Vortices and Spontaneous Symmetry Breaking in Rotating Bose Gases

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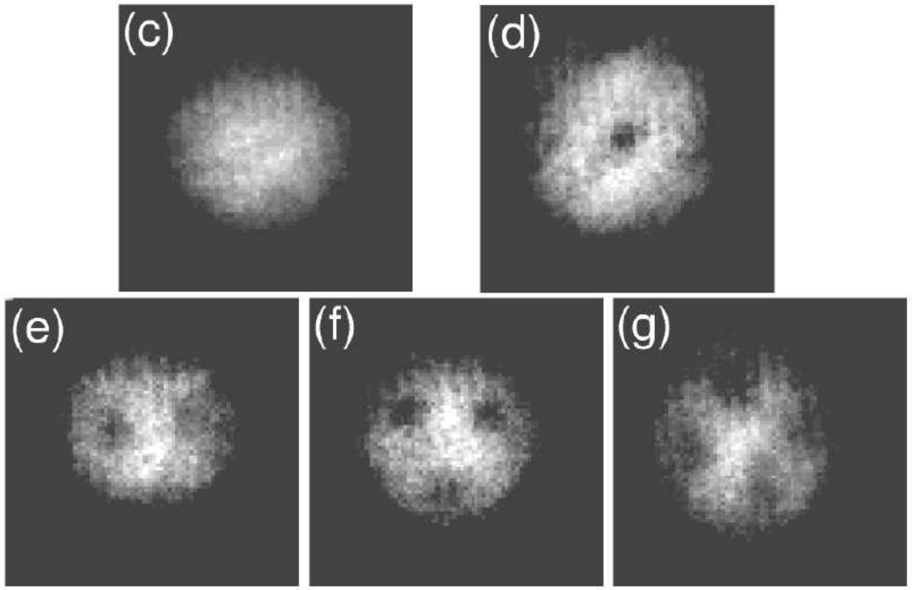
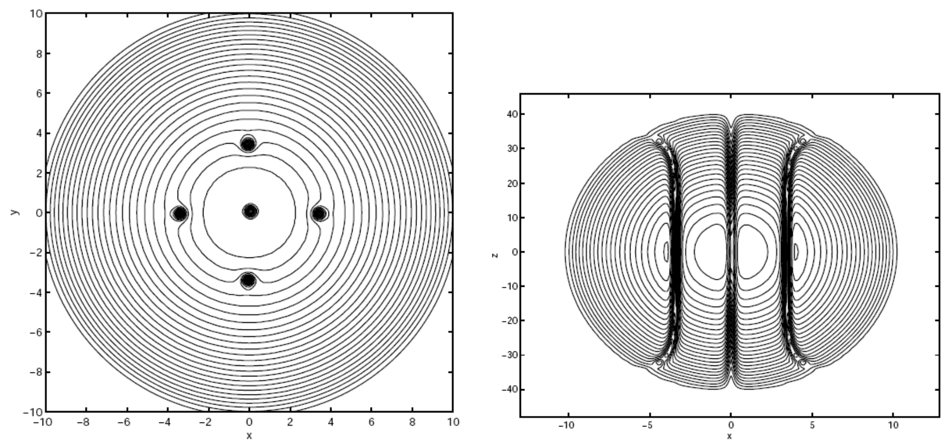
Rotating Bose Gases

Ultra-cold dilute Bose gases in rotating traps show appearance of **quantized vortices**. These are well described by the Gross-Pitaevskii (GP) equation:

Experiments: [Madison *et at.*, Phys. Rev. Lett. **84**, 806 (2000)]

Prediction of **GP equation**: [Castin, Dum, Eur. Phys. J. D **7**, 399 (1999)]





The Gross-Pitaevskii Equation

The GP equation originates from the **GP energy functional**

$$\mathcal{E}^{\mathrm{GP}}[\phi] = \langle \phi | H_0 | \phi \rangle + 4\pi g \int_{\mathbb{R}^3} |\phi(x)|^4 d^3x \ .$$

