



Supporting Online Material for

Bose-Einstein Condensation in Microgravity

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Published 18 June 2010, *Science* **328**, 1540 (2010)
DOI: 10.1126/science.1189164

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Materials and methods

In order to simulate in an adequate, yet efficient way the long-time evolution of a Bose-Einstein condensate (BEC) in microgravity, we employ two different methods: (i) a full numerical simulation of the three-dimensional, time-dependent Gross-Pitaevskii equation (GPE), and (ii) a generalized (S1) scaling approach (S2–S4) that applies to BECs in the Thomas-Fermi (TF) regime for time-dependent, rotating traps. Building upon the modeling of magnetic fields associated with the trapping potential, we briefly discuss the time-dependent TF approximation and the resulting half-widths Δz and Δx of the BEC. We then sketch the essential ideas used in the numerical solution of the GPE and conclude by comparing the theoretical predictions to the observation of the long time evolution of the atomic wave packet expanding under conditions set by the drop tower environment.

Trapping potential and time sequence

We adopt a semi-classical approach describing the quantum dynamics of a BEC as it evolves along a classical trajectory $\mathcal{R}(t)$. For this purpose, we numerically solve the classical equations of motion assuming that our elongated condensate is initially at rest at the minimum of the trap which translates into the initial conditions $\mathcal{R}(t_0) = \mathcal{R}_0$ and $\mathcal{P}(t_0) = 0$ for the center of mass and total momentum. This trap originates from various magnetic field contributions acting on the ^{87}Rb atoms and the resulting potential energy reads

$$V(t, \mathbf{x}) = \mu_B g_F m_F |\mathbf{B}(t, \mathbf{x})|. \quad (1)$$

Here, μ_B denotes the Bohr magneton, $g_F = 0.5$ the Landé factor and $m_F = 2$ the hyperfine state of the ^{87}Rb atoms.

Next we perform an expansion of $V(t, \mathbf{x})$ given by (1) around the center-of-mass trajectory

$\mathcal{R}(t)$ of the BEC up to second order:

$$V(t, \mathbf{x}) = V(t, \mathcal{R}(t)) + m \mathbf{a}(t) (\mathbf{x} - \mathcal{R}(t)) + \frac{m}{2} (\mathbf{x} - \mathcal{R}(t))^T \Omega^2(t) (\mathbf{x} - \mathcal{R}(t)) ,$$

where the first and second order contributions

$$\mathbf{a}(t) = \frac{\mu_B g_F m_F}{m} \left[\nabla |\mathbf{B}(t, \mathbf{x})| \right]_{\mathbf{x}=\mathcal{R}(t)} \quad \text{and} \quad (\Omega^2(t))_{ik} = \frac{\mu_B g_F m_F}{m} \left[\frac{\partial^2 |\mathbf{B}(t, \mathbf{x})|}{\partial x_i \partial x_k} \right]_{\mathbf{x}=\mathcal{R}(t)}$$

depend on the gradient and the curvature of the magnetic field, respectively. Here m denotes the mass of the ^{87}Rb atoms, whereas the eigenvalues of the matrix $\Omega^2(t)$ correspond to the squares of the angular frequencies $\omega_i^2(t)$ of the trap. The validity of this approximation for our configuration was checked numerically.

Our simulations start directly after evaporation at $t_0 = -770$ ms, include the adiabatic opening of the trap within 752 ms and a subsequent phase in the time-independent final trap of 18 ms. At this point ($t = 0$ ms) the BEC is released and its expansion is simulated up to 1 s. During this phase of the experiment the currents through the chip wires and the Helmholtz coils are off. In our simulations we also account for homogeneous magnetic stray fields inside the vacuum chamber. Their magnitude was determined in ground-based experiments while optimizing the optical molasses phase.

Our simulations show that in the course of the opening sequence, $\mathcal{R}(t)$ moves adiabatically away from the chip – from its initial z -position at 110 μm to 800 μm just before release. During this sequence, the change of the trap frequencies from $\omega_x/(2\pi) = 18.5$ Hz and $\omega_y/(2\pi) = \omega_z/(2\pi) = 2245$ Hz to their final values of 10, 22 and 27 Hz is accompanied by a significant rotation of the principal axes of the harmonic potential.

