Numerical Study of BEC Phase Transition in Hartree-Fock Approximation

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Motivation: Hartree-Fock (HF) approximation is the simplest way to study finite-temperature properties of Bose-Einstein condensates. However, the order of the Bose-Einstein condensation (BEC) phase transition for a trapped weakly interacting Bose gas in this approximation is not known. As a first step in resolving this question, we present a numerical study of the BEC phase transition using the semiclassical approximation (SC) for thermal states [1].

HF description of BEC

- **Weakly interacting Bose gas - functional integral formulation**
  - for ultra-cold dilute gases we assume contact interaction [2]

$$V_{\rm int}(\vec{r}-\vec{r}\,') = g\,\delta(\vec{r}-\vec{r}\,')$$

  - grand-canonical partition function

$$\mathcal{Z} = \oint \mathcal{D}\psi^* \oint \mathcal{D}\psi\, \exp\left(-\mathcal{A}[\psi^*,\psi]/\hbar\right)$$

$$\mathcal{A}[\psi^*,\psi] = \int_0^{\hbar\beta} d\tau \int d^3\vec{r}\, \psi^*(\vec{r},\tau)\left[\hbar\frac{\partial}{\partial\tau} - \frac{\hbar^2}{2M}\Delta + V(\vec{r}) - \mu\right]\psi(\vec{r},\tau) + \frac{g}{2}\int_0^{\hbar\beta} d\tau \int d^3\vec{r}\,\psi^*(\vec{r},\tau)\psi(\vec{r},\tau)\psi^*(\vec{r},\tau)\psi(\vec{r},\tau)$$

  - for trapping we assume isotropic harmonic potential $V(\vec{r}) = \frac{1}{2}M\omega^2 r^2$
  - we split ψ into the ground-state (condensate) and thermal contribution

$$\psi(\vec{r},\tau) = \psi_0(\vec{r},\tau) + \delta\psi(\vec{r},\tau)$$

  - the action now contains terms up to $4^{\rm th}$ order in $\delta\psi$
  - numerous approximation techniques treat $\delta\psi^4$ terms differently [2, 3]
- **HF-SC approximation**
  - mean-field approach

$$\delta\psi^*\delta\psi\delta\psi^*\delta\psi \approx 4\langle\delta\psi^*\delta\psi\rangle\delta\psi^*\delta\psi - 2\langle\delta\psi^*\delta\psi\rangle\langle\delta\psi^*\delta\psi\rangle,$$

  where $\langle\bullet\rangle$ denotes self-consistently calculated mean value
  - by extremizing the HF action, we obtain HF equations

$$\left(-\frac{\hbar^2}{2M}\Delta + V(\vec{r}) + gn_0(\vec{r}) + 2gn_{\rm th}(\vec{r})\right)\psi_0(\vec{r}) = \mu\,\psi_0(\vec{r})$$

$$n_{\rm th}(\vec{r}) = \sum_{\vec{k}} |\psi_{\vec{k}}(\vec{r})|^2 \frac{1}{\exp(\beta(E_{\vec{k}}-\mu))-1}$$

$$\left(-\frac{\hbar^2}{2M}\Delta + V(\vec{r}) + 2gn_0(\vec{r}) + 2gn_{\rm th}(\vec{r})\right)\psi_{\vec{k}}(\vec{r}) = E_{\vec{k}}\,\psi_{\vec{k}}(\vec{r})$$

  - we further apply SC approximation to calculate thermal contributions; in this approximation, the last two equations are combined and replaced by

$$n_{\rm th}(r) = \frac{1}{\lambda^3}\zeta_{3/2}\left(e^{\beta(\mu-2g(n_0(r)+n_{\rm th}(r))-V(r))}\right),$$

  where $\lambda = \sqrt{\frac{2\pi\hbar^2\beta}{M}}$ and $\zeta_{3/2}(z) = \sum_{j=1}^{\infty}\frac{z^j}{j^{3/2}}$

Numerical solution of HF-SC equations

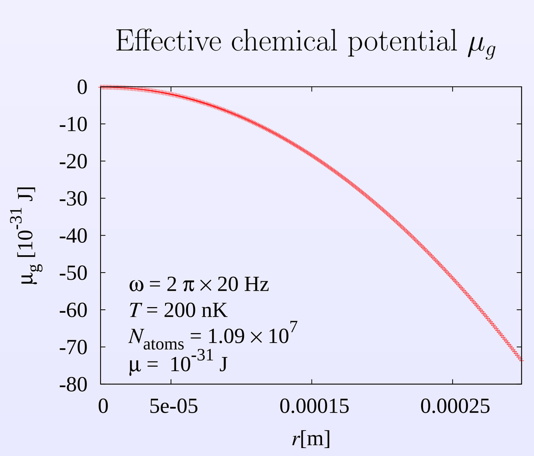
- **Gas phase**
  - when condensate is absent ($n_0 = 0$), HF-SC equations reduce to

$$n_{\rm th}(r) = \frac{1}{\lambda^3}\zeta_{3/2}\left(e^{\beta(\mu-2gn_{\rm th}(r)-V(r))}\right)$$

