Instability of a repulsive Bose gas near the BEC transition

M. Männel[1,*], K. Morawetz[1,2] and P. Lipavský[3]

[1]Department Physical Engineering, Münster University of Applied Science, 48565 Steinfurt, Germany
[2]International Institute of Physics, Universidade Federal do Rio grande do Norte, 59.072-970 Natal-RN, Brazil
[3]Faculty of Mathematics and Physics, Charles University, Ke Karlovu 3, 12116 Prague 2, Czech Republic

Fachhochschule Münster University of Applied Sciences

CHARLES UNIVERSITY PRAGUE faculty of mathematics and physics

UFRN

International Institute of Physics Federal University of Rio Grande do Norte

TT 45.109

Abstract

We investigate a Bose gas with finite-range interaction using a scheme to eliminate self-interaction in the T-matrix approximation. In this way the corrected T-matrix becomes suitable to calculate properties below the critical temperature, without the use of anomalous functions [1–3]. In the vicinity of the onset of Bose-Einstein condensation (BEC) chemical potential and pressure show a van-der-Waals like behavior indicating a first-order phase transition although there is no long-range attraction. Furthermore for sufficiently strong interaction the equation of state becomes multivalued near the BEC transition. For a Hatree-Fock or Hartree-Fock-Bogoliubov approximation such a multivalued region can be avoided by a Maxwell construction. However, for the T-matrix approximation there remains a multivalued region even after a Maxwell construction.

Renormalized Kadanoff-Martin approximation (T-matrix approximation)

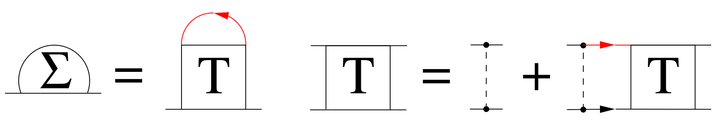

FIG. 1. Diagrams for the self energy and T-matrix [4], red arrows mark reduced propagators.

To avoid self-interaction, the full Green functions in the upper loop of the self energy were replaced by reduced ones, which do not include the singular contribution $n_0^2\mathcal{T}^2(\boldsymbol{q})$ [2,3]. The resulting full Green functions have the same structure as those obtained with anomalous propagators [1]

$$G(\boldsymbol{q}, iz_\nu) \approx \frac{iz_\nu + \epsilon_{\boldsymbol{q}}}{iz_\nu^2 - \epsilon_{\boldsymbol{q}}^2 + n_0^2\mathcal{T}^2(\boldsymbol{q})} ,$$

$$\epsilon_{\boldsymbol{q}} = \frac{\hbar^2 q^2}{2m} - \mu + 2n\mathcal{T}(\boldsymbol{0}) .$$

Medium effects are covered by the many-body T-matrix $\mathcal{T}(\boldsymbol{q})$. The dispersion in the BEC phase is

$$E_{\boldsymbol{k}} = \sqrt{\left(\frac{\hbar^2 k^2}{2m} + n_0\mathcal{T}(\boldsymbol{0})\right)^2 - n_0^2\mathcal{T}^2(\boldsymbol{k})} .$$

We consider a homogeneous interacting Bose gas in equilibrium with the Hamiltonian

$$\hat{H} = \sum_{\boldsymbol{k}} \frac{\hbar^2 k^2}{2m} \hat{a}^\dagger_{\boldsymbol{k}} \hat{a}_{\boldsymbol{k}} + \frac{\lambda}{2\Omega} \sum_{\boldsymbol{q},\boldsymbol{p},\boldsymbol{k}} \hat{a}^\dagger_{\boldsymbol{p}} \hat{a}^\dagger_{\boldsymbol{q}-\boldsymbol{p}}\, g_{\boldsymbol{p}-\frac{\boldsymbol{q}}{2}}\, g_{\boldsymbol{k}-\frac{\boldsymbol{q}}{2}}\, \hat{a}_{\boldsymbol{k}} \hat{a}_{\boldsymbol{q}-\boldsymbol{k}}$$

and assume a separable interaction with Yamaguchi form factors $g_{\boldsymbol{p}} = \left(1 + \frac{p^2}{\gamma^2}\right)^{-1}$ [5].

References

[1] K. Morawetz. *Phys. Rev. B*, 82:092501, 2010.
[2] M. Männel et al. *New J. Phys.*, 12:033013, 2010.
[3] B. Šopík et al. *Phys. Rev. B*, 84:094529, 2011.
[4] L. P. Kadanoff et al. *Phys. Rev.*, 124:670, 1961.
[5] Y. Yamaguchi. *Phys. Rev.*, 95:1628, 1954.
[6] N. Bogolubov. *J. Phys. (USSR)*, 11:23, 1947.
[7] K. Huang and C. N. Yang. *Phys. Rev.*, 105:767, 1957.
[8] K. Huang et al. *Phys. Rev.*, 105:776, 1957.