Dynamics of the Bose-Einstein Condensate: a Thomas-Fermi approach

Due to the rotation of the harmonic potential, it is advantageous to employ a generalization (S1) of the familiar scaling method (S2–S4). Provided the condensate is in the TF regime, the initial

density distribution of the ground state of the BEC can be approximated by

$$|\phi_{TF}(\mathbf{x})|^2 = \frac{1}{g} \cdot \Theta \left[\mu_{TF} - \frac{m}{2} (\mathbf{x} - \mathbf{R}_0)^T \Omega^2(t_0) (\mathbf{x} - \mathbf{R}_0) \right]$$

with the chemical potential

$$\mu_{TF} \equiv \frac{\hbar\bar{\omega}}{2} \left(15Na \sqrt{\frac{m\bar{\omega}}{\hbar}} \right)^{\frac{2}{5}}.$$

In these expressions, Θ denotes the Heaviside function, N is the number of atoms in the BEC and $\bar{\omega} = \sqrt[3]{\det\Omega(t_0)}$ defines the geometric mean of the initial angular frequencies of the trap. Moreover, the coupling constant g is related to the s -wave scattering length a according to $g \equiv 4\pi\hbar^2 a/m$.

The generalized scaling approach (*SI*) for a rotating BEC in the TF regime states that the main contributions arising from the internal dynamics of the condensate can be absorbed in a time-dependent, linear transformation of the spatial coordinates. The corresponding transformation matrix $\Lambda(t)$ satisfies the matrix differential equation

$$\Lambda^T(t) \left(\frac{d^2\Lambda}{dt^2} + \Omega^2(t) \Lambda(t) \right) = \frac{\Omega^2(t_0)}{\det\Lambda(t)} \quad (2)$$

with the initial conditions $\Lambda(t_0) = \mathbf{1}$ and $\dot{\Lambda}(t_0) = 0$.

Based on the solution $\Lambda(t)$ of Eq. 2 and the center-of-mass position $\mathbf{R}(t)$ discussed in the previous subsection, the time evolution of the BEC in the time-dependent TF approximation is given by

$$|\psi_{TF}(t, \mathbf{x})|^2 = \frac{1}{g\sqrt{\det(\Omega^2(t_0)\Sigma(t))}} \Theta \left[\mu_{TF} - \frac{m}{2} (\mathbf{x} - \mathbf{R}(t))^T \Sigma^{-1}(t) (\mathbf{x} - \mathbf{R}(t)) \right].$$

Here, the positive definite matrix $\Sigma(t) = \Lambda(t)(\Omega^2(t_0))^{-1}\Lambda^T(t)$ characterizes the orientation and the width of the ellipsoidal condensate. In order to compare the theoretical predictions with the observed BEC images, we depict in Fig. 4 (black curves) the corresponding projected

half-widths

$$\Delta x(t) = \sqrt{\frac{2\mu_{TF} \Sigma_{11}(t)}{m}} \quad \text{and} \quad \Delta z(t) = \sqrt{\frac{2\mu_{TF} \Sigma_{33}(t)}{m}},$$

which follow directly from the elements Σ_{11} and Σ_{33} of the matrix $\Sigma(t)$.

Numerical solution of the Gross-Pitaevskii equation

In our experiment the condensates are prepared with typically 10^4 atoms remaining after evaporation. Combined with the low trap frequencies just before release, the validity of the TF approximation has to be checked. Therefore, we test the applicability of the scaling method by numerically examining the solutions of the GPE

$$i\hbar \frac{\partial \psi}{\partial t} = \left[-\frac{\hbar^2}{2m} \nabla^2 + V(t, \mathbf{x}) + g |\psi(t, \mathbf{x})|^2 \right] \psi(t, \mathbf{x}).$$

Since the size of the BEC increases by a few orders of magnitude within 1 s after release, an efficient numerical representation of the macroscopic wave function $\psi(t, \mathbf{x})$ is crucial. To this end, we take advantage of the linear coordinate transformation $\boldsymbol{\xi} \equiv \Lambda^{-1}(t) \mathbf{x}$ and introduce a new time coordinate $\tau \equiv t$ for the sake of an unambiguous notation. This transformation includes the solution $\Lambda(t)$ of the matrix differential Eq. 2 and is accompanied by the transformation

$$\psi(t, \mathbf{x}) = \frac{1}{\sqrt{\det \Lambda(t)}} \exp \left[\frac{i}{\hbar} (\mathcal{B}(t) + \mathcal{P}(t) \mathbf{x} - \mathcal{R}(t) \hat{\mathbf{p}}) \right] \exp \left[\frac{i}{\hbar} \mathbf{x}^T S(t) \mathbf{x} \right] \psi_{\Lambda}(\tau, \boldsymbol{\xi})$$

of the wave function. In this substitution the scalar $\mathcal{B}(t)$ depends on the chemical potential μ of the initial ground state, the matrix $\Lambda(t)$ and the action (S5–S8) along the classical trajectory $\mathcal{R}(t)$. Moreover, we have defined the symmetric matrix $S(t) \equiv \frac{m}{2} \dot{\Lambda}(t) \Lambda^{-1}(t)$ and have denoted the momentum operator in position representation by $\hat{\mathbf{p}} = \frac{\hbar}{i} \nabla$.

