded by faint outer rings, and it grows to about 30 droplets at 6.5 and about 60 to 70 at 10. The energy rises smoothly with BetaDipole, and the difference between the x and y mean-square radii serves as a simple marker of broken rotational symmetry. Among the converged runs, the cost of convergence is highest close to the onset: 55,213 iterations at 6.25, compared with 3,693 at 5. A time-step test shows that $\text{Deltat} = 1\text{e-}2$ and $\text{Deltat} = 1\text{e-}3$ give the same state, the larger step did converge within 20,000 iterations in the lattice region and gave a saving in CPU time.

Keywords. Dipolar Bose-Einstein condensate; GPELab; ground state; imaginary-time propagation; droplet lattice; rotational symmetry breaking; Gross-Pitaevskii equation.

Аннотация: Мы используем готовую имитационную модель из набора инструментов GPELab для MATLAB, чтобы вычислить основные состояния двумерного дипольного бозе-эйнштейновского конденсата (БЭК) при изменении дипольной константы BetaDipole от 5 до 10 при фиксированной константе контактного взаимодействия $\text{Beta} = 3000$. Основные состояния получены методом распространения по мнимому времени со схемой BESP. При BetaDipole = 5 и 6 основное состояние представляет собой вращательно-симметричный набор концентрических колец. Гексагональная решётка капель плотности появляется между BetaDipole = 6,1 и 6,2: сначала в виде ядра примерно из 19 капель, окружённого слабыми внешними кольцами, затем она разрастается до примерно 30 капель при 6,5 и до примерно 60–70 при 10. Энергия плавно растёт с увеличением BetaDipole, а разность между средними квадратами радиусов по x и y служит простым индикатором нарушения вращательной симметрии. Среди сошедшихся расчётов затраты на сходимость максимальны вблизи порога возникновения решётки: 55 213 итераций при 6,25 против 3 693 при 5. Тест временного шага показывает, что $\text{Deltat} = 1\text{e-}2$ и $\text{Deltat} = 1\text{e-}3$ дают одно и то же состояние; больший шаг сошёлся за 20 000 итераций в области решётки и дал экономию процессорного времени.

Ключевые слова: Дипольный бозе-эйнштейновский конденсат; GPELab; основное состояние; распространение по мнимому времени; решётка капель; нарушение вращательной симметрии; уравнение Гросса–Питаевского.

Annotatsiya: Biz MATLAB uchun GPELab tayyor simulyatsiya modelidan foydalanib, kontakt ta'sir konstantasi $\text{Beta} = 3000$ qayd etilgan holda dipol konstantasi BetaDipole 5 dan 10 gacha o'zgartirilganda ikki o'lchamli dipolar Boze–Eynshteyn kondensati (BEK)ning asosiy holatlarini hisoblaymiz. Asosiy holatlar BESP sxemasi yordamida mavhum vaqt bo'yicha tarqatish usulida olingan. BetaDipole = 5 va 6 da asosiy holat konsentrik halqalarning aylanma simmetrik to'plamidan iborat. Zichlik tomchilarining geksagonal panjarasi BetaDipole = 6,1 va 6,2 oralig'ida paydo bo'ladi: avval xira tashqi halqalar bilan o'ralgan taxminan 19 ta tomchidan iborat yadro ko'rinishida, so'ngra u 6,5 da taxminan 30 ta, 10 da esa taxminan 60–70 ta tomchigacha o'sadi. Energiya BetaDipole ortishi bilan silliq oshadi, x va y bo'yicha o'rtacha kvadratik radiuslar farqi esa aylanma simmetriya buzilishining oddiy ko'rsatkichi bo'lib xizmat qiladi. Yaqinlashgan hisoblashlar orasida yaqinlashish uchun sarf paydo bo'lish chegarasi yaqinida eng yuqori: 6,25 da 55 213 iteratsiya, 5 da esa 3 693. Vaqt qadami testi $\text{Deltat} = 1\text{e-}2$ va $\text{Deltat} = 1\text{e-}3$ bir xil holatni berishini ko'rsatadi; katta qadam panjara sohasida 20 000 iteratsiya ichida yaqinlashdi va protsessor vaqtini tejash imkonini berdi.





Kalit soʻzlar: Dipolar Bose–Eynshteyn kondensati; GPESLab; asosiy holat; mavhum vaqt boʻyicha tarqatish; tomchilar panjarasi; aylanma simmetriyaning buzilishi; Gross–Pitaevskiy tenglamasi.

