Maths physics meeting on cold atoms,
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Two component Bose Einstein condensates: Thomas-Fermi limit, phase separation and defects

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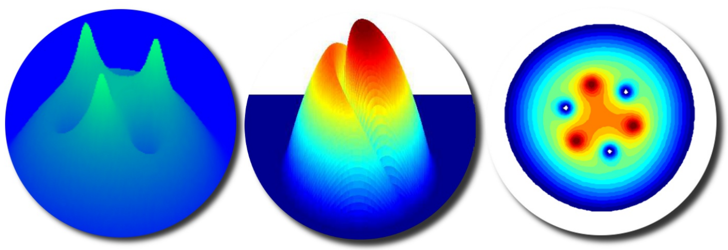
Joint works with

Peter Mason (PRA 2012 and PRA 2013)
Peter Mason and Juncheng Wei (PRA 2012)
Benedetta Noris and Christos Sourdis (in preparation)
Jimena Royo Letelier (to appera in Calculus of Variations and PDE's)
Juncheng Wei (in preparation)



Outline of the talk

I. Main mathematical results for a single condensate

II. Two component condensates: numerical simulations

III. Two component condensates: rigorous results

IV. Spin orbit coupling

Gross Pitaevskii energy for a single condensate

A single BEC, set under rotation $\Omega = \Omega e_z$, is in a state which minimizes

$$E(\psi) = \int_{\mathbb{R}^2} \frac{1}{2}|\nabla\psi - i\Omega \times r\psi|^2 + \frac{1}{2}(1-\Omega^2)r^2|\psi|^2 + \frac{1}{2}g|\psi|^4,$$

Two mathematical limits

• g large, Thomas Fermi limit: analogue of Bethuel Brezis Helein analysis of vortices, also Jerrard, Sandier-Serfaty. vortex core of size $1/\sqrt{g}$ is much smaller than the distance between vortices. Triangular lattice.

• Rapid rotation: $\Omega \to 1$. vortex cores start to overlap: reduction to a single particle state: the lowest Landau level (LLL).

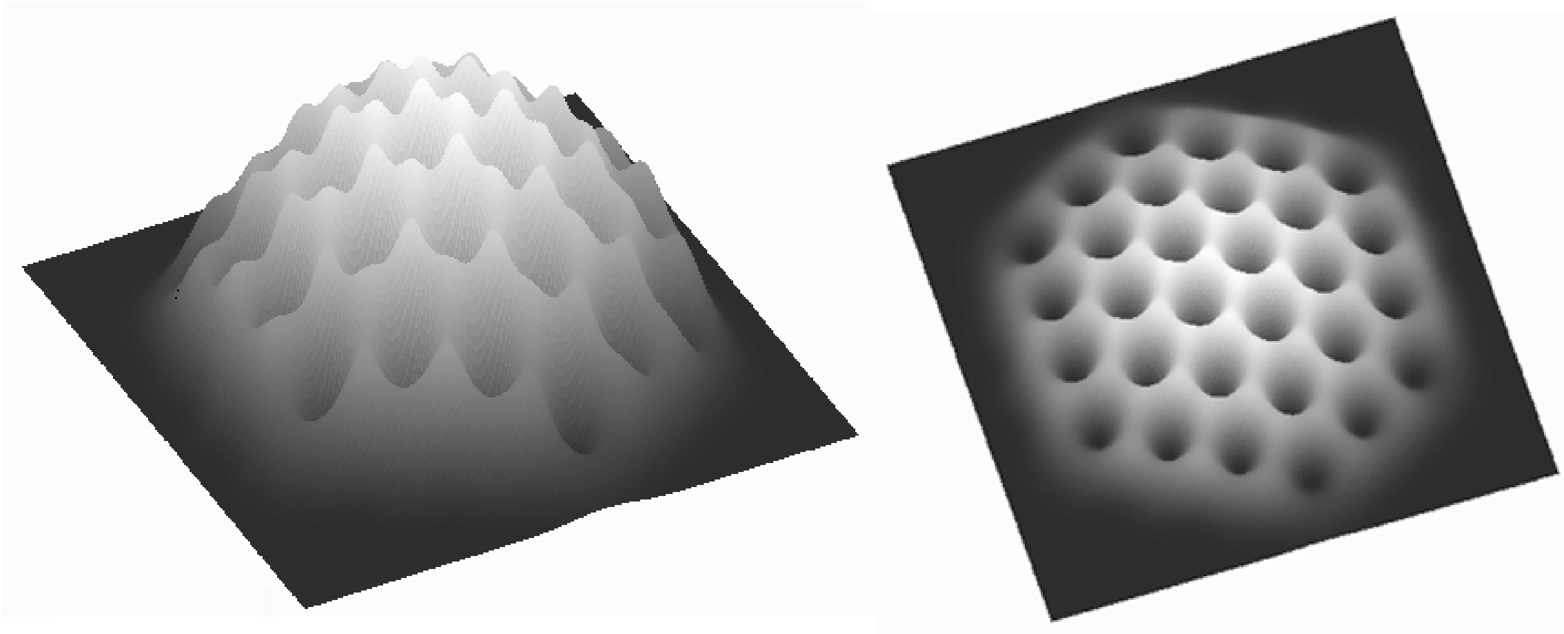


Figure 1: Numerical simulations illustrating experiments in the group of Jean Dalibard