Weak repulsive interaction

The total energy in T-matrix approximation is

$$U = \underbrace{\sum_{\boldsymbol{k}\neq\boldsymbol{0}} E_{\boldsymbol{k}} f_{\mathrm{B}}(E_{\boldsymbol{k}})}_{\text{quasi particles}} + \underbrace{\sum_{\boldsymbol{k}\neq\boldsymbol{0}} \frac{n_0^2\mathcal{T}^2(\boldsymbol{k})}{4E_{\boldsymbol{k}}}(1 + 2f_{\mathrm{B}}(E_{\boldsymbol{k}}))}_{\text{depletion}} - \underbrace{\sum_{\boldsymbol{k}\neq\boldsymbol{0}} E_{\boldsymbol{k}} v_{\boldsymbol{k}}^2}_{\text{attraction in momentum space}} + \frac{\mathcal{T}(\boldsymbol{0})}{\Omega}\left(N^2 - NN_{\boldsymbol{0}} + \tfrac{1}{2}N_{\boldsymbol{0}}^2\right)$$

and the total number of particles

$$N = N_{\boldsymbol{0}} + \underbrace{\sum_{\boldsymbol{k}\neq\boldsymbol{0}} f_{\mathrm{B}}(E_{\boldsymbol{k}})}_{\text{quasi particles}} + \underbrace{\sum_{\boldsymbol{k}\neq\boldsymbol{0}} v_{\boldsymbol{k}}^2}_{\text{depletion}} + \sum_{\boldsymbol{k}\neq\boldsymbol{0}} 2v_{\boldsymbol{k}}^2 f_{\mathrm{B}}(E_{\boldsymbol{k}}) .$$

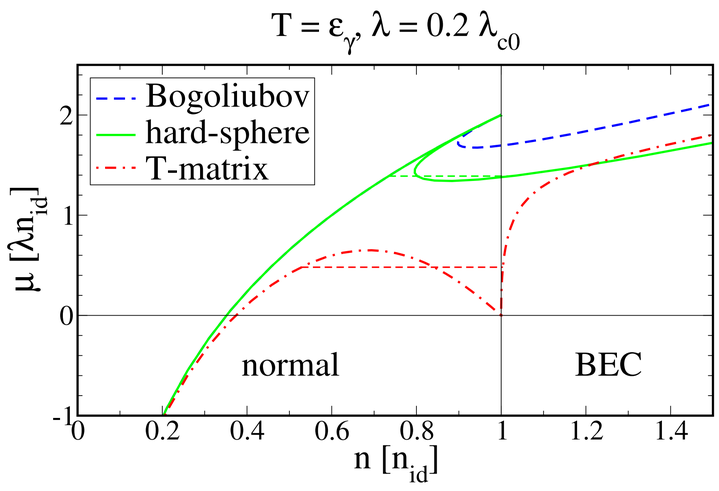

FIG. 2. Chemical potential in Hartree-Fock-Bogoliubov, hard-sphere and T-matrix approximation, $n_{id} \approx 0.059\gamma^3$ is the ideal critical density for Bose condensation, the constant quantities are given above the diagram, $\varepsilon_\gamma = \hbar^2\gamma^2/2m$, $\lambda_{c0} = 8\pi\hbar^2/m\gamma$.

The Bogoliubov and hard-sphere approximation [6–8] show an unphysical behavior of the chemical potential due to an overestimation of the attraction in momentum space. Furthermore there is a drop of the chemical potential when BEC sets in signaling an instability of the system and a first-order phase-transition. The multivalued region can be avoided with a Maxwell construction. For the T-matrix approximation medium effects compensate the repulsive interaction near the onset of BEC. Therefore the attraction in momentum space is compensated. Nevertheless the vanishing of the interaction leads again to an instability and a first-order phase-transition.

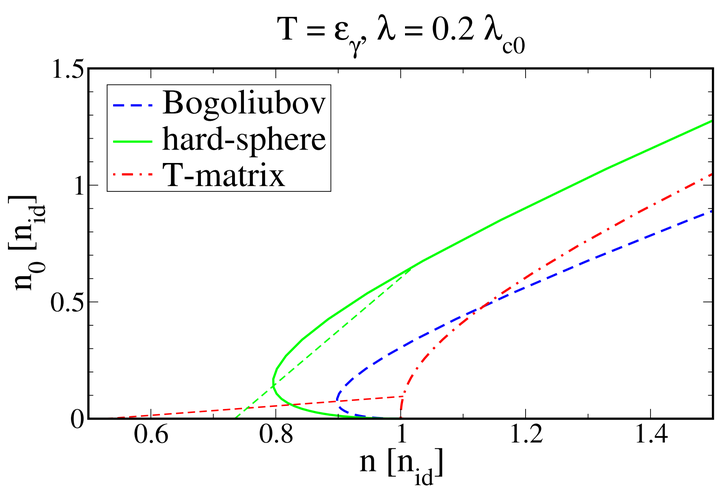

FIG. 3. Condensate density in Hartree-Fock-Bogoliubov, hard-sphere and T-matrix approximation.