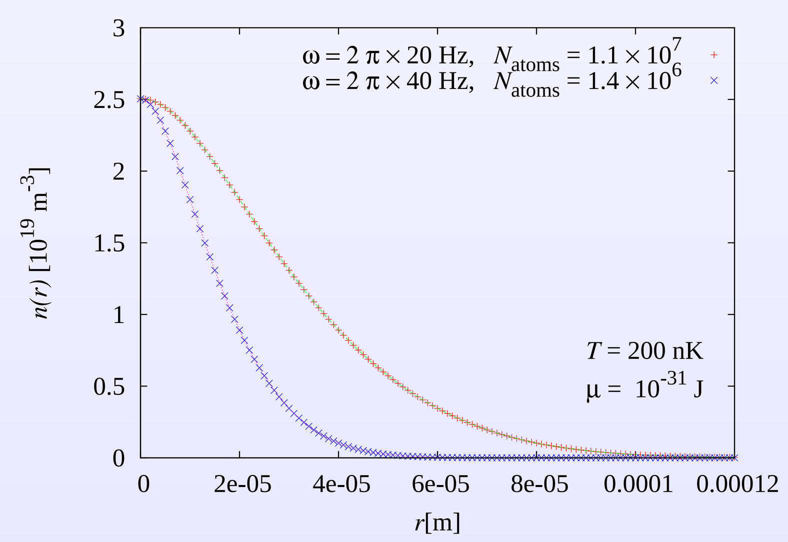
  - for a given μ, we solve the equation numerically in the range of r
  - total number of atoms: $N_{\rm atoms} = 4\pi\int_0^\infty dr\, r^2\, n_{\rm th}(r)$
  - consistency check: to ensure the convergence of $\zeta_{3/2}$ function, we need to verify that $\mu_g(r) = \mu - 2gn_{\rm th}(r) - V(r) < 0$

  - **Numerical results**

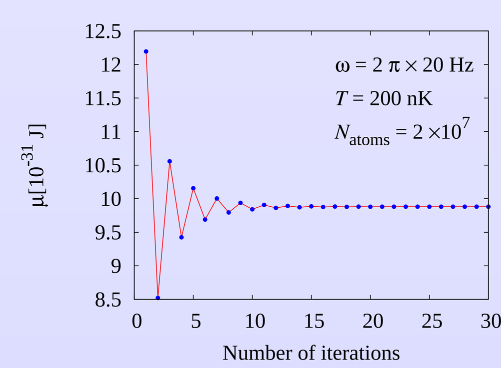
Effective chemical potential μ_g



Density of atoms



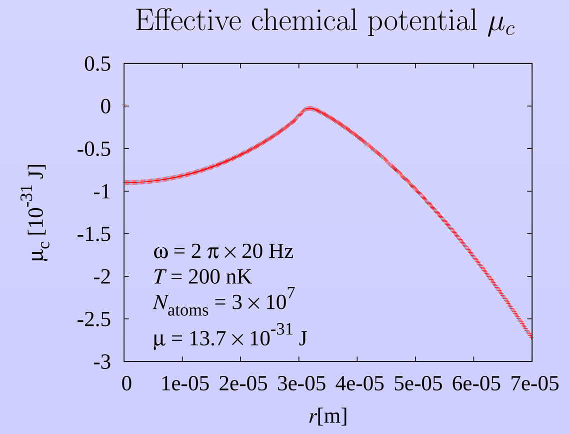
- **Condensate phase**
  - in the condensate phase we solve the full system of two HF-SC equations
  - the total number of atoms $N_{\rm atoms}$ is held fixed and we calculate the chemical potential μ
  - we use an iterative procedure to solve the HF-SC equation
  - the convergence is achieved after small number of iterative steps



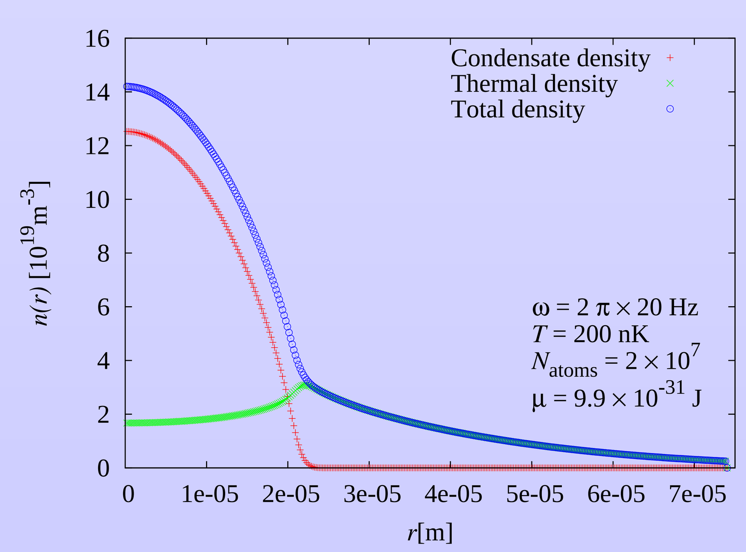
  - the generalized form of Gross-Pitaevskii equation is solved using propagation in imaginary time
  - again we have to ensure the convergence of $\zeta_{3/2}$ function by verifying that $\mu_c(r) = \mu - 2g(n_0(r) + n_{\rm th}(r)) - V(r) < 0$