Minimize the Gross Pitaevskii energy in the Thomas Fermi limit, g large:

$$E(\psi)=\int \frac{1}{2}|\nabla\psi - i\Omega\times r\psi|^2+\frac{1}{2}r^2|\psi|^2(1-\Omega^2)+\frac{1}{2}g|\psi|^4,$$

under $\int_{\mathbb{R}^2}|\psi|^2=1$, $r=(x,y)$. Difficulty, the problem is set on $\mathbb{R}^2$ with a constraint and a trapping potential. One can rewrite the energy as

$$E(\psi)=\int \frac{1}{2}|\nabla\psi - i\Omega\times r\psi|^2+\frac{1}{2}g(|\psi|^2-a(r))^2-\frac{1}{2}ga^2(r)|\psi|^2,$$

where $a(r)=\frac{1-\Omega^2}{2g}(R^2-r^2)$, a_+, a_- denote the positive and negative parts of a, and R is determined by the constraint $\int a_+=1$.

Leading order, inverted parabola profile:
$|\psi|^2=a_+(r)$.

Splitting of energy. (Trick due to Mironescu) to get the energy of the vortex balls

Let η be the minimizer at $\Omega = 0$, then $\eta^2 \sim a_+(r)$ and let $v = \psi/\eta$, then

$$E(\psi) - E(\eta) = \int \frac{1}{2}\eta^2 |\nabla v - i\Omega \times rv|^2 + \frac{1}{2} g\eta^4 (|v|^2 - 1)^2$$

Next order: computation of the critical velocity Ω_c for the nucleation of the first vortex. The ground state stays real valued until Ω_c.

Next order vortex balls of size $1/\sqrt{g}$. The behaviour of the vortex core is given by $f(r)e^{i\theta}$ where $f(0) = 0$, and f is the solution tending to 1 at infinity of

$$f'' + \frac{f'}{r} - \frac{f}{r^2} + f(1 - f^2) = 0.$$

Vortex location miminize the vortex interaction energy

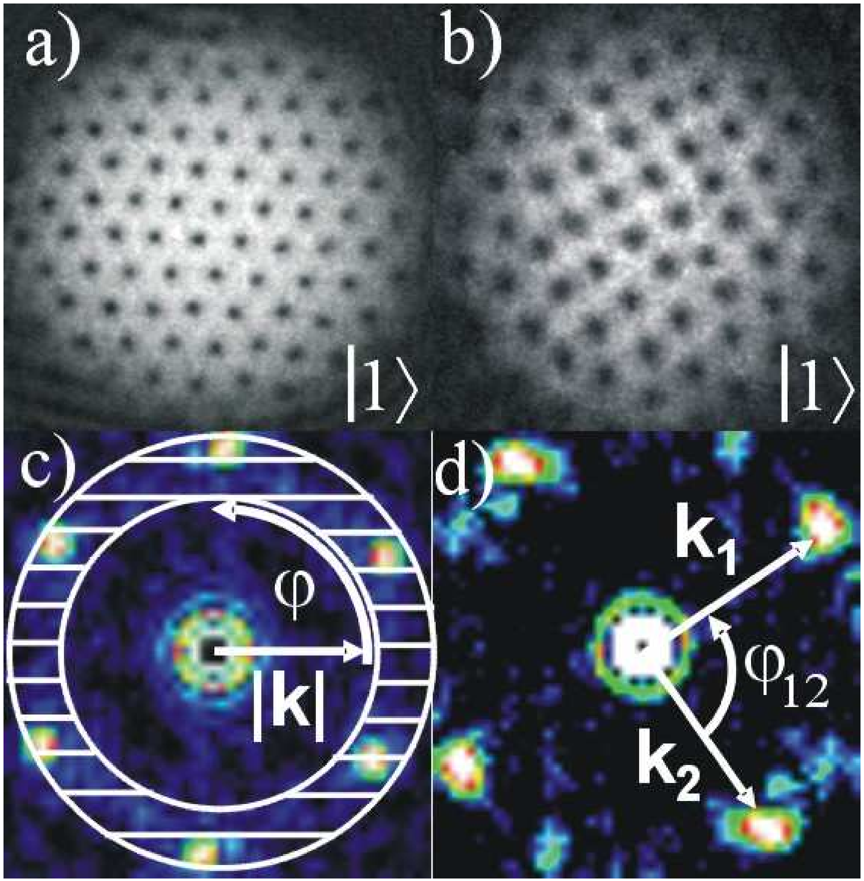
$$\sum_i |p_i|^2 - \sum_{i,j} \log |p_i - p_j|$$

Numerically, almost a triangular lattice.

II. Two component condensates: numerical simulations

2 component condensate: 2 wave functions, new phases and defects.

V. Schweikhard, I. Coddington, P. Engels, S. Tung, and E. A. Cornell (2004): a square lattice is stabilized in a two component condensate.