1. Introduction. Bose–Einstein condensates of atoms with a large magnetic dipole moment interact through a long-range, anisotropic interaction in addition to the usual short-range contact interaction. When the two interactions are balanced, dipolar condensates can form self-bound density droplets and, in some regimes, supersolid states in which a density modulation coexists with global phase coherence. Mean-field calculations based on the Gross–Pitaevskii equation (GPE) are a standard first tool for exploring such states.

GPESLab is a MATLAB toolbox for computing stationary states and dynamics of GPEs [5, 6]. It ships with ready-made examples, including a two-dimensional dipolar "supersolid" example. In this thesis we use that example without changing the model. We only vary its dipolar strength and the numerical settings. The aims are:

1. to map how the ground-state structure changes as BetaDipole increases,
2. to record how expensive each ground state is to compute, and
3. to test whether a larger time step gives the same states at lower cost.

2. Model and Numerical Method

2.1 Model and parameters. The example computes the ground state of a single-component, two-dimensional GPE with a kinetic term (prefactor Delta = 0.5, i.e. the usual $-\frac{1}{2}\nabla^2$), a contact interaction of strength Beta, and a nonlocal dipolar interaction of strength BetaDipole. The remaining parameters of the example are gamma = 5 and R0 = 1.5. In all runs Beta = 3000, Delta = 0.5, gamma = 5 and R0 = 1.5 were kept fixed, and only BetaDipole was changed.

For each ground state we report the energy, the chemical potential, the root-mean-square radii in x and y, the peak density, the number of iterations and the CPU time. The difference between the x and y mean-square radii is used as a simple marker of broken rotational symmetry.

2.2 Numerical method. Ground states are computed by imaginary-time propagation with the Backward Euler Spectral (BESP) scheme of GPESLab. Most runs used Deltat = 1e-3 with the stopping tolerance printed by GPESLab as 1e-9. Two runs used Deltat = 1e-2 with a printed tolerance of 1e-8, and the time-step test in Section 3.6 compares the two. The solver stops when the evolution criterion falls below the tolerance or when the iteration cap (Max_iter) is reached. The initial data are the default ones of the example. Each BetaDipole value was run once. CPU times were measured on one personal computer and are only roughly comparable between runs.

3. Results



3.1 Overview. Table 1 lists all runs. The run at BetaDipole = 6.2 stopped making progress at iteration 22,305 and was interrupted, so its numbers are provisional.

Table 1. Ground states as a function of BetaDipole (Beta = 3000).

BetaDipole	Deltat	Iterations	Energy	Chem. potential	rms radius (x / y)	Peak density	Structure
5	1e-3	3,693	359.07	366.73	3.748 / 3.748	about 0.008	Weak concentric rings, maximum at the center
6	1e-3	10,226	392.80	400.06	3.926 / 3.926	about 0.0095	strong rings, central dip
6.1	1e-2	5,036	396.11	403.42	3.942 / 3.942	about 0.0098	about 5 rings, small central dip
6.2 (provisional)	1e-3	not converged (22,305)	400.95	409.77	3.957 / 3.957	about 0.02	core of about 19 droplets, faint hexagonal outer rings
6.25	1e-3	55,213	403.36	412.94	3.965 / 3.965	about 0.019	core of about 19 droplets, hexagonal outer rings
6.5	1e-3	18,618	413.56	425.27	4.003 / 4.004	about 0.025	about 30 droplets, faint outer ring
7	1e-3	11,044	431.45	445.73	4.075 / 4.078	about 0.027	hexagonal lattice, about 30 to 40 droplets
10	1e-2	4,340	516.575	535.657	4.445 / 4.445	about 0.033	hexagonal lattice

At BetaDipole = 10 the run with Deltat = 1e-3 was interrupted at iteration 22,680 with a criterion of 1.7e-7, before reaching its 1e-9 target. It gave an energy of 516.587 and a chemical potential of 535.687. Droplet counts were estimated by eye from the density plots.