The resulting GPE in transformed coordinates

$$i\hbar \frac{\partial \psi_{\Lambda}}{\partial \tau} = -\frac{\hbar^2}{2m} \left(\nabla_{\boldsymbol{\xi}}^T [\Lambda^T(\tau) \Lambda(\tau)]^{-1} \nabla_{\boldsymbol{\xi}} \right) \psi_{\Lambda}(\tau, \boldsymbol{\xi}) + \frac{1}{\det \Lambda(\tau)} \left(\frac{m}{2} \boldsymbol{\xi}^T \Omega^2(t_0) \boldsymbol{\xi} + g |\psi_{\Lambda}(\tau, \boldsymbol{\xi})|^2 - \mu \right) \psi_{\Lambda}(\tau, \boldsymbol{\xi}) \quad (3)$$

is an advantageous starting point for full 3D numerical simulations, and this for several reasons: (i) the main part of the inner dynamics is absorbed by the linear coordinate transformation of the generalized scaling approach. As a result, Eq. 3 allows for an efficient simulation of the long-time evolution using a static discretization in the coordinates ξ . (ii) Any change in the density distribution of the BEC during the numerical integration of the transformed GPE reveals additional aspects of the BEC dynamics which cannot be described by the generalized scaling approach. Hence, the numerical simulation of the long-time evolution of a BEC based on the transformed GPE provides us with a direct test of the validity of the scaling method. Under the conditions of our experiment, the results of the numerical simulation of the transformed GPE deviate slightly from those of the scaling approach. However, these differences are negligible when contrasted to the resolution of the observed density distributions making the generalized scaling method an efficient numerical tool to explore the dynamics of our BEC.

Long time evolution of the BEC in free fall

Figures 3 and 4 display the center of mass and the expansion of the BEC during the free fall. Moreover, in Fig. 4 we compare this expansion to the prediction (black solid curve) of the generalized scaling approach (S1). For short times (up to 120 ms) we find a good agreement between experiment and theory but observe a deviation for larger times.

Our theoretical approach outlined above allows us to include residual magnetic fields. In order to gain a qualitative understanding of the observed sizes of the BEC after expansion, we assume a magnetic field curvature defined by the three time-independent components

$\partial_{xx}B_x = 0.43 \mu\text{T}/\text{mm}^2$, $\partial_{xz}B_x = -0.016 \mu\text{T}/\text{mm}^2$ and $\partial_{zz}B_x = -0.024 \mu\text{T}/\text{mm}^2$. Additional coefficients $\partial_{yy}B_x$, $\partial_{xx}B_z$, $\partial_{xz}B_z$ and $\partial_{zz}B_z$ were included in our simulation in order to satisfy the stationary Maxwell equations. With these parameters we achieve a qualitative agreement with the data (black dotted curves in Fig. 4).

To convey a feeling for the stray fields, we have complemented the gallery of figure 3 (A,B,C) with a graph (Fig. 3D) which represents the center of mass of the BECs for several TOFs. For long time scales we observe a displacement of the BEC and a scattering of the data which stands in sharp contrast to the stable and highly reproducible results for short TOFs. This figure suggests that weak magnetic field inhomogeneities such as time-dependent gradients or curvatures cause an observable effect at large time scales difficult to reach in earth-bound experiments. In spite of the restricted number of drops, we have deliberately made more experiments at 500 ms and 1000 ms to estimate the scattering of the data.

In conclusion, accounting for these weak field curvatures that could originate from the experimental environment of the drop tower, we obtain a good agreement between the computed expansion (black dotted curves) and the corresponding experimental data for both short and long time scales as shown in Fig. 4. Our experiment demonstrates that atoms in magnetic hyperfine states such as $F = 2, m_F = 2$ (in our case) are sensitive probes for tiny fields when exposed for long times. A coherent transfer of the BEC into the magnetically insensitive hyperfine state $F = 2, m_F = 0$ is underway and should dramatically reduce the effects of residual magnetic fields.

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