  - **Numerical results**

Effective chemical potential μ_c



Density of atoms

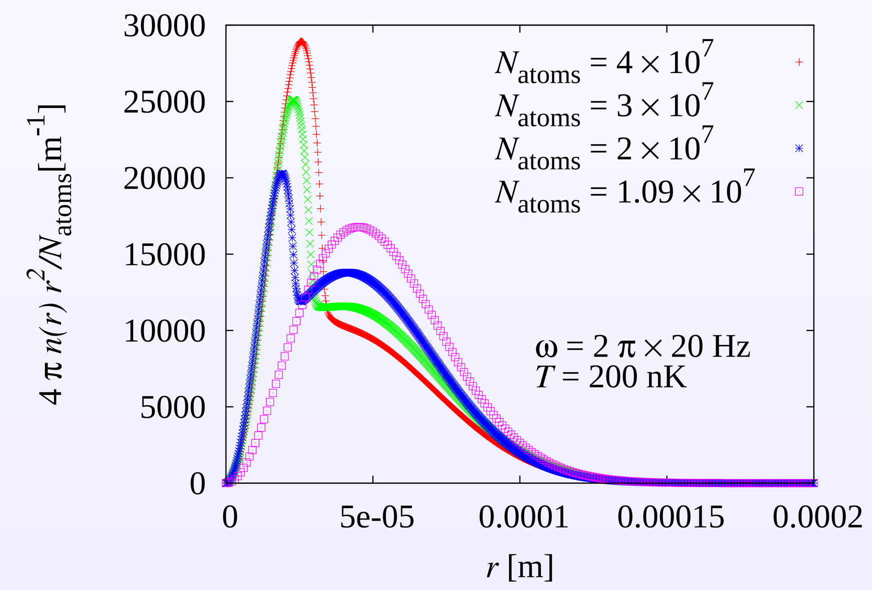


BEC phase transition

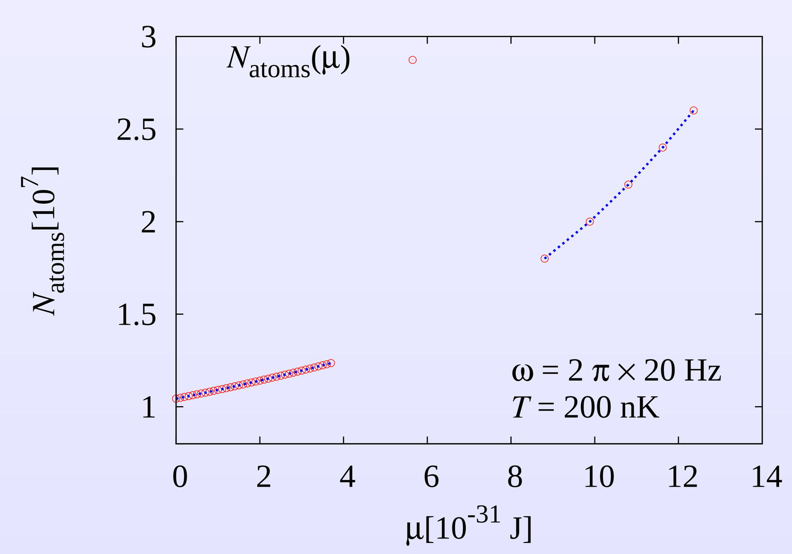
- **Setup**

The temperature and trap frequency are fixed while we decrease $N_{\rm atoms}$ in the trap and observe transition from the condensate to the gas phase.

If we plot the normalized radial density distribution $4\pi r^2 n(r)/N_{\rm atoms}$, the prominent peak for smaller values of r corresponds to the presence of Bose-Einstein condensate. This peak disappears as we decrease the total number of atoms.



- **Phase diagram**



Left branch of the phase diagram describes the gas phase, while the right one corresponds to the condensate phase. The central part, where the phase transition is located, is inaccessible due to the SC approximation limitation (convergence of $\zeta_{3/2}$) [1].

Summary and outlook

- HF-SC equations fail to describe the behavior of ultra-cold atomic gases in the vicinity of the phase transition from BEC to the gas phase, since it is not possible to find self-consistent solution of equations, in agreement with earlier studies [4-6]
- thus, we cannot characterize the order of the BEC phase transition using the simple HF-SC approach
- to resolve this, we need to go beyond the standard SC approximation in the Hartree-Fock approach

References

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