With Ω the **angular velocity** vector and $V(x)$ the trap potential,

$$H_0 = -\Delta + V(x) - \Omega \cdot L$$

The GP energy is

$$E^{\mathrm{GP}}(g, \Omega) = \inf_{\|\phi\|_2 = 1} \mathcal{E}^{\mathrm{GP}}[\phi] \, ,$$

and any minimizer satisfies the **GP equation**

$$\boxed{- \Delta\phi(x) + V(x)\phi(x) - \Omega \cdot L \, \phi(x) + 8\pi g |\phi(x)|^2 \phi(x) = \mu\phi(x)}$$

For axially symmetric $V(x)$ and $\Omega \neq 0$, **symmetry is broken** $\Rightarrow$ many GP minimizers!

The Many-Body Problem

Hamiltonian for N bosons with repulsive pair interaction $v_a(x)$:

$$H_N = \sum_{i=1}^{N} H_0^{(i)} + \sum_{1\leq i<j\leq N} v_a(x_i - x_j)\,.$$

Acts on $\mathcal{H}_N$, the **symmetric** functions in $\bigotimes^N L^2(\mathbb{R}^3)$.

As before, $H_0 = -\Delta + V(x) - \Omega\cdot L$, with $\lim_{|x|\to\infty}\left(V(x) - \frac{1}{4}|\Omega\wedge x|^2\right) = \infty$.

$v_a(x) \geq 0$, short range, with finite **scattering length** a. (Example: hard spheres of diameter a.) We write

$$v_a(x) = a^{-2} w(x/a)\,,$$

with $w(x) \geq 0$ having scattering length 1. We can then vary a (equivalent to scaling the trap potential!). In particular,

$$E_0 = \inf\operatorname{spec} H_N = E_0(N,a,\Omega)\,.$$

Main Theorem 1

Expect

$$E_0(N, a, \Omega) \approx N E^{\mathrm{GP}}(Na, \Omega)$$

for **dilute** gases, i.e, when $a^3\bar{\rho} \ll 1$. In particular satisfied if $N \gg 1$, $Na = O(1)$.

Theorem 1. *For any* $g \geq 0$,

$$\boxed{\lim_{N\to\infty} \frac{E_0(N, g/N, \Omega)}{N} = E^{\mathrm{GP}}(g, \Omega)}$$

Theorem 1 holds for all angular velocities Ω. It extends previous results on the case $\Omega = 0$ [Lieb, Seiringer, Yngvason, PRA **61**, 043602 (2000)].

It is essential to restrict to symmetric wave functions (bosons) in Theorem 1!

Note the independence of $w(x)$. In dilute limit only scattering length matters. Note also that the result **cannot** be obtained by simple perturbation theory; in particular, the $\int |\phi|^4$ term in the GP functional is partly **kinetic** energy!

Bose-Einstein Condensation

The GP minimizers also tell us something about the one-particle density matrix

$$\gamma_N^{(1)}(x,x') = N \int_{\mathbb{R}^{3(N-1)}} \Psi_0(x,x_2,\ldots,x_N)\Psi_0^*(x',x_2,\ldots,x_N) d^3x_2 \cdots d^3x_N$$

and about **Bose-Einstein condensation** (BEC) in the ground state of H_N.

BEC means that $\gamma_N^{(1)}$ has an eigenvalue of order N. The corresponding eigenfunction is the **condensate wave function**. For dilute systems, one expects **complete** BEC, and $\gamma_N^{(1)}(x,x') \approx N\phi^{\mathrm{GP}}(x)\phi^{\mathrm{GP}}(x')$.

For $\Omega = 0$ it was shown [Lieb, Seiringer, PRL **88**, 170409 (2002)] that

$$\boxed{\lim_{N\to\infty} \frac{1}{N}\gamma_N^{(1)}(x,x') = \phi_g^{\mathrm{GP}}(x)\phi_g^{\mathrm{GP}}(x')}$$

in the GP limit $N \to \infty$, $Na \to g$. Here, ϕ_g^{GP} is the GP minimizer for coupling constant $g \geq 0$, which is **unique** for $\Omega = 0$.