In the coexistence region the condensate density changes linearly.

* maennel@fh-muenster.de

Strong repulsive interaction

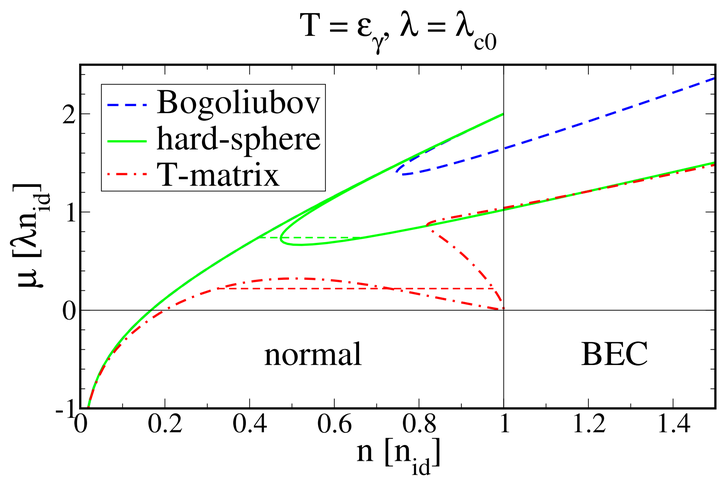

FIG. 4. Chemical potential.

For a strong repulsive interaction the attraction in momentum space is too strong to be compensated by medium effects, therefore also the T-matrix approximation yields a multivalued region, which cannot be avoided by a Maxwell construction.

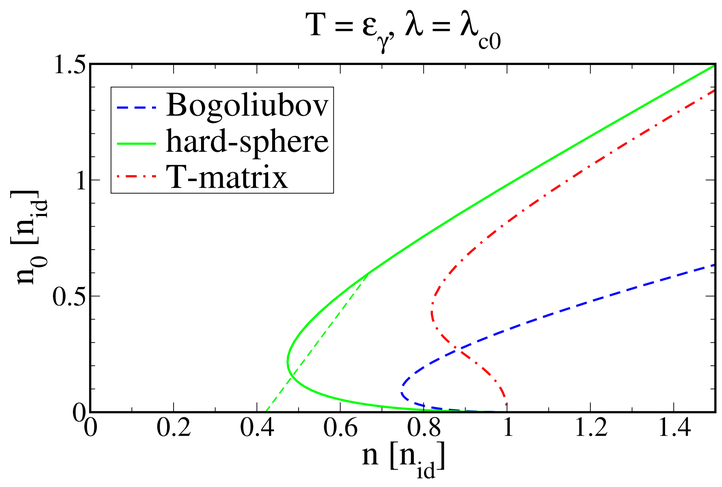

FIG. 5. Condensate density.

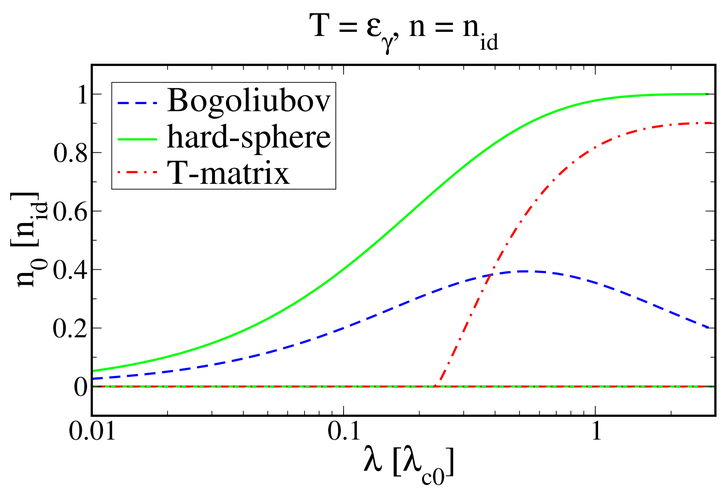

FIG. 6. Solutions for the condensate density at $n = n_{id}$.

The Bogoliubov and hard-sphere approximation always have two solutions for the condensate density $n_{\boldsymbol{0}}$ at the ideal critical density n_{id}. For the T-matrix approximation the second solution appears only above a critical interaction strength.

Summary and conclusions

The appearance of BEC destabilizes the repulsive Bose gas due to the attraction in momentum space or medium effects, leading to a first-order phase transition. The BEC sets in with the first-order phase transition, therefore the critical density is decreased. During the first-order phase transition the condensate density increases linearly.