Upper bound for the grand canonical free energy of the Bose gas in the Gross–Pitaevskii limit

Andreas Deuchert
(joint work with Chiara Boccato and David Stocker)

The dilute Bose gas, that is, a bosonic system with rare but strong collisions, is one of the most fundamental and interesting models in quantum statistical mechanics. Its prominence is mostly due to the occurrence of the Bose–Einstein condensation (BEC) phase transition and its numerous phenomenological consequences. Triggered by the experimental realization of BEC in ultra cold alkali gases in 1995, see [1, 5], and by the subsequent experimental progress, in the past two decades there have been numerous mathematical investigations of dilute Bose gases in different parameter regimes. I refer to [11, 10, 12, 14, 15, 2, 3, 4, 6, 7, 8, 9] and to references therein for examples concerning questions in equilibrium statistical mechanics.

In the article I was presenting in my talk in Oberwolfach, we consider a system of bosons confined to a three-dimensional flat torus Λ with side length L in the grand canonical ensemble. The Hamiltonian of the system is given by

$$\mathcal{H}_N = \int_\Lambda \nabla a_x^* \nabla a_x \mathrm{d}x + \frac{1}{2}\int_{\Lambda^2} a_x^* a_y^* v_N(d(x,y)) a_y a_x \mathrm{d}(x,y) \tag{1}$$

and acts on a dense domain in the bosonic Fock space. By a_x^*, a_x I denote the usual bosonic creation and annihilation operators (actually operator-valued distributions) of a particle at the point $x \in \Lambda$ that satisfy the canonical commutation relations $[a_x, a_y^*] = \delta(x-y), [a_x, a_y] = 0 = [a_x^*, a_y^*]$. Here $\delta(x)$ is Dirac's delta distribution with unit mass at the origin. The interaction potential is of the form $v_N(d(x,y)) = N^2 v(N d(x,y))$ with a nonnegative function v and a parameter $N > 0$ that we choose as the expected number of particles in the system. By $d(x,y)$ I denote the distance between x and y in Λ. The scattering length a_N of v_N, which is a combined measure for its range and strength, scales as $a_N/L \sim N^{-1}$. This assures that the interaction energy per particle is of the same order as the spectral gap of the Laplacian in Λ.

The quantity we are interested in is the grand canonical free energy at inverse temperatue β related to the Hamiltonian $\mathcal{H}_N$. It is defined as

$$F(\beta, N, L) = -\frac{1}{\beta} \ln\left(\mathrm{Tr}[\exp(-\beta(\mathcal{H}_N - \mu\mathcal{N}))]\right) + \mu N, \tag{2}$$

where the chemical potential μ is chosen such that the grand canonical Gibbs state

$$G = \frac{\exp(-\beta(\mathcal{H}_N - \mu\mathcal{N}))}{\mathrm{Tr}[\exp(-\beta(\mathcal{H}_N - \mu\mathcal{N}))]} \tag{3}$$

satisfies $\mathrm{Tr}[\mathcal{N}G] = N$ ($\mathcal{N}$ is the particle number operator).

The main result in our article is the following theorem. For the sake of simplicity I state it only in the special case $\beta = \kappa\beta_c$ with $\kappa \in (1,\infty)$ and the inverse critical temperature for BEC β_c in the ideal gas (condensed phase).

Theorem 1: *Assume that the function $v : [0,\infty) \to [0,\infty]$ is nonnegative, compactly supported, satisfies $v(|\cdot|) \in L^3(\Lambda)$, and is strictly positive on a set of* *positive measure. By $\varrho = N/L^3$ we denote the particle density. We consider the combined limit $N \to \infty$, $\beta = \kappa\beta_c$ with $\kappa \in (1,\infty)$. The free energy in* (2) *satisfies the upper bound*

$$
\begin{aligned}
F(\beta, N, L) \leq\; & F_0^+(\beta, N, L) + 4\pi\mathfrak{a}_N L^3 \left(2\varrho^2 - \varrho_0^2(\beta, N, L)\right) + \frac{\ln\left(4\beta\mathfrak{a}_N/L^3\right)}{2\beta} \\
& - \frac{1}{2\beta} \sum_{p \in (2\pi/L)\mathbb{Z}^3\setminus\{0\}} \left[\frac{16\pi\mathfrak{a}_N \varrho_0(\beta, N, L)}{p^2} - \ln\left(1 + \frac{16\pi\mathfrak{a}_N\varrho_0(\beta, N, L)}{p^2}\right)\right] \\
& + O(L^{-2}N^{7/12}). \qquad (4)
\end{aligned}
$$