Two component condensates (Aftalion-Mason)

2 different isotopes of the same alkali atom, isotopes of different atoms, or a single isotope in 2 different hyperfine spin states: 2 wave functions ψ_1 and ψ_2 with $\int |\psi_1|^2 = N_1$, $\int |\psi_2|^2 = N_2$

$$E_{\Omega,g}(\psi) = \int \frac{1}{2}|\nabla\psi - i\Omega \times r\psi|^2 + \frac{1}{2}r^2|\psi|^2(1-\Omega^2) + \frac{1}{2}g|\psi|^4,$$

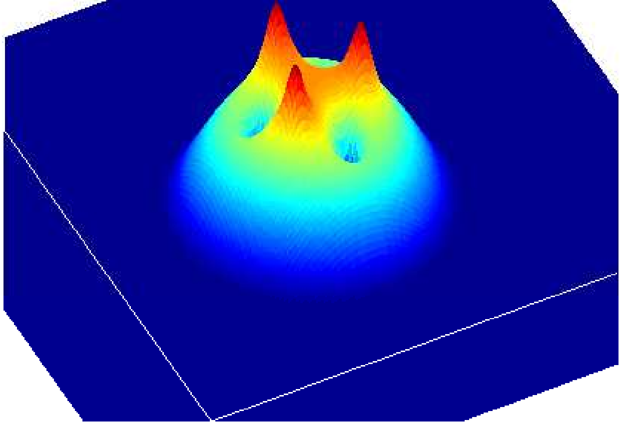
$$E = E_{\Omega,g_1}(\psi_1) + E_{\Omega,g_2}(\psi_2) + g_{12}\int |\psi_1|^2|\psi_2|^2$$

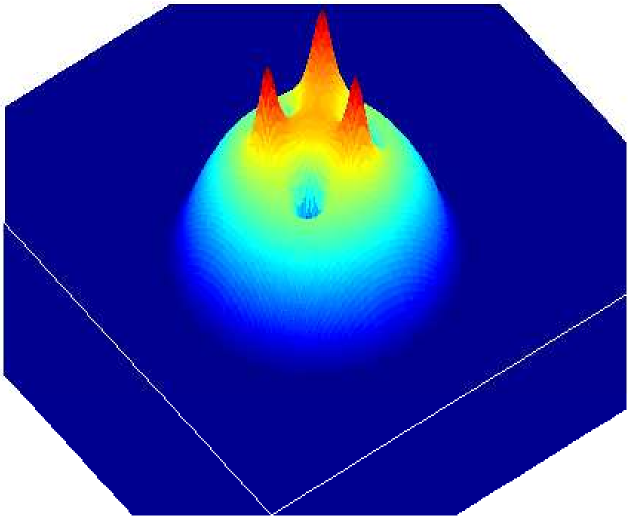
- g_{12} small: 2 components are disk-shaped with vortex lattices. a vortex in component 1 corresponds to a peak in component 2. Square lattice.

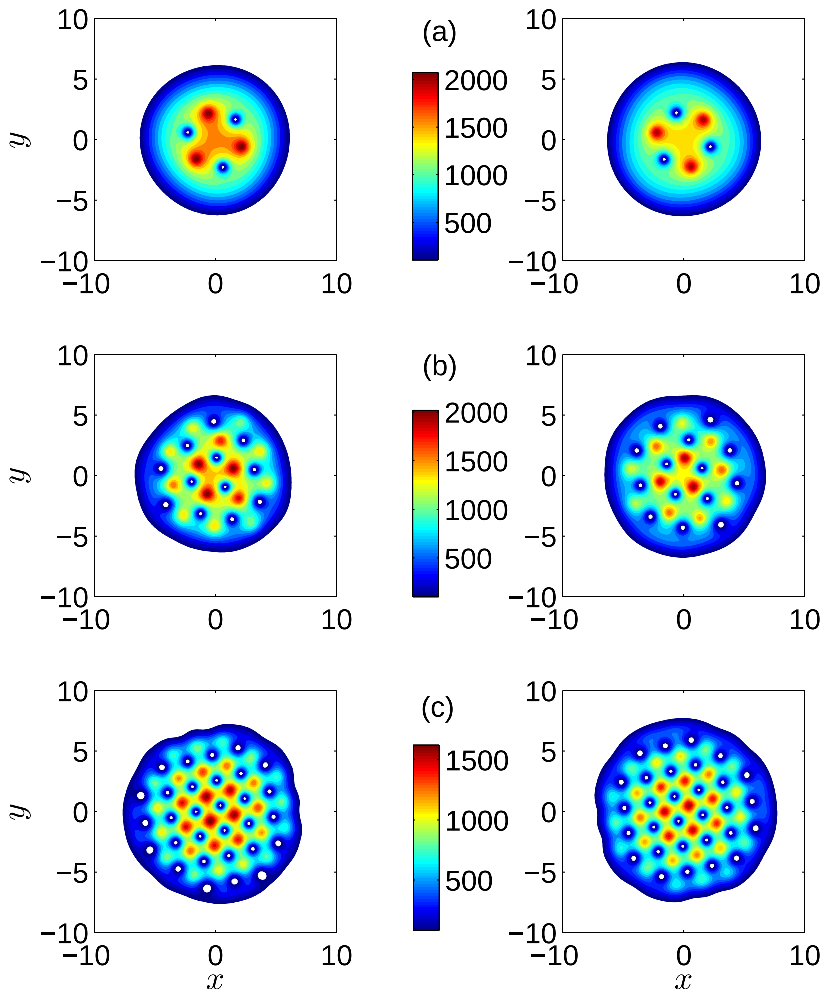
- g_{12} large: phase separation and breaking of symmetry: rotating droplets

- intermediate regime: phase separation but no breaking of symmetry, one component is a disk, the other is an annulus. Skyrmion in the boundary layer

