Bose-Einstein condensate of bosonic atoms: Gross-Pitaevskii equation and hydrodynamic expansion

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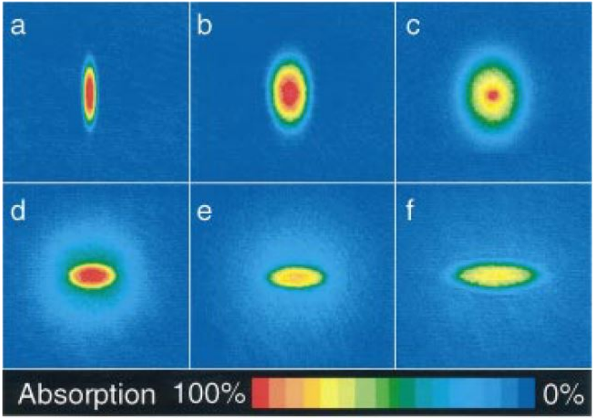
What is going on here?

Bose-Einstein condensate of sodium atoms in a confining, axially symmetric harmonic potential is released
(Experimentally realized by the Ketterle Group at MIT 1996 [1])



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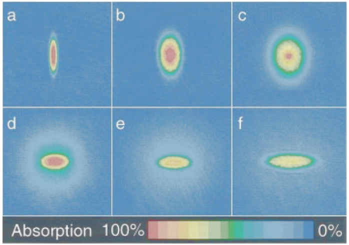

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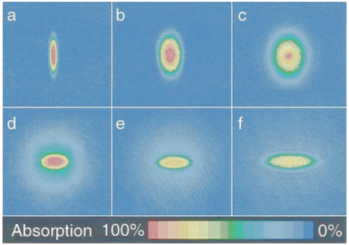
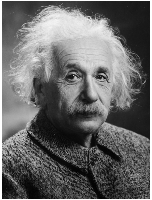


Theoretical Prediction

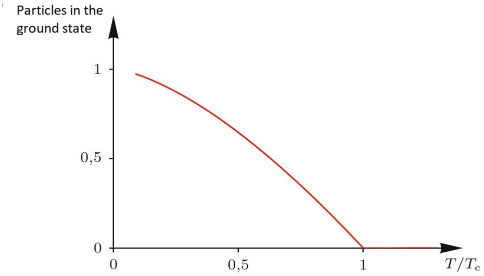
- First theoretical prediction by Bose [2] and Einstein [3] in 1924
- Bose first proposed a derivation of the radiation law of photons without the use of classical physics leading to Bose statistics
- Einstein then recognized that at low temperatures the ground state will be macroscopically occupied by bosons, hence the name **Bose-Einstein condensate**
- Modern description uses quantum statistics for derivation

Satyendranath Bose



Albert Einstein

Theoretical properties of an ideal Bose-Einstein condensate



- Bose and Einstein description assumed an **ideal Bose gas**, i.e. non-interacting bosonic particles
- A critical temperature can be computed below which the ground state begins to be more and more occupied

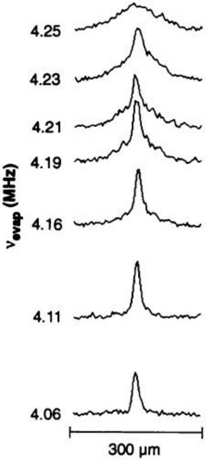
$$T_c = \frac{2\pi\hbar^2}{k_B m}\left(\frac{\rho}{2.612}\right)^{2/3}$$

- Experimentally a lower critical temperature is measured, which is a first hint that interaction must be considered

Experimental realization of a Bose-Einstein condensate

- Only after more than 70 years a condensate was produced by Wieman and Cornell with rubidium atoms [4] and by Ketterle with sodium atoms [5] in 1995
- In 2001 they won the Nobel prize "for the achievement of Bose-Einstein condensation in dilute gases of alkali atoms, and for early fundamental studies of the properties of the condensates"

E.A. Cornell, C.E. Wieman and W. Ketterle

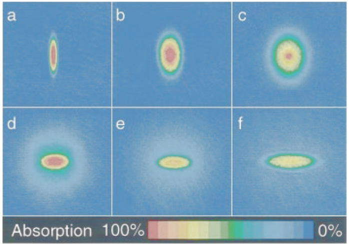


Velocity distribution of Rb^{87} at JILA [4]