In the above formula $F_0^+(\beta, N, L)$ denotes the free energy of the non-condensed particles in the ideal gas with the chemical potential $\mu_0(\beta, N, L)$, and $\varrho_0(\beta, N, L)$ is the related condensate density. The first two terms in (4) had been justified for the first time for the dilute Bose gas in the thermodynamic limit, see [13, 15]. They also appeared in [7], where the asymptotics of the canonical free energy in the GP limit has been established with a remainder of the size $o(L^{-2}N)$ (The aim of this article was to give a proof of the BEC phase transition.). It is, however, expected that the canonical and the grand canonical free energies agree on that level of accuracy. The main novelty of the upper bound in (4) is therefore the appearance of the last two terms on the r.h.s., which are of the order $N^{2/3}\ln(N)$ and $N^{2/3}$, respectively. We highlight that the first two terms in (4) scale as $L^{-2}N^{5/3}$ and $L^{-2}N$, respectively. In the following I briefly discuss the origin of our new terms.

The third term on the r.h.s. of (4) is the free energy of the fluctuations of the interacting BEC. It originates from the following effective free energy:

$$
\begin{aligned}
F^{\mathrm{BEC}}(\beta, N_0, L, \mathfrak{a}_N) =& -\frac{1}{\beta}\ln\left(\int_{\mathbb{C}} \exp\left(-\beta\left(4\pi\mathfrak{a}_N L^{-3}|z|^4 - \mu|z|^2\right)\right)\mathrm{d}z\right) \\
& + \mu\varrho_0(\beta, N, L)L^3. \qquad (5)
\end{aligned}
$$

Here $\mathrm{d}z = \mathrm{d}x\mathrm{d}y/\pi$, where x and y denote the real and imaginary part of the complex number z, respectively. The chemical potential μ in (5) is chosen such that the Gibbs distribution

$$
g(z) = \frac{\exp\left(-\beta\left(4\pi\mathfrak{a}_N L^{-3}|z|^4 - \mu|z|^2\right)\right)}{\int_{\mathbb{C}}\exp\left(-\beta\left(4\pi\mathfrak{a}_N L^{-3}|z|^4 - \mu|z|^2\right)\right)\mathrm{d}z} \qquad (6)
$$

satisfies $\int_{\mathbb{C}} |z|^2 g(z)\mathrm{d}z = \varrho_0(\beta, N, L)L^3$ ($|z|^2$ should be interpreted as a particle number). Under the assumption of Theorem 1 we have

$$
F^{\mathrm{BEC}}(\beta, N_0, L, \mathfrak{a}_N) = 4\pi\mathfrak{a}_N L^3\varrho_0^2 + \frac{\ln\left(4\beta\mathfrak{a}_N/L^3\right)}{2\beta} + O\left(L^{-2}\exp\left(-cN^{1/6}\right)\right). \qquad (7)
$$

In combination with $\int |z|^2 g(z)\mathrm{d}z = \varrho_0 L^3$, this implies

$$4\pi\mathfrak{a}_N L^{-3}\left(\int_{\mathbb{C}}|z|^4 g(z)\mathrm{d}z - \left(\int_{\mathbb{C}}|z|^2 g(z)\mathrm{d}z\right)^2\right) - \frac{1}{\beta}S(g) = \frac{\ln\left(16\beta\mathfrak{a}_N/L^3\right)}{2\beta} + O\left(L^{-2}\exp\left(-cN^{1/6}\right)\right), \tag{8}$$

where $S(g) = -\int g(z)\ln(g(z))\mathrm{d}z$ denotes the classical entropy of g. This explains my claim about the physical interpretation of the term on the r.h.s. from above.