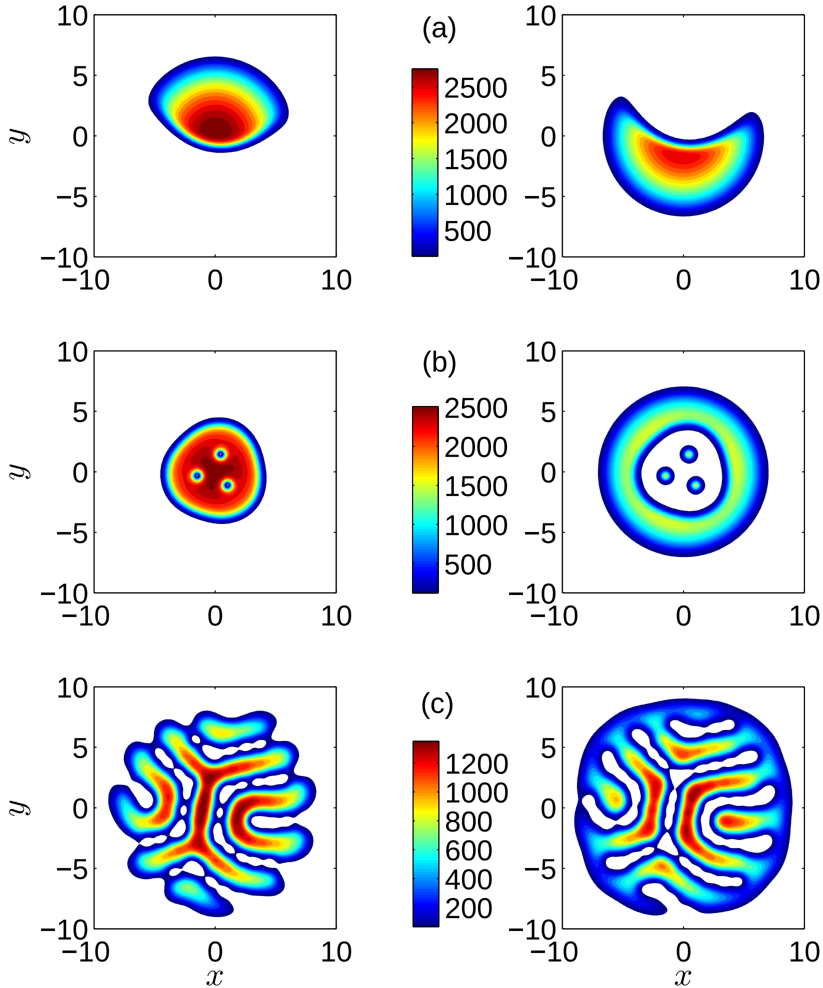
- vortex sheets



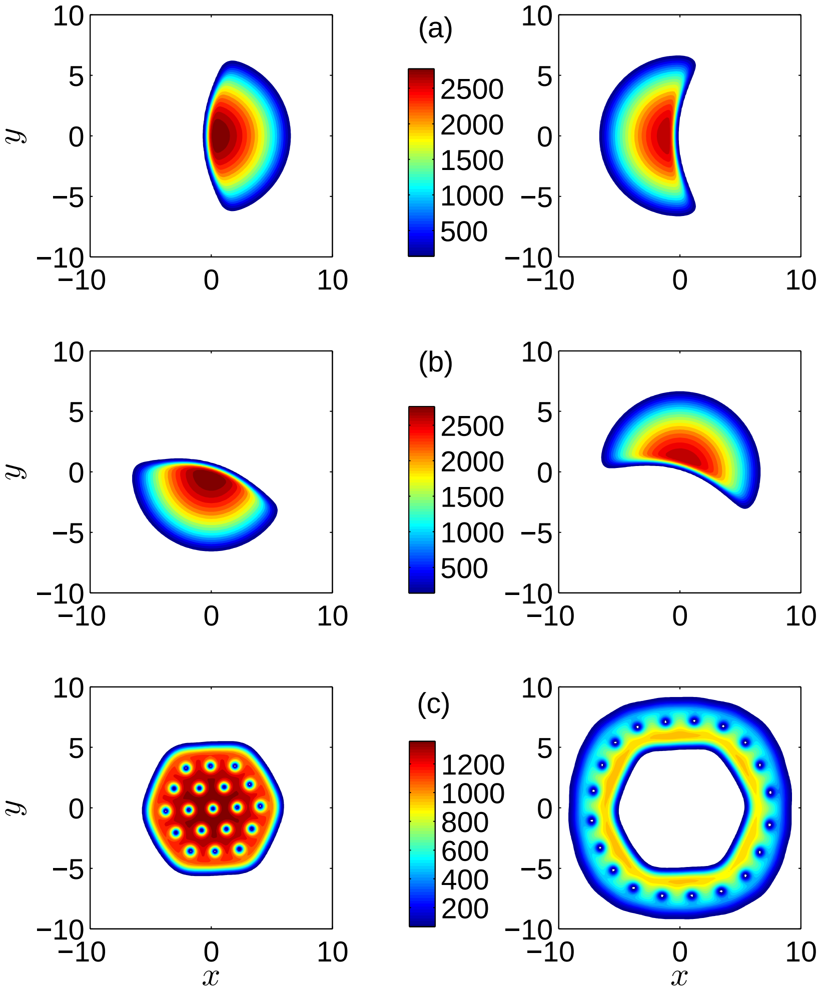




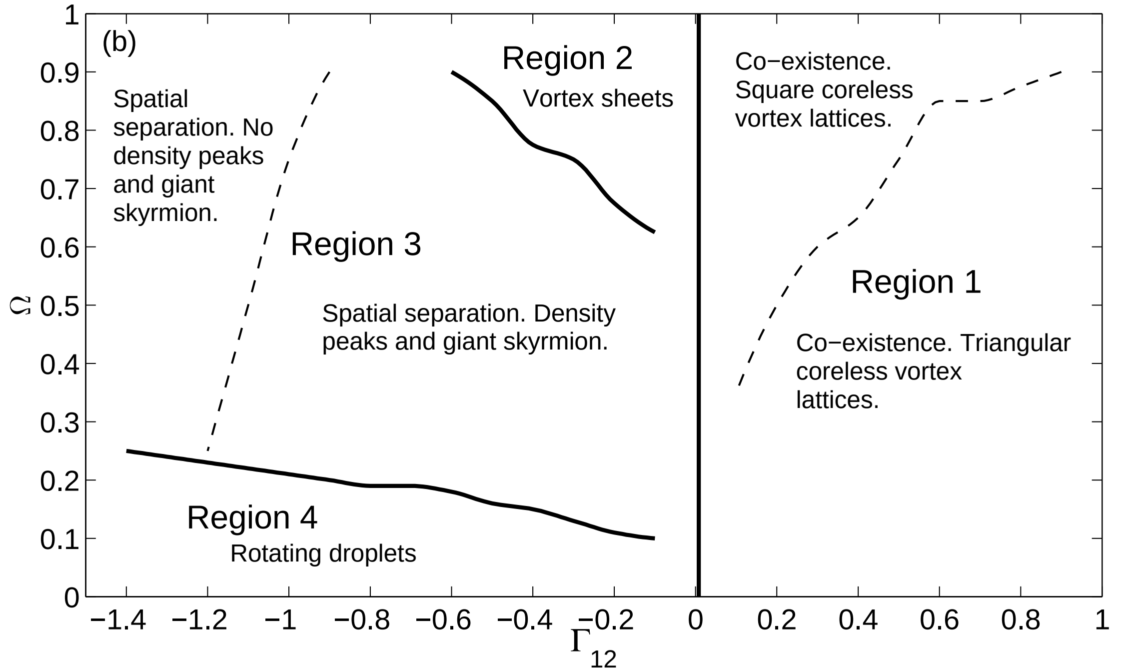
left column $|\psi_1|^2$
right column $|\psi_2|^2$
Ω = (a) 0.25, (b) 0.5, (c) 0.75
$g_1 = 0.0078$, $g_2 = 0.0083$, $N_1 = N_2 = 10^5$, $m_1 = m_2$, $g_{12} = 0.0057$



g_{12} large: phase separation left column $|\psi_1|^2$ right column $|\psi_2|^2$ $g_1 = 0.0078$, $g_2 = 0.0083$, $N_1 = N_2 = 10^5$, $g_{12} = 0.0092$, $\Omega =$ (a) 0.1, (b) 0.5, (c) 0.9



g_{12} larger
left column $|\psi_1|^2$
right column $|\psi_2|^2$
$g_1 = 0.0078$, $g_2 = 0.0083$, $N_1 = N_2 = 10^5$, $g_{12} = 0.0122$), $\Omega =$ (a) 0, (b) 0.1, and (c) 0.9.



$\Omega - \Gamma_{12}$ phase diagrams $g_1 = 0.0078$, $g_2 = 0.0083$, $N_1 = N_2 = 10^5$ $\Gamma_{12} = 1 - \frac{g_{12}^2}{g_1 g_2}$

III. Two component condensates: rigorous results

What can be proved

We recall $\Gamma_{12} = 1 - \frac{g_{12}^2}{g_1 g_2}$.

• If $\Gamma_{12} > 0$, we expect phase coexistence. If g_1, g_2, g_{12} are large, TF limit ($g_1 = \alpha_1 g$, $g_2 = \alpha_2 g$, $g_{12} = \alpha_{12} g$ with g large).

– leading order, inverted parabola profile. The computation of the limiting profile involves the coupling

$$\alpha_1 |\psi_1|^2 + \alpha_{12} |\psi_2|^2 = \lambda_1 - \frac{1}{2}(1 - \Omega^2) r^2$$

$$\alpha_{12} |\psi_1|^2 + \alpha_2 |\psi_2|^2 = \lambda_2 - \frac{1}{2}(1 - \Omega^2) r^2$$

Either 2 disks with different radii or a disk and an annulus. Convergence in the TF limit. No vortex in the exterior until the first critical velocity (Aftalion-Noris-Sourdis following Aftalion-Jerrard-Letelier and Karali-Sourdis).

What we can prove in ANS:

• uniqueness of the ground state at $\Omega = 0$. Either 2 disks or a disk+annulus.

• precise estimate of the convergence to the Thomas-Fermi limit. Proved by constructing an approximate solution. Then using the linearized operator, we perturb it to a genuine solution. By uniqueness, it is the ground state. Related to the talk of C.Gallo.

• until the first vortex, the minimizer is unique and real valued. Done by division of the ground state at Ω, by the ground state at $\Omega = 0$ and with jacobian estimates, we prove that the ratio is 1. It means that the ground state stays real valued until the first vortex.