A new field in physics

- With the experimental realization of BECs a new field in physics was established: **Ultracold quantum gases**
- New phenomena were measured such as quantum vortices in condensates, different oscillation modes and (most importantly in this presentation) **hydrodynamic expansion of Bose-Einstein condensates**
- Consideration of an ideal Bose gas is not sufficient! New techniques to describe interacting Bose gases had to be found
- This lead to the rediscovery of the already formulated **Gross-Pitaevskii equation**

Outline

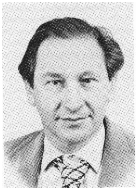


Historic introduction

- First developed independently by L. P. Pitaevskii [6] and E. P. Gross [7]
- Historic motivation was the description of quantum vortices in condensates, but there are far more applications
- In general, the Gross-Pitaevskii equation describes **nonuniform**, **interacting** bosons at **very low (zero) temperatures**

$$i\hbar\frac{\partial}{\partial t}\Phi(\mathbf{r},t) = \left(-\frac{\hbar^2}{2m}\nabla^2 + V_{\text{ext}}(\mathbf{r},t) + g|\Phi(\mathbf{r},t)|^2\right)\Phi(\mathbf{r},t)$$

Lev P. Pitaevskii (1933-)



Eugene P. Gross (1926-1991)

Short reminder: Second quantization

- Mostly developed by Dirac in 1927 [8] to describe **quantum many-body systems**
- Classical fields are replaced by field operators:
  Most importantly, the **quantum field operators** $\hat{\Psi}(\mathbf{r}, t)$ and $\hat{\Psi}^\dagger(\mathbf{r}, t)$
- The Hamiltonian of a many-body system with a two-particle interaction $U(\mathbf{r} - \mathbf{r}')$ and an external potential $V_{\text{ext}}(\mathbf{r}, t)$ is given by

$$\hat{H} = \int \mathrm{d}\mathbf{r}\, \hat{\Psi}^\dagger(\mathbf{r}, t)\left(-\frac{\hbar^2}{2m}\nabla^2 + V_{\text{ext}}(\mathbf{r}, t)\right)\hat{\Psi}(\mathbf{r}, t) + \frac{1}{2}\int \mathrm{d}\mathbf{r}\,\mathrm{d}\mathbf{r}'\, \hat{\Psi}^\dagger(\mathbf{r}, t)\hat{\Psi}^\dagger(\mathbf{r}', t)U(\mathbf{r} - \mathbf{r}')\hat{\Psi}(\mathbf{r}', t)\hat{\Psi}(\mathbf{r}, t)$$

Short reminder: Second quantization

- The field operators describe the creation/annihilation of a particle in position space
- In the case of **bosons** they obey the following commutation relation

$$\left[\hat{\Psi}(\mathbf{r},t),\hat{\Psi}^{\dagger}(\mathbf{r}',t)\right]=\delta(\mathbf{r}-\mathbf{r}')$$

- Then, together with the Heisenberg equation $i\hbar\,\partial_t\Psi=[\Psi,H]$ an equation of motion for the field operator can be derived

$$i\hbar\frac{\partial}{\partial t}\hat{\Psi}(\mathbf{r},t)=$$
$$\left(-\frac{\hbar^2}{2m}\nabla^2+V_{\mathrm{ext}}(\mathbf{r},t)+\int \mathrm{d}\mathbf{r}'\,\hat{\Psi}^{\dagger}(\mathbf{r}',t)U(\mathbf{r}-\mathbf{r}')\hat{\Psi}(\mathbf{r}',t)\right)\hat{\Psi}(\mathbf{r},t)$$

First assumption: Mean field or zero temperature

- Firstly, expand the field operator in the following way

$$\hat{\Psi}(\mathbf{r},t) = \Phi(\mathbf{r},t) + \hat{\psi}(\mathbf{r},t) \quad \text{with} \quad \left\langle \hat{\Psi}(\mathbf{r},t) \right\rangle = \Phi(\mathbf{r},t)$$