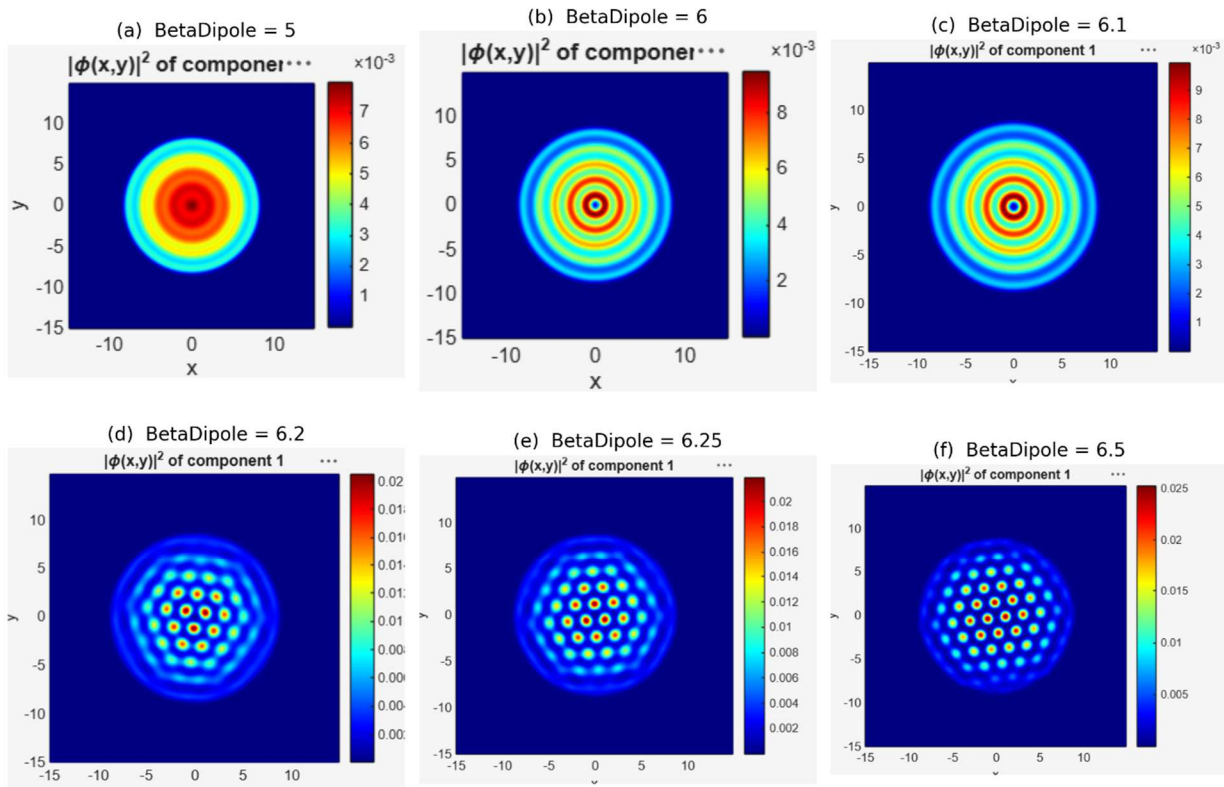


Figure 1. density plots $|\varphi(x, y)|^2$ for $\text{BetaDipole} = 5, 6, 6.1, 6.25$

3.2 Structure of the ground states

At $\text{BetaDipole} = 5$ the density is a smooth, rotationally symmetric set of concentric rings with a density maximum at the centre. At $\text{BetaDipole} = 6$ the rings are much more strongly modulated and the centre has become a dip (origin density 0.0012, about 12% of the peak). At 6.1 the state is still a ring state. From 6.2 on, the centre of the cloud is a hexagonal array of separated droplets surrounded by fainter rings with a hexagonal outline. At 6.25 the core has about 19 droplets. The core grows to about 30 droplets at 6.5 and the outer ring weakens. At 7 and 10 the droplets fill the whole cloud, and the cloud becomes larger and the peaks sharper as BetaDipole increases (peak density about 0.027 at 7 and 0.033 at 10).

3.3 Onset of the droplet lattice.

The lattice appears between $\text{BetaDipole} = 6.1$, where only rings are found, and 6.2, where a droplet core is already present. The onset is therefore located within an interval of width 0.1. This conclusion rests on the provisional 6.2 run, and the 6.2 state may still rearrange as it converges. The x and y mean-square radii agree to better than $1e-8$ for $\text{BetaDipole} = 5, 6$ and 6.1, and begin to differ at 6.2 and 6.25 (by about $2e-6$) and clearly at 6.5 and 7 (by about $2e-3$). The radii difference therefore tracks the breaking of rotational symmetry. It is not monotonic, because



at $\text{BetaDipole} = 10$ the larger and nearly hexagonal lattice has a difference of only about $7e-5$, so it should be read together with the density plots.

3.4 Energy.

The energy increases smoothly with BetaDipole , from 359.07 at 5 to 516.59 at 10, with no visible jump. The increase per unit of BetaDipole is about 34 from 5 to 6 and from 6 to 6.1 (the ring branch), about 48 between 6.1 and 6.25, about 41 from 6.25 to 6.5, about 36 from 6.5 to 7 and about 28 from 7 to 10. The slope is therefore steepest around the onset of the lattice. This is suggestive but rests on single runs, and the 6.1 point used a different time step.