– computation of the critical velocity for the 1st vortex, called Ω_c (in component with larger radius). (Aftalion-Mason-Wei)

– vortex peak interaction. The equation of the vortex core has to be replaced by a system of vortex/spike $(f(r)e^{i\theta}, S(r))$ where $(f(r), S(r))$ satisfies

$$\frac{(rf')'}{r} - \frac{f}{r^2} + \alpha_1 f(1 - f^2) + \alpha_{12} S^2 f = 0,$$

$$\frac{(rS')'}{r} + \alpha_2 S(1 - S^2) + \alpha_{12} f^2 S = 0.$$

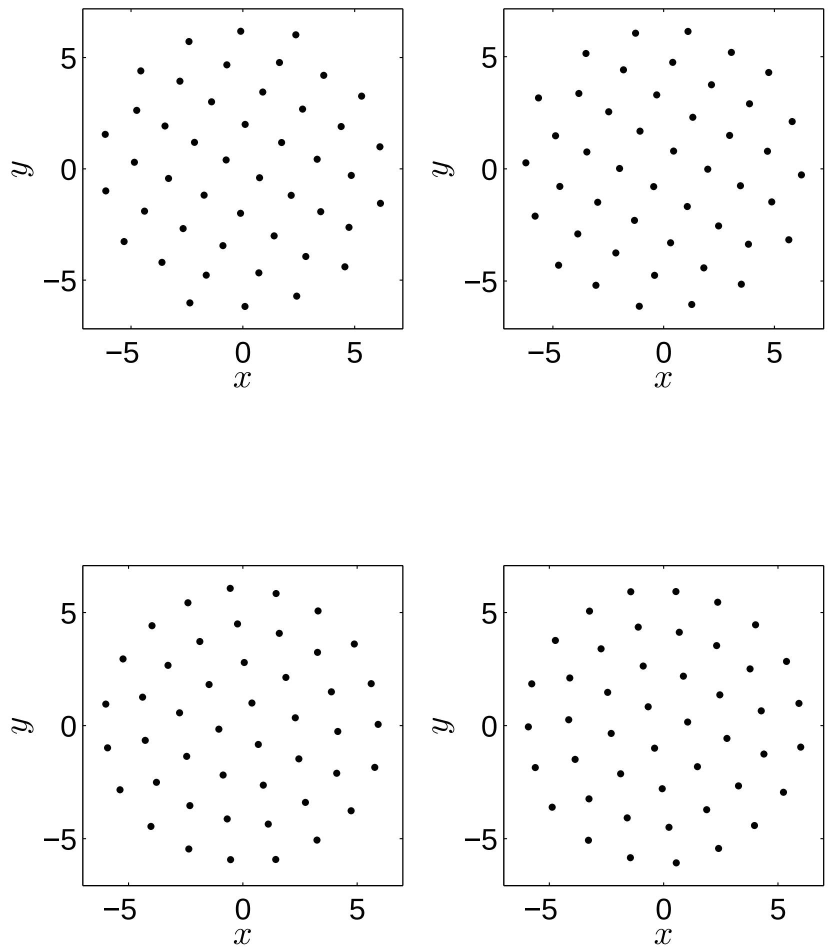
Related results by Eto, Kasamatsu, Nitta, Takeuchi, Tsubota, in the case of a homogeneous condensate.

Existence of a non degenerate solution, upper bound for the full problem (Aftalion-Wei). Related results: Alama-Bronsard-Mironescu.

$$-\sum_{i,j}(\log|p_i - p_j| + \log|q_i - q_j|) + \sum_i (|p_i|^2 + |q_i|^2) + \sum_{i,j} \frac{c_\Omega}{|p_i - q_j|^2}$$

where p_i are the vortices for component 1, q_j are the vortices for component

2 and $c_\Omega = \frac{\pi(1-\Gamma_{12})|\log g_1|^2}{8\Gamma_{12}^2 N_1 g_1}(2\frac{\Omega}{\Omega_c} - 1)$. At some critical value of c_Ω, the lattice goes from triangular to square: relation between Γ_{12} and Ω.



y
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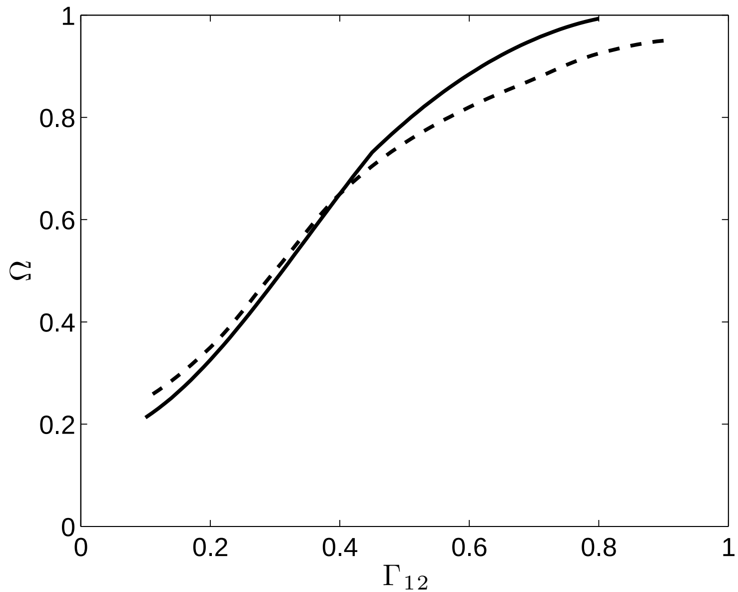
−5


1
0.8
0.6
0.4
0.2
0
Ω
0
0.2
0.4
0.6
0.8
1
Γ_{12}

Formal Abrikosov computation by Kasamatsu, Tsubota, Ueda (Int. J. Mod. Phys. B, 2005)

Using the reciprocical lattice, they compute the lattice displacement and how, as Γ_{12} varies, the lattice goes from triangular to rectangular.