  This was initially done by Bogoliubov 1947 [9] but with a constant exp. value
- At low temperatures, the expectation value can be related with the particle number density of the condensate

$$|\Phi(\mathbf{r},t)|^2 = n(\mathbf{r},t) \quad \text{with} \quad \int \mathrm{d}\mathbf{r}\, n(\mathbf{r},t) = N$$

- At zero temperature, all **depletion** from the condensate can be neglected, so that the field operator is totally replaced by the complex exp. value:

  $\Phi(\mathbf{r},t)$ is called **order parameter/wave function of the condensate**

Second assumption: Dilution or pseudo-potential

- Scattering of a particle in quantum mechanics can be described by a scattering amplitude. At low energies it can be replaced by a simple number, the **(s-wave) scattering length a**

$$\psi(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} + f(\mathbf{k}, \mathbf{r}/r)\,\frac{e^{ikr}}{r} \longrightarrow 1 - \frac{a}{r}$$

- If the scattering length is much larger than the mean distance between particles, i.e. the condensate is **dilute** $\overline{n}\,|a|^3 \ll 1$, a pseudo-potential can be introduced

$$U(\mathbf{r}-\mathbf{r}') = g\,\delta(\mathbf{r}-\mathbf{r}') \quad \text{with} \quad g = \frac{4\pi a\hbar^2}{m}$$

- The scattering length a is positive for a **repulsive** interaction and negative for an **attractive** one

Set-up of the Gross-Pitaevskii equation

Starting from the equation of motion of an arbitrary field operator...

$$i\hbar\frac{\partial}{\partial t}\hat{\Psi}(\mathbf{r},t) = \left(-\frac{\hbar^2}{2m}\nabla^2 + V_{\text{ext}}(\mathbf{r},t) + \int \mathrm{d}\mathbf{r}'\; \hat{\Psi}^\dagger(\mathbf{r}',t)U(\mathbf{r}-\mathbf{r}')\hat{\Psi}(\mathbf{r}',t)\right)\hat{\Psi}(\mathbf{r},t)$$

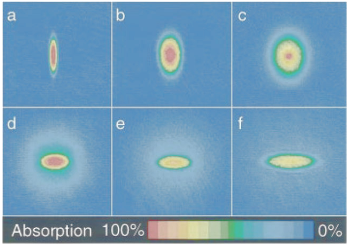
...using the following assumptions...

- Neglecting all depletion (zero temperature): $\hat{\Psi}(\mathbf{r},t) = \Phi(\mathbf{r},t)$
- Assuming a dilute condensate ($\overline{n}\,|a|^3 \ll 1$): $U(\mathbf{r}-\mathbf{r}') = g\,\delta(\mathbf{r}-\mathbf{r}')$

... we end up at the **Gross-Pitaevskii equation**:

$$\boxed{i\hbar\frac{\partial}{\partial t}\Phi(\mathbf{r},t) = \left(-\frac{\hbar^2}{2m}\nabla^2 + V_{\text{ext}}(\mathbf{r},t) + g|\Phi(\mathbf{r},t)|^2\right)\Phi(\mathbf{r},t)}$$

Outline



Scales of the Gross-Pitaevskii equation

- The scattering length for sodium was measured to be $a = 2.75\,\mathrm{nm}$ (Tiesinga et al., 1996) [10]. With density values ranging from $10^{13}\,\mathrm{cm}^{-3}$ to $10^{15}\,\mathrm{cm}^{-3}$ the dilution parameter is of order:

$$\overline{n}\,|a|^3 < 10^{-3}$$

- The confining, harmonic trap introduces another length scale

$$V_{\mathrm{ext}}(\mathbf{r}) = \frac{m}{2}\sum \omega_i^2 r_i^2 \quad \text{namely} \quad a_{\mathrm{ho}}^2 = \frac{\hbar}{m\omega_{\mathrm{ho}}} \quad \text{with} \quad \omega_{\mathrm{ho}} = \sqrt[3]{\omega_1\omega_2\omega_3}$$