3.5 Cost of convergence.

Among runs with $\text{Deltat} = 1e-3$ the number of iterations needed to reach the tolerance was 3,693 at $\text{BetaDipole} = 5$, 10,226 at 6, 55,213 at 6.25, 18,618 at 6.5 and 11,044 at 7. The run at 6.2 did not converge within 22,305 iterations. The cost per iteration was about 0.2 s throughout, so the differences are almost entirely differences in iteration count. The solver therefore works hardest close to the onset of the lattice, where the state changes character. A likely explanation is that several nearly equal configurations compete there, but we have not tested this. At $\text{BetaDipole} = 10$ the run was interrupted after 22,680 iterations at a criterion of $1.7e-7$, so its full cost at $1e-9$ is not known.

3.6 Effect of the time step

The time step was tested at $\text{BetaDipole} = 6.25$ and 10.

	$\text{Deltat} = 1e-3$	$\text{Deltat} = 1e-2$
6.25: outcome	converged, 55,213 iterations	cap reached at 20,000, criterion $4.3e-5$
6.25: energy	403.363	403.326
6.25: chem. potential	412.937	412.867
10: outcome	interrupted at 22,680, criterion $1.7e-7$	converged, 4,340 iterations
10: energy	516.587	516.575

Both time steps give the same state: the density plots agree, the rms radii agree to about five digits at 6.25, and the energies differ by about $1e-4$ relative at 6.25 and $2e-5$ relative at 10. The larger step is therefore adequate for exploring the structure. It did not, however, reduce the cost. The 6.25 run with $\text{Deltat} = 1e-2$ did not converge within 20,000 iterations (200 units of imaginary time, against about 55 for the converged $1e-3$ run). The runs with $\text{Deltat} = 1e-2$ also cost about 0.4 to 0.5 s per iteration, against about 0.2 s for $\text{Deltat} = 1e-3$. We do not know whether the larger step stalls near the lattice onset or would converge with more iterations.

4. Discussion and Limitations

The scan shows a continuous change from a rotationally symmetric ring state to a hexagonal droplet lattice as BetaDipole increases through about 6.1 to 6.2. The ground-state



energy has no jump over the scanned range, and the largest convergence cost occurs near the onset. The following limitations apply.

- **Single runs from default initial data.** Dipolar systems with droplets can have several nearly degenerate local minima. We did not test other initial guesses, so we cannot say whether the states found are the lowest-energy ones.
- **Mixed numerical settings.** Most runs used $\text{Deltat} = 1\text{e-}3$ and a printed tolerance of $1\text{e-}9$, but $\text{BetaDipole} = 6.1$ used $\text{Deltat} = 1\text{e-}2$ and $1\text{e-}8$, and $\text{BetaDipole} = 10$ is reported at $\text{Deltat} = 1\text{e-}2$. The 6.2 run did not converge.
- **No supersolid claim.** The density between droplets was not analysed. At $\text{BetaDipole} = 6.25$ to 7 the origin density is only 1 to 2% of the peak density, which suggests that neighbouring droplets are only weakly connected, but the origin need not be the point of lowest density, and at 10 it lies on a droplet. A supersolid requires a connecting superfluid background, so the states found here are described as droplet-lattice states.
- **Droplet counts** were estimated by eye from the density plots.
- **Model scope.** We used the example as supplied. Whether it includes beyond-mean-field stabilisation terms, and how it relates to a specific experiment, was not checked.

5. Conclusions

Using GPELab's supersolid example with $\text{Beta} = 3000$, we found that the ground state changes from concentric rings at $\text{BetaDipole} = 5$ and 6 to a hexagonal droplet lattice for BetaDipole of about 6.2 and above. The droplet core first has about 19 droplets and grows to about 60 to 70 at $\text{BetaDipole} = 10$. The energy rises smoothly across the transition. The cost of convergence is highest near the onset (55,213 iterations at 6.25). $\text{Deltat} = 1\text{e-}2$ reproduces the states found with $1\text{e-}3$ but did not save computing time and did not converge at 6.25 within 20,000 iterations.

Further work should (i) refine the scan between 6.1 and 6.2 and finish the 6.2 run, (ii) repeat each point from several initial guesses and keep the lowest energy, (iii) analyse the density between droplets, (iv) compare other GPELab ground-state solvers and preconditioners at the critical points, and (v) vary Beta .

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ZAMONAVIY TA'LIMDA ISLOHOTLAR VA TEXNIK TAFAKKUR

ZAMONAVIY TA'LIMDA ISLOHOTLAR & TEXNIK TAFAKKUR

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