BEC in Rotating Case

For $\Omega \neq 0$, the result is more complicated because of non-uniqueness of ϕ^{GP}.

Look at set of all **approximate ground states**: A sequence of bosonic N-particle density matrices γ_N with $\operatorname{Tr} H_N \gamma_N \approx N E^{\mathrm{GP}}$.

One can then expect that the reduced one-particle density matrix $\gamma_N^{(1)}$ of any such approximate ground state is a convex combination

$$\gamma_N^{(1)}(x, x') \approx \sum_i \lambda_i \phi_i^{\mathrm{GP}}(x) \phi_i^{\mathrm{GP}}(x')^*$$

where ϕ_i^{GP} is a GP minimizer, and $\sum_i \lambda_i = N$.

The mathematical precise formulation is complicated by the fact that the set of GP minimizers is, in general, not countable.

Main Theorem 2

Let Γ be the set of all limit points of 1pdm of approximate ground states:

$$\Gamma = \left\{ \gamma \,:\, \exists \text{ sequence } \gamma_N, \lim_{N\to\infty,\, Na\to g} \frac{1}{N} \mathrm{Tr}\, H_N \gamma_N = E^{\mathrm{GP}}(g,\Omega), \ \lim_{N\to\infty} \frac{1}{N} \gamma_N^{(1)} = \gamma \right\}.$$

Compactness implies that $\mathrm{Tr}\,\gamma = 1$ for all $\gamma \in \Gamma$.

Theorem 2. *(i) Γ is a compact and convex subset of the set of all trace class operators.*

(ii) Let $\Gamma_{\mathrm{ext}} \subset \Gamma$ denote the set of **extreme points** *in Γ. We have $\Gamma_{\mathrm{ext}} = \{|\phi\rangle\langle\phi| : \mathcal{E}^{\mathrm{GP}}[\phi] = E^{\mathrm{GP}}(g,\Omega)\}$.*

(iii) For each $\gamma \in \Gamma$, there is a positive (regular Borel) measure $d\mu_\gamma$, supported in Γ_{ext}, with $\int_{\Gamma_{\mathrm{ext}}} d\mu_\gamma(\phi) = 1$, such that (in weak sense)

$$\boxed{\gamma = \int_{\Gamma_{\mathrm{ext}}} d\mu_\gamma(\phi)\, |\phi\rangle\langle\phi|}$$

Remarks

- As typical for **superfluids**, angular momentum is acquired by the system in terms of **quantized vortices**. These can be seen by solving the GP equation.
- Theorem 2 shows the occurrence of **spontaneous symmetry breaking**. Axial symmetry of the trap $V(x) \Rightarrow$ non-uniqueness of GP minimizer for g large enough [Seiringer, CMP **229**, 491 (2002)]. Uniqueness can be restored by perturbing H_0 to break the symmetry and favor one of the minimizers. This then leads to **complete BEC**.
- As in the case of the energy discussed above, the situation is very different for the **absolute ground state**. The set Γ consists of only one element in this case (namely the minimizer of the density matrix functional discussed below, which is unique for any value of Ω and g). In particular, there is no spontaneous symmetry breaking in the absolute ground state.

The Absolute Ground State

The **absolute** ground state can be described by a GP **density matrix** functional

$$\mathcal{E}^{\mathrm{DM}}[\gamma] = \mathrm{Tr}\left[(-\Delta - \Omega \cdot L + V)\,\gamma\right] + 4\pi g \int \rho_\gamma(x)^2 d^3x.$$

This functional always has a **unique** minimizer γ^{DM} (under the normalization condition $\mathrm{Tr}\,\gamma = 1$)! Denote the corresponding energy by $E^{\mathrm{DM}}(g,\Omega) = \mathcal{E}^{\mathrm{DM}}[\gamma^{\mathrm{DM}}]$, and the absolute ground state energy of H_N by $E_{\mathrm{abs}}(N,a,\Omega)$.