- Using these scales one can make the GPE dimensionless, e.g. $\mathbf{r}^2 \to a_{\mathrm{ho}}^2\tilde{\mathbf{r}}^2$, $t \to \omega_{\mathrm{ho}}^{-1}\,\tilde{t}$, $\Phi(\mathbf{r},t) \to a_{\mathrm{ho}}^{-3/2}\sqrt{N}\,\tilde{\Phi}(\tilde{\mathbf{r}},\tilde{t})$ (with $\tilde{\Phi}$ normalized to 1)

Scales of the Gross-Pitaevskii equation

- Plugging all these new quantities with tilde in the GPE yields

$$2i\frac{\partial}{\partial\tilde{t}}\tilde{\Phi} = \left(-\tilde{\nabla}^2 + \tilde{\mathbf{r}}^2 + 8\pi\frac{Na}{a_{\text{ho}}}\left|\tilde{\Phi}\right|^2\right)\tilde{\Phi}$$

- The ratio Na/a_{ho} plays an important role! It can be shown (with use of the virial theorem) [11]

$$\frac{E_{\text{int}}}{E_{\text{kin}}} \propto \frac{N|a|}{a_{\text{ho}}}$$

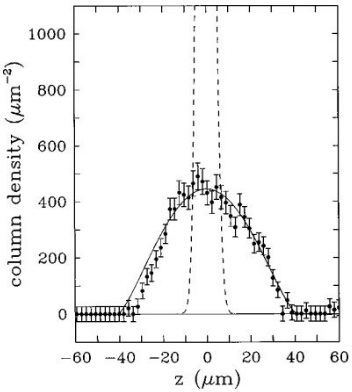
- The experiments with sodium yield a relative large number of atoms (10^6-10^7) [1, 5], so that $Na/a_{\text{ho}} \propto 10^3 - 10^4$

Repulsive interaction is much stronger than kinetic energy!

Thomas-Fermi approximation

- Repulsive interaction flattens the density distribution
- Variation of the density can be neglected, i.e. kinetic distribution in the GPE
- GPE takes the form (**Thomas-Fermi approximation**):

$$i\hbar\frac{\partial}{\partial t}\Phi(\mathbf{r},t) = \left(V_{\text{ext}}(\mathbf{r}) + g|\Phi(\mathbf{r},t)|^2\right)\Phi(\mathbf{r},t)$$



Density distribution of 80 000 sodium atoms in the trap of Hau et al. (1998) [12] as a function of the axial coordinate. Dashed line: Non-interacting bosons. (Figure from [11])

Static solution of the Gross-Pitaevskii equation

- Constructing a static solution by making the typical ansatz:

$$\Phi(\mathbf{r},t) = \Phi(\mathbf{r})\, e^{-i\frac{\mu}{\hbar}t}$$

- For the spatial part of the wave function this yields (enforcing the Thomas-Fermi approximation)

$$\mu\,\Phi(\mathbf{r}) = \left(V_{\text{ext}}(\mathbf{r}) + g|\Phi(\mathbf{r})|^2\right)\Phi(\mathbf{r}) \quad \rightarrow \quad \boxed{n(\mathbf{r}) = \frac{\mu - V_{\text{ext}}(\mathbf{r})}{g}}$$

  for $\mu > V_{\text{ext}}$ else $n = 0$. $n(\mathbf{r})$ is then called the **Thomas-Fermi density**
- The chemical potential can be determined by calculating the total number of particles

$$N = \int \mathrm{d}\mathbf{r}\, n(\mathbf{r}) \quad \rightarrow \quad \mu = \frac{\hbar\omega_{\text{ho}}}{2}\left(\frac{15Na}{a_{\text{ho}}}\right)^{2/5}$$

Collisionless hydrodynamics and superfluidity

- Looking at a system with many particles, the condensate can be described by hydrodynamics as a superfluid at zero temperature (Stringari, 1996 [13])
- To that end, the wave function can be parameterized as

$$\Phi(\mathbf{r}, t) = \sqrt{n(\mathbf{r}, t)}\, e^{i\theta(\mathbf{r}, t)}$$

- The different derivatives appearing in the GEP can be calculated to

$$\partial_t \Phi = \left(\frac{\partial_t n}{2n} + i \partial_t \theta \right) \Phi$$

$$\nabla^2 \Phi = \nabla \left[\left(\frac{\nabla n}{2n} + i \nabla \theta \right) \Phi \right] = \left(\frac{\nabla^2 \sqrt{n}}{\sqrt{n}} - (\nabla \theta)^2 + i \nabla^2 \theta + i \frac{\nabla n}{n} \nabla \theta \right) \Phi$$