If $\Gamma_{12} = 1 - \frac{g_{12}^2}{g_1 g_2} < 0$, phase separation is expected: asymptotic limit $\Gamma_{12} \to -\infty$, or $g_{12} \to \infty$. The coexistence region gets asymptotically small. Two droplets are expected.

We define $\rho_T = |\psi_1|^2 + |\psi_2|^2$, $\psi_k = \sqrt{\rho_T}\chi_k$, $\chi_k = |\chi_k| e^{i\theta_k}$ so that $|\chi_1|^2 + |\chi_2|^2 = 1$ and $S_z = |\chi_1|^2 - |\chi_2|^2$. We have $S_z = 1$ when only component 1 is present, $S_z = -1$, when only component 2 is present.

- $\Omega = 0$ and g_1, g_2 large, $\Gamma_{12} \to -\infty$: Thomas Fermi regime with inverted parabola profile for $\rho_T = |\psi_1|^2 + |\psi_2|^2$. Gamma convergence to a De Giorgi type problem (Aftalion, Royo-Letelier).

Write $S_z = \cos\phi$, then the energy becomes (for $g_1 = g_2$ and $\Omega = 0$)

$$\int |\nabla \sqrt{\rho}_T|^2 + \frac{\rho_T}{2}|\nabla\phi|^2 + \frac{1}{2}r^2\rho_T + g_{12}\frac{\rho_T^2}{4}(1-\cos^2\phi) + g_1\frac{\rho_T^2}{4}(1+\cos^2\phi)$$

If g_{12} is large, then $\cos^2\phi \sim 1$ almost everywhere, except on a boundary layer.
ρ_T is almost TF, and vanishes at interface.

We go back to the GP energy for a single condensate with $1/\varepsilon^2 = g_1 = g_2$:

$$E_\varepsilon(\eta) = \int \frac{1}{2}|\nabla\eta|^2 + \frac{1}{2}r^2|\eta|^2 + \frac{1}{2\varepsilon^2}|\eta|^4.$$

under $\int \eta^2 = N_1 + N_2$. We call η the ground state. Let $\rho_T = \eta v$. Then the energy splits into

$$E_\varepsilon(\eta) + F_\varepsilon(v) + G_\varepsilon(\phi)$$

with

$$F_\varepsilon(v) = \int \frac{1}{2}\eta^2|\nabla v|^2 + \frac{1}{2\varepsilon^2}\eta^4(1 - |v|^2)^2$$

$$G_\varepsilon(\phi) = \int \frac{1}{2}\eta^2 v^2|\nabla\phi|^2 + \frac{g}{2}(1 - \frac{1}{g\varepsilon^2})\eta^4 v^4(1 - \cos^2\phi)$$

F_ε is a Modica Mortola type energy with weight.

$|v|$ is 1 almost everywhere, but goes to zero on the interface region between the two components.

We prove that G_ε converges to 0 and F_ε converges to $c_* \int_{interface} \eta^3$.

Limiting problem

defined by the inverted parabola $\eta^2 = (\lambda - \frac{1}{2}r^2)_+$, where D is the disk of radius $\sqrt{\lambda}/2$ and $\int_D \eta^2 = N_1 + N_2$.

Find the optimal D_1 and D_2 such that

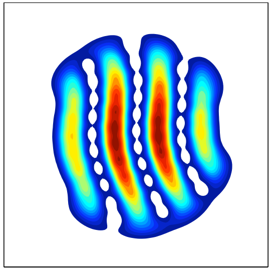
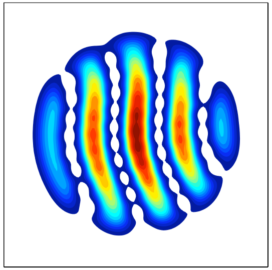
$D = D_1 \cup D_2$, $\int_{D_1} \eta^2 = N_1$, $\int_{D_2} \eta^2 = N_2$ and they minimize

$\int_{\partial D_1 \cap \partial D_2} \eta^3$.

Better to have half spaces than disk+annulus to minimize this interface integral.

Related results of Berestycki-Lin-Wei (no trapping potential)

Vortex sheets

Add rotation. This requires to understand the equation for S_z (or ϕ) at leading order.

IV. Spin orbit coupling

Spin orbit coupled condensates

$$\int \sum_{k=1,2} \left(\frac{1}{2}|\nabla \psi_k|^2 + \frac{1}{2} r^2 |\psi_k|^2 - \Omega \psi_k^* L_z \Psi_k + \frac{g_k}{2} |\psi_k|^4 \right) + g_{12}|\psi_1|^2|\psi_2|^2$$

$$-\kappa \psi_1^* \left(i \frac{\partial \psi_2}{\partial x} + \frac{\partial \psi_2}{\partial y} \right) - \kappa \psi_2^* \left(i \frac{\partial \psi_1}{\partial x} - \frac{\partial \psi_1}{\partial y} \right)$$

under the constraint $\int |\psi_1|^2 + |\psi_2|^2 = 1$.