Theorem 3. *For any fixed $g \geq 0$ and Ω,*

$$\boxed{\lim_{N\to\infty} \frac{E_{\mathrm{abs}}(N, g/N, \Omega)}{N} = E^{\mathrm{DM}}(g,\Omega) \qquad \text{and} \qquad \lim_{N\to\infty} \frac{1}{N}\gamma^{(1)}_{\mathrm{abs}} = \gamma^{\mathrm{DM}}}$$

Note that $\mathcal{E}^{\mathrm{GP}}$ is the **restriction** of $\mathcal{E}^{\mathrm{DM}}$ to rank one projections. In the case of symmetry breaking (i.e., for g large enough), $\mathrm{rank}\,\gamma^{\mathrm{DM}} \geq 2$, and hence $E^{\mathrm{DM}} < E^{\mathrm{GP}}$. The absolute and bosonic ground state differ significantly!

Ideas in the Proof of Theorem 1

On **bosonic Fock space** $\mathcal{F} = \bigoplus_N \mathcal{H}_N$, the Hamiltonian can be written in terms of $a_j^\dagger$ and a_j, the creation and annihilation operators of φ_j:

$$H = \sum_{j \geq 1} e_j a_j^\dagger a_j + \tfrac{1}{2} \sum_{ijkl} a_i^\dagger a_j^\dagger a_k a_l W_{ijkl} \,, \tag{1}$$

where $H_0 = \sum_j e_j |\varphi_j\rangle\langle\varphi_j|$ and $W_{ijkl} = \langle \varphi_i \otimes \varphi_j | v_a | \varphi_k \otimes \varphi_l \rangle$.

Two **main steps**:

1. Eq. (1) not necessarily well defined (e.g. $W_{ijkl} \equiv \infty$ for hard-core interaction). Show that, for a lower bound, one can replace v_a by a "soft" and smooth potential $U(x)$ (with the same scattering length), at the expense of the high-momentum part of the kinetic energy.
2. Show that one can replace the operators $a_j^\dagger$ and a_j by complex numbers $z_j \Longrightarrow$ GP functional $\mathcal{E}^{\mathrm{GP}}[\phi_{\mathbf{z}}]$ with $\phi_{\mathbf{z}}(x) = \sum_j z_j \varphi_j(x)$.

Step 1: Generalized Dyson Lemma

Separate high momentum from **low** momentum. High momentum for scattering of two particles, low momentum for H_0-part in GP functional.

Lemma 1. *Let v have scattering length a and range R_0. Let θ_R be the characteristic function of $\{|x| < R\}$. Let $0 \leq \chi(p) \leq 1$, such that $h(x) \equiv \widehat{1 - \chi}(x)$ is bounded and integrable,*

$$f_R(x) = \sup_{|y| \leq R} |h(x-y) - h(x)|, \quad \textit{and} \quad w_R(x) = \frac{2}{\pi^2} f_R(x) \int_{\mathbb{R}^3} f_R(y) d^3y.$$

Then for any $\varepsilon > 0$ and any positive radial function $U_R(x)$ supported in $R_0 \leq |x| \leq R$ with $\int U_R = 4\pi$ we have the operator inequality