Collisionless hydrodynamics and superfluidity

- Plugging these derivatives into the GEP

$$i\hbar\frac{\partial}{\partial t}\Phi = \left(-\frac{\hbar^2}{2m}\nabla^2 + V_{\text{ext}} + g|\Phi|^2\right)\Phi$$

and splitting the equation into a real and imaginary part yields

$$\partial_t n = -\frac{\hbar}{m}\left(n\nabla^2\theta + \nabla n\nabla\theta\right)$$
$$\hbar\,\partial_t\theta = \frac{\hbar^2}{2m}\left(\frac{\nabla^2\sqrt{n}}{\sqrt{n}} - (\nabla\theta)^2\right) - V_{\text{ext}} - gn$$

- Introducing the velocity field $\mathbf{v} = \hbar/m\,\nabla\theta$ and applying the Thomas-Fermi approx., the equations can be finally modified to...

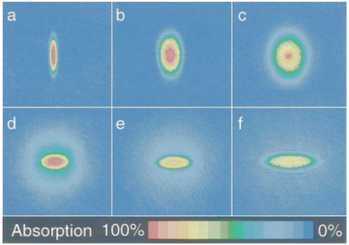
Collisionless hydrodynamics and superfluidity

$$\frac{\partial}{\partial t} n + \nabla \cdot (n\mathbf{v}) = 0 \quad \text{continuity eq.}$$

$$m \frac{\partial}{\partial t} \mathbf{v} + \nabla \left(\frac{m\mathbf{v}^2}{2} + V_{\text{ext}} + gn \right) = 0 \quad \text{Euler eq.}$$

- **Hydrodynamic equations of a superfluid**
- First equation: Continuity equation of the particle density and total particle number conservation
- Second equation: Euler equation of frictionless fluid (zero viscosity!). Also: irrotational velocity field and pressure given by $p = gn^2/2$

Outline



Expansion of an atomic cloud

- Much information of Bose condensed gases is extracted from expanded atomic clouds
- For example: Temperature of the gas, the release energy and the **aspect ratio of the density profile**
- Problem concerns non-linear dynamics of many particles, i.e. easiest way to attack it by hydrodynamic description
- Equations can be solved in the Thomas-Fermi approx., which is fulfilled by the experiments at MIT [1] and some others (e.g. with Rubidium atoms in Konstanz [14])

Ansatz: Time evolution conserves parabolic shape

- Consider the general case of an anisotropic potential with time dependent trapping frequencies

$$V_{\text{ext}}(\mathbf{r},t) = \frac{m}{2}\sum \omega_i^2(t) r_i^2$$

- The static values $\omega_i(t=0) = \omega_{0i}$ determine the initial equilibrium distribution which is given by the Thomas-Fermi density

$$n(\mathbf{r},t=0) = \frac{\mu - V_{\text{ext}}}{g} = \frac{1}{g}\left(\mu - \frac{m}{2}\sum \omega_{0i}^2 r_i^2\right)$$

- Equilibrium distribution exhibits a parabolic shape! We assume it to be conserved in the time evolution

Ansatz: Time evolution conserves parabolic shape

- We are making the following ansatz for the density and velocity profile:

$$n(\mathbf{r},t) = a_0(t) - a_x(t)\,x^2 - a_y(t)\,y^2 - a_z(t)\,z^2$$
$$\mathbf{v}(\mathbf{r},t) = \frac{1}{2}\nabla\left(\alpha_x(t)\,x^2 + \alpha_y(t)\,y^2 + \alpha_z(t)\,z^2\right)$$

  where a_0 is fixed by the total particle number $a_0 = (15N/8\pi)^{2/5}(a_x a_y a_z)^{1/5}$
- The initial coefficients are fixed by the equilibrium density distribution to be

$$a_i(t=0) = \frac{m\omega_{0i}^2}{2g} \quad \text{and} \quad \alpha_i(t=0) = 0$$