The last term in (4) is related to the free energy of the Bogoliubov Hamiltonian

$$\mathcal{H}^{\mathrm{Bog}} = \sum_{p\neq 0} p^2 a_p^* a_p + 4\pi\mathfrak{a}_N\varrho_0(\beta,N,L)\sum_{p\neq 0}\left(2a_p^*a_p + a_p^*a_{-p}^* + a_p a_{-p}\right), \tag{9}$$

which depends on β via $\varrho_0(\beta,N,L)$ (From a physics point of view this Hamiltonian can be motivated by the c-number substitution $a_0^*, a_0 \mapsto \sqrt{\varrho_0(\beta,N,L)L^3}$.). The operators a_p^* and a_p create and annihilate a particle with momentum $p \in 2\pi\mathbb{Z}^3/L$, respectively. To see the relation between $\mathcal{H}^{\mathrm{Bog}}$ and the last term in (4), we note that

$$\begin{aligned}-\frac{1}{\beta}\ln\operatorname{Tr}\exp(-\beta\mathcal{H}^{\mathrm{Bog}}) = & \frac{1}{\beta}\sum_{p\neq 0}\ln\left(1-\exp\left(-\beta\sqrt{p^2-\mu_0}\sqrt{p^2-\mu_0+16\pi\mathfrak{a}_N\varrho_0}\right)\right)\\ = & \frac{1}{\beta}\sum_{p\neq 0}\ln\left(1-\exp\left(-\beta(p^2-\mu_0)\right)\right) + 8\pi\mathfrak{a}_N L^3(\varrho-\varrho_0)\varrho_0\\ & -\frac{1}{2\beta}\sum_{p\neq 0}\left[\frac{16\pi\mathfrak{a}_N\varrho_0}{p^2} - \ln\left(1+\frac{16\pi\mathfrak{a}_N\varrho_0}{p^2}\right)\right] + o(L^{-2}N^{2/3}).\end{aligned}$$

The first and the second term on the r.h.s. contribute to F_0^+ and to the second term on the r.h.s. of (4), respectively. The third term is the novel contribution in the second line of (4).

References

[1] M.H. Anderson, J.R. Ensher, M.R. Matthews, C.E. Wieman, E.A. Cornell, *Observation of bose-einstein condensation in a dilute atomic vapor*, Science **269**, 198 (1995)

[2] G. Basti, S. Cenatiempo, B. Schlein, *A new second order upper bound for the ground state energy of dilute Bose gases*, Forum Math. Sigma **9**, e74 (2021)

[3] C. Boccato, C. Brennecke, S. Cenatiempo, B. Schlein, *Optimal Rate for Bose–Einstein Condensation in the Gross–Pitaevskii Regime*, Commun. Math. Phys. 1–85, (2019)

[4] C. Boccato, C. Brennecke, S. Cenatiempo, B. Schlein, *Bogoliubov Theory in the Gross-Pitaevskii Limit*, Acta Mathematica **222**, 219 (2019)

[5] K.B. Davis, M.-O. Mewes, M.R. Andrews, N.J. van Druten, D.S. Durfee, D.M. Kurn, W. Ketterle, *Bose-Einstein Condensation in a Gas of Sodium Atoms*, Phys. Rev. Lett. **75**, 3969 (1995)

[6] A. Deuchert, R. Seiringer, J. Yngvason, *Bose-Einstein Condensation for a Dilute Trapped Gas at Positive Temperature*, Commun. Math. Phys. **368**, 723 (2019)

[7] A. Deuchert, R. Seiringer, *Gross–Pitaevskii Limit of a Homogeneous Bose Gas at Positive Temperature*, Arch. Ration. Mech. **236**(3), 1217 (2020)

[8] S. Fournais, J.P. Solovej, *The energy of dilute Bose gases*, Ann. Math. **192**, No. 3, 893 (2020)

[9] S. Fournais, J.P. Solovej, *The energy of dilute Bose gases II: The general case*, Invent. math. **232**, 863 (2023)

[10] E.H. Lieb, R. Seiringer, J. P. Solovej, J. Yngvason, *The Mathematics of the Bose Gas and its Condensation*, Birkhäuser, Basel (2005)

[11] E.H. Lieb, J. Yngvason, *Ground State Energy of the Low Density Bose Gas*, Phys. Rev. Lett. **80**, 2504 (1998)

[12] N. Rougerie, *Scaling limits of bosonic ground states, from many-body to nonlinear Schrödinger*, arXiv:2002.02678 [math.AP] (2020)

[13] R. Seiringer, *Free Energy of a Dilute Bose Gas: Lower Bound*, Comm. Math. Phys. **279**, 595 (2008)

[14] H.-T. Yau, J. Yin, *The Second Order Upper Bound for the Ground Energy of a Bose Gas*, J. Stat. Phys. **136**, 453 (2009)

[15] J. Yin, *Free Energies of Dilute Bose Gases: Upper Gound*, J. Stat. Phys. **141**, 683 (2010)