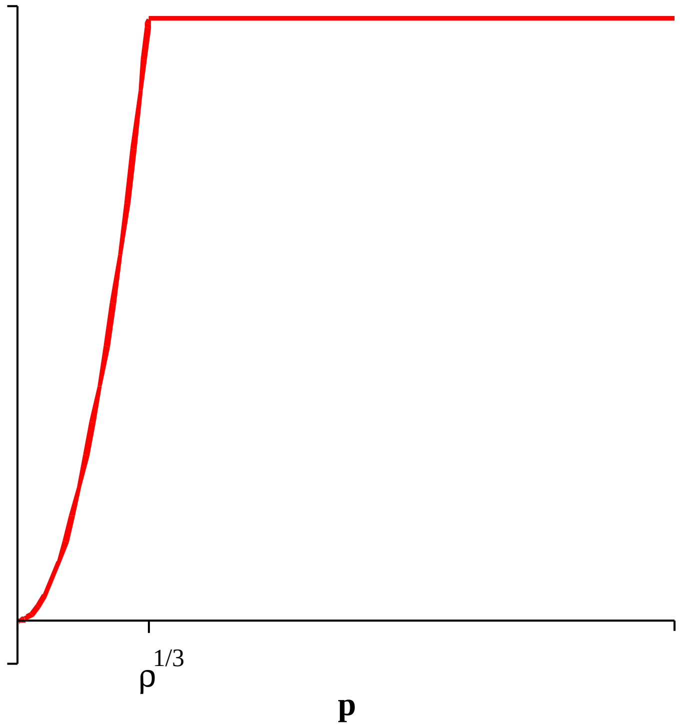
$$-\nabla \chi(p) \theta_R(x) \chi(p) \nabla + \tfrac{1}{2} v(x) \geq (1 - \varepsilon) a U_R(x) - \frac{a}{\varepsilon} w_R(x).$$

The parameter R is chosen such that $a \ll R \ll N^{-1/3}$.

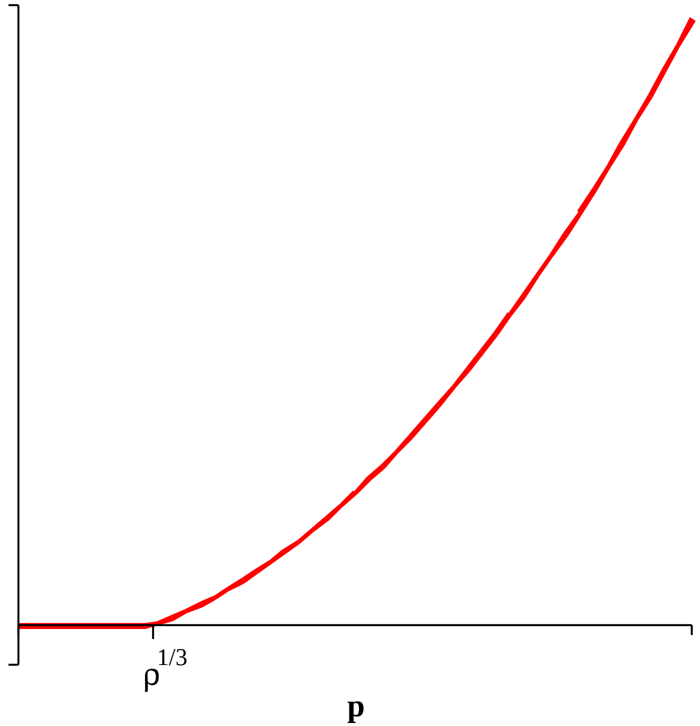
Proof: [Lieb, Seiringer, Solovej, PRA **71**, 053605 (2005)]

The Kinetic Energy Separation

$p^2(1-\chi(p)^2)$
Low momentum regime



$p^2\chi(p)^2$
High momentum regime



Step 2: Coherent States

$\mathcal{F} = \bigotimes_j \mathcal{F}_j$, with $\mathcal{F}_j$ spanned by $(a_j^\dagger)^n|0\rangle$. Coherent state $|z_j\rangle = \exp[-|z_j|^2/2 + z_j a_j^\dagger]\,|0\rangle$ for $z_j \in \mathbb{C}$. **Completeness** property $\int dz|z\rangle\langle z| = \mathbb{I}$.