- The evolution can then be determined by the hydrodynamic equations

Ansatz: Time evolution conserves parabolic shape

- Short reminder what the hydrodynamic equations look like

$$\frac{\partial}{\partial t}n + \nabla \cdot (n\mathbf{v}) = 0 \quad \text{and} \quad m\frac{\partial}{\partial t}\mathbf{v} + \nabla\left(\frac{m\mathbf{v}^2}{2} + V_{\text{ext}} + gn\right) = 0$$

- Plugging the ansatz yields

$$\dot{a}_0 - \sum \dot{a}_i r_i^2 + \left(a_0 - \sum a_i r_i^2\right)\sum \alpha_j - 2\sum \alpha_i a_i r_i^2 = 0$$
$$\sum \mathbf{e}_i \left(m\dot{\alpha}_i r_i + m\alpha_i^2 r_i + m\omega_i^2 r_i - 2g a_i r_i\right) = 0$$

- Comparing the different variables and directions gives

$$\dot{a}_i + 2a_i\alpha_i + a_i\sum \alpha_j = 0$$
$$\dot{\alpha}_i + \alpha_i^2 + \omega_i^2 - \frac{2g}{m}a_i = 0$$

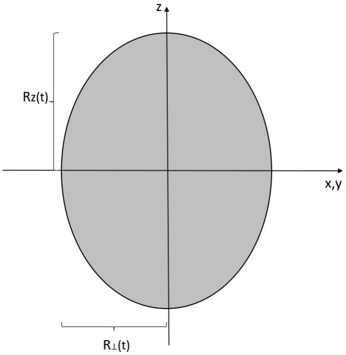
Choosing different parameterization

- New parameterization can be chosen such that the equations reduce to three
- Consider the density profile radii at which the cloud vanishes:

$$R_i(t) = \sqrt{\frac{a_0(t)}{a_i(t)}} = R_i(0)\, b_i(t) = \sqrt{\frac{2\mu}{m\omega_{0i}^2}} b_i(t)$$

- With that the coefficients can then be expressed by the b_i as:

$$a_i = \frac{m\omega_{0i}^2}{2g b_x b_y b_z b_i^2}$$



Schematic density profile of a bosonic condensate cloud

Choosing different parameterization

- The evolution equations for the intrinsic parameterization

$$\dot{a}_i + 2a_i\alpha_i + a_i \sum \alpha_j = 0 \quad \text{and} \quad \dot{\alpha}_i + \alpha_i^2 + \omega_i^2 - \frac{2g}{m} a_i = 0$$

then reduces to $\alpha_i = \dot{b}_i / b_i$ and

$$\boxed{\ddot{b}_i + \omega_i^2 b_i - \frac{\omega_{0i}^2}{b_i b_x b_y b_z} = 0}$$

- Only three ordinary coupled differential equations! Great simplification to initial problem
- Equation first formulated by Castin and Dum [15] and later by Kagan, Surkov and Shlyapnikov [16] and finally by Dalfovo, Minniti, Stringari and Pitaevskii [17] (all in 1996-1997)

Comparison to experiment

$$\boxed{\ddot{b}_i + \omega_i^2 b_i - \frac{\omega_{0i}^2}{b_i b_x b_y b_z} = 0}$$

- In the experiment at MIT [1] the bosons are trapped until $t = 0$. Then the trap is switched off and the bosons can expand freely.
- The trap is axially symmetric so there are two independent frequencies $\omega_\perp = \omega_x = \omega_y$ and ω_z
- The equation of the evolution of the parameters b_i then becomes

$$\ddot{b}_\perp - \frac{\omega_\perp^2}{b_\perp^3 b_z} = 0 \quad \text{and} \quad \ddot{b}_z - \frac{\omega_z^2}{b_\perp^2 b_z^2} = 0$$

with boundary conditions $b_\perp(t = 0) = 1$ and $b_z(t = 0) = 1$

Comparison to experiment

- Interested in the evolution of the **aspect ratio** (Reminder: The equilibrium were $R_i(0) \propto \omega_{0i}^{-1}$)

$$\frac{R_\perp}{R_z} = \frac{\omega_z}{\omega_\perp}\frac{b_\perp}{b_z} = \lambda\frac{b_\perp}{b_z}$$