We assume $g_1 = g_2 = g$ and define $\delta = g_{12}/g$.

Aftalion-Mason, PRA 2013

We define $\rho_T = |\psi_1|^2 + |\psi_2|^2$, $\psi_k = \sqrt{\rho_T}\chi_k$, $\chi_k = |\chi_k| e^{i\theta_k}$ so that $|\chi_1|^2 + |\chi_2|^2 = 1$ and $S_z = |\chi_1|^2 - |\chi_2|^2$, $S_x = \chi_1^*\chi_2 + \chi_2^*\chi_1$, $S_y = -i(\chi_1^*\chi_2 - \chi_2^*\chi_1)$.

$\delta > 1$: segregation: at $\kappa = 0$, one component is empty. As κ increases, to a giant skyrmion (disk+ think annulus circulation 1), to multiple annuli and eventually stripes.

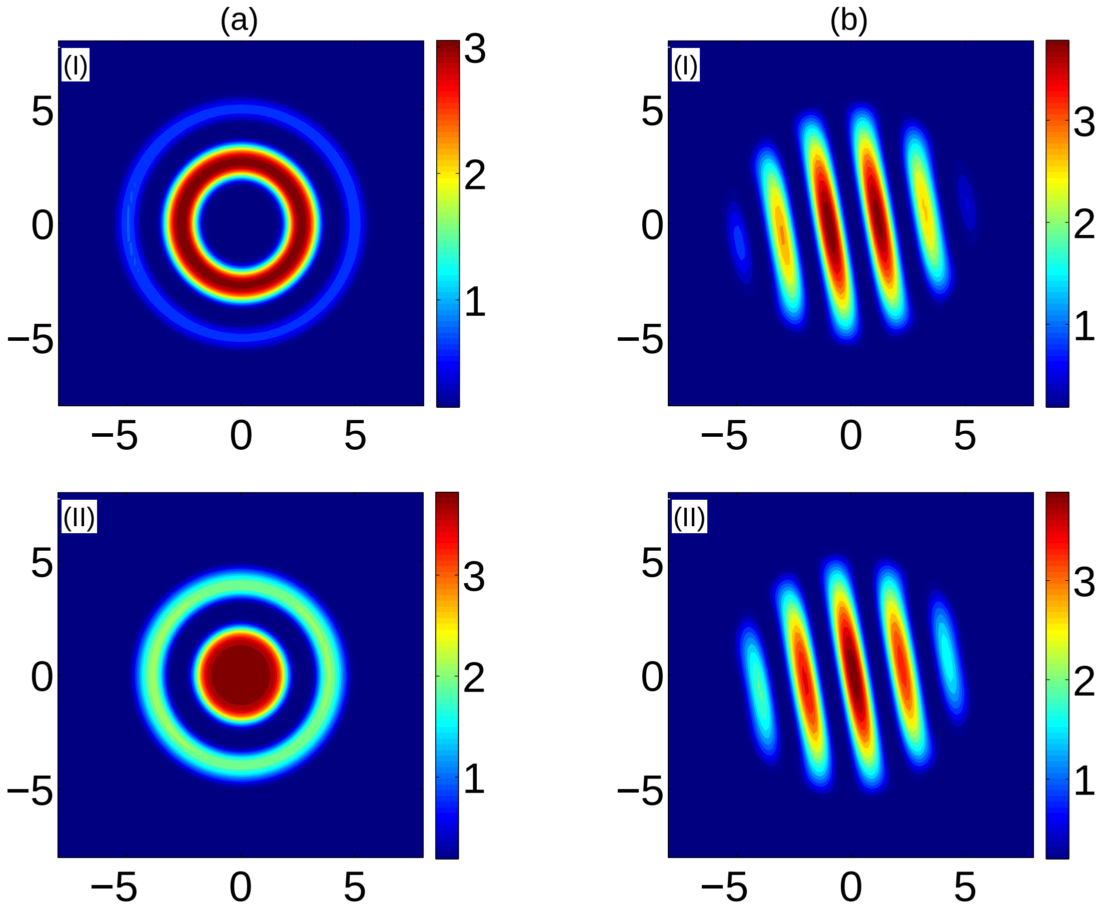


Figure 2: Left column (a): $(\delta, \kappa) = (1.5, 1.25)$ and right column (b): $(\delta, \kappa) = (1.5, 1.5)$. Density plots (frame (I), component-1, and (II), component-2).

Question: understand the Gamma limit of the spin orbit term in the segregation case?

$$-\kappa\psi_2^* \left(i\frac{\partial\psi_1}{\partial x} - \frac{\partial\psi_1}{\partial y} \right)$$

Formally in the case disk+annulus, we find that the circulation in each annulus is 1.

$\Omega = 0$, $\delta < 1$: coexistence of the components, the global phase $\theta = \theta_1 + \theta_2$ is such that $\nabla\theta = -2\kappa S_\perp$: relation with a ferromagnetic problem.

MORE IN THE TALK OF PETER MASON....

Conclusion

We have seen mathematical techniques to deal with two component condensates in the case of

• coexistence: TF approximation, core of vortex - peak, vortex energy, LLL open mathematically

• segregation: Γ convergence in the case of no rotation. Open for vortex sheets or spin orbit coupling