Upper symbols: $a_j = \int dz_j\, z_j|z_j\rangle\langle z_j|$, but $a_j^\dagger a_j = \int dz_j\,(|z_j|^2 - 1)|z_j\rangle\langle z_j|$. The (-1) is unwanted! Hence we introduce coherent states only for modes $j \leq J$ for some $J \gg 1$.

I.e., $\mathcal{F} = \mathcal{F}_< \otimes \mathcal{F}_>$. For $\mathbf{z} = (z_1, \ldots, z_J) \in \mathbb{C}^J$ and $\Pi(\mathbf{z}) = |z_1 \otimes \cdots \otimes z_J\rangle\langle z_1 \otimes \cdots \otimes z_J|$, we can then write

$$H = \int d\mathbf{z}\,\Pi(\mathbf{z}) \otimes U(\mathbf{z})\,,$$

where, for fixed $\mathbf{z}$, $U(\mathbf{z})$ is an operator on $\mathcal{F}_>$. Hence $\inf\operatorname{spec} H \geq \inf_{\mathbf{z}} \inf\operatorname{spec} U(\mathbf{z})$.

One then shows that $U(\mathbf{z}) \approx \mathcal{E}^{\mathrm{GP}}[\phi_{\mathbf{z}}] - \text{controllable terms}$. These terms are **operators** on $\mathcal{F}_>$ which describe the interaction between particles in modes $j \leq J$ and $j > J$.

Ideas in the Proof of Theorem 2

Griffiths' argument together with first order perturbation theory yields:
For any $\gamma \in \Gamma$, and any bounded hermitian operator S,

$$\mathrm{Tr}\, S\gamma \geq \min_{\phi=\phi^{\mathrm{GP}}} \langle \phi | S | \phi \rangle \,. \tag{2}$$

It is not too difficult to show that $|\phi^{\mathrm{GP}}\rangle\langle\phi^{\mathrm{GP}}| \in \Gamma$. Now use **convexity theory**.

An **exposed point** of a convex set $\mathcal{C}$ is an extreme point p with the additional property that there is a tangent plane to $\mathcal{C}$ containing p but containing no other point of $\mathcal{C}$.
Hence, for $\widetilde{\gamma} \in \Gamma$ an exposed point, there exists an S such that

$$\mathrm{Tr}\, S\widetilde{\gamma} \leq \mathrm{Tr}\, S\gamma \quad \text{for all } \gamma \in \Gamma \,. \tag{3}$$

with equality **if and only if** $\gamma = \widetilde{\gamma}$. Hence, with ϕ^{GP} minimizing the right side of (2) for this S, and $\gamma = |\phi^{\mathrm{GP}}\rangle\langle\phi^{\mathrm{GP}}| \Rightarrow \widetilde{\gamma} = |\phi^{\mathrm{GP}}\rangle\langle\phi^{\mathrm{GP}}|$, i.e., all exposed points are of this form!!

Extension to **all** extreme points: **Straszewicz's Theorem**: the exposed points are a dense subset of the extreme points (at least in finite dimensions).

Conclusions

- **Rigorous justification** of Gross-Pitaevskii approximation for sufficiently dilute rotating Bose gases. For large N and both Na and Ω of order 1, the ground state of the Bose gas is well approximated by the solution to the GP equation. This is true both for the energy and the reduced density matrices.

- In particular, appearance of **quantized vortices** and **spontaneous symmetry breaking** for either g or Ω large enough.

- GP equation in **2D** can be derived by scaling $V(x)$:

$$V(x) = r^{-2}V^{\perp}(x^{\perp}/r) + \ell^{-2}V^{\|}(z/\ell) \quad , \quad x = (x^{\perp}, z)$$

  with $a \ll \ell \ll r$. Effective 2D parameter g depends non-trivially on the particular scaling limit. [J. Yin, 2007]

- **For the future:** Study the case of very **rapid rotation**, i.e., $\Omega \gg 1$ for super-harmonic traps, or $\Omega \to \Omega_c$ for harmonic traps. The GP description is expected to break down once the number of vortices is comparable to the number of particles.