- Rewrite the equations in terms of λ by introducing a dimensionless time $\tau = \omega_\perp t$

$$\frac{\mathrm{d}^2}{\mathrm{d}\tau^2}b_\perp = \frac{1}{b_\perp^3 b_z} \quad \text{and} \quad \frac{\mathrm{d}^2}{\mathrm{d}\tau^2}b_z = \frac{\lambda^2}{b_\perp^2 b_z^2}$$

- The experimental values of the trap are $\omega_z = 2\pi \times 16.23\,\mathrm{Hz}$ and $\omega_\perp = 2\pi \times 248\,\mathrm{Hz}$ (cigar shaped trap). The ratio then calculates to $\lambda = 0.065 \ll 1$. In this limit the equations can be analytically solved [15]!

Comparison to experiment

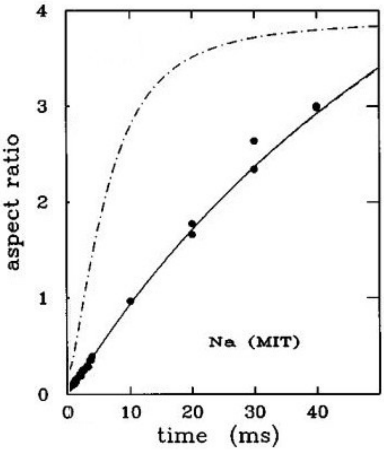
- In the small lambda limit $\lambda \ll 1$ the equations are solved by

$$b_\perp(\tau) = \sqrt{1+\tau^2}$$
$$b_z(\tau) = 1 + \lambda^2\left(\tau \arctan \tau - \ln\sqrt{1+\tau^2}\right)$$

- So the aspect ratio calculates to

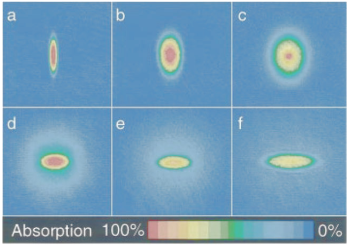
$$\frac{R_\perp}{R_z} = \frac{\lambda\sqrt{1+\tau^2}}{1 + \lambda^2\left(\tau \arctan \tau - \ln\sqrt{1+\tau^2}\right)}$$

with $\lim_{\tau\to\infty}(R_\perp/R_z) = 2/(\pi\lambda) = 9.794$



Aspect ratio of the expanding cloud at MIT [1] (Figure from [11])

Outline

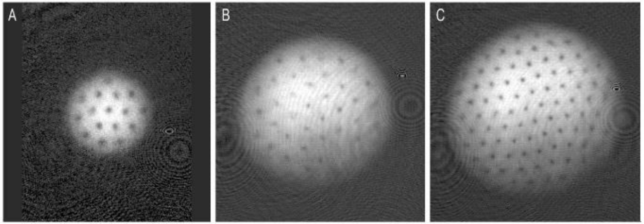


Summary

- Whole new field of physics established by the first achievement of a Bose-Einstein condensate by Ketterle [5] and Cornell and Wieman [4]: **Ultracold quantum gases**
- Description is needed for interacting bosons at low temperatures: **Gross-Pitaevskii equation**
  - Description of nonuniform, dilute bosonic condensate at zero temperature
- Experimentally observed that condensates expand after being released from the trap [1]
- Hydrodynamic description was delivered shorty after observation by Castin and Dum 1996 [15]
  - Condensate expands while preserving shape (given by the trap)
  - Expands faster in the direction the trap was more confining

Outlook

- With the Gross-Pitaevskii equation collective oscillation can be determined, e.g. the Bogoliubov dispersion relation [9] can be recovered
- Quantum vortices can be described by the Gross-Pitaevskii equation (as was the original motivation). These can even be experimentally realized, as was done here [18]



- Many more applications! For a nice introduction I recommend the review by Dalfovo, Giorgini, Pitaevskii and Stringari [11]

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