Statistical mechanics of shell-shaped Bose-Einstein condensates on board of the International Space Station

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Introduction

Bose-Einstein condensates (BECs) made of ultracold alkali-metal atoms under microgravity were achieved dropping the BEC down a 146-meter-long drop chamber[1], but also rocketing the BEC and conducting experiments during in-space flight.[2]

In 2020 a BEC in harmonic trap[3] was observed with the NASA's Cold Atom Laboratory on board of the International Space Station (ISS). Moreover, in 2022 the same team reported the observation of ultracold atomic bubbles confined on a thin ellipsoidal shell.[4]

[1] T. van Zoest, et al., Science **328**, 1540 (2010)
[2] D. Becker et al., Nature **562**, 391 (2018).
[3] D.C. Aveline et al., Nature **582**, 193 (2020).
[4] R.A. Carollo et al., Nature **606**, 281 (2022).

Bose gas on the surface of a sphere

Our theoretical study of a Bose gas on the surface of a sphere is triggered by the experimental confinement the atoms on a bubble trap,[5] which needs microgravity conditions.[6]

The energy of a particle of mass m moving on the surface of a sphere of radius R is quantized according to the formula

$$\epsilon_l = \frac{\hbar^2}{2mR^2} l(l+1) \;, \qquad (1)$$

where $\hbar$ is the reduced Planck constant and $l = 0, 1, 2, ...$ is the **integer quantum number** of the angular momentum. This energy level has the degeneracy $2l + 1$ due to the magnetic quantum number $m_l = -l, -l + 1, ..., l - 1, l$ of the third component of the angular momentum.

[5] B. M. Garraway and H. Perrin, J. Phys. B **49**, 172001 (2016).

[6] E.R. Elliott et al., npj Microgravity **4**, 16 (2018); R.A. Carollo et al., Nature **606**, 281 (2022).

Non-interacting bosons: BEC critical temperature (I)

In quantum statistical mechanics the total number N of non-interacting bosons moving on the surface of a sphere and at equilibrium with a thermal bath of absolute temperature T is given by

$$N = \sum_{l=0}^{+\infty} \frac{2l+1}{e^{(\epsilon_l - \mu)/(k_B T)} - 1} \, , \tag{2}$$

where k_B is the Boltzmann constant and μ is the chemical potential. In the Bose-condensed phase, we can set[7] $\mu = 0$ and

$$N = N_0 + \sum_{l=1}^{+\infty} \frac{2l+1}{e^{\epsilon_l/(k_B T)} - 1} \, , \tag{3}$$

where N_0 is the number of bosons in the lowest single-particle energy state, i.e. the number of bosons in the Bose-Einstein condensate (BEC).

[7] For details, see Martina Russo, BSc thesis, Supervisor: LS, Univ. of Padova (2019).

Non-interacting bosons: BEC critical temperature (II)

Within the semiclassical approximation, where $\sum_{l=1}^{+\infty} \to \int_1^{+\infty} dl$, the previous equation becomes

$$n = n_0 + \frac{mk_B T}{2\pi\hbar^2}\left(\frac{\hbar^2}{mR^2 k_B T} - \ln\left(e^{\hbar^2/(mR^2 k_B T)} - 1\right)\right) , \qquad (4)$$

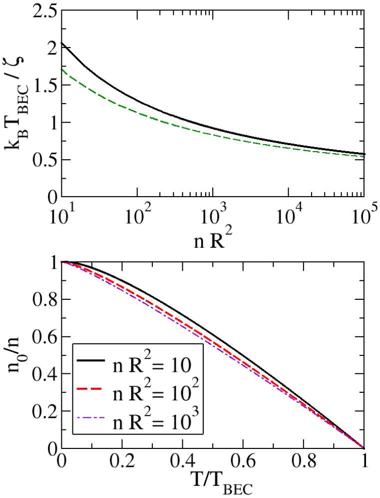
where $n = N/(4\pi R^2)$ is the 2D number density and $n_0 = N_0/(4\pi R^2)$ is the 2D condensate density.
At the critical temperature T_{BEC}, where $n_0 = 0$, one then finds[8]

$$k_B T_{BEC} = \frac{\frac{2\pi\hbar^2}{m} n}{\frac{\hbar^2}{mR^2 k_B T_{BEC}} - \ln\left(e^{\hbar^2/(mR^2 k_B T_{BEC})} - 1\right)} . \qquad (5)$$

As expected, in the limit $R \to +\infty$ one gets $T_{BEC} \to 0$, in agreement with the Mermin-Wagner theorem.[9] However, for any finite value of R the critical temperature T_{BEC} is larger than zero.

[8] A. Tononi and LS, Phys. Rev. Lett. **123**, 160403 (2019).
[9] N. D. Mermin and H. Wagner, Phys. Rev. Lett. **17**, 1133 (1966).

Non-interacting bosons: BEC critical temperature (III)



Top panel: T_{BEC} vs nR^2, with $\zeta = \hbar^2 n/m$. Solid line: semiclassical approximation (solid line); dashed line: numerical evaluation of the sum.
Bottom panel: condensate fraction n_0/n vs temperature T/T_{BEC}.

Interacting bosons: path-integral statistical mechanics (I)

We now consider a system of interacting bosons on the surface of a sphere of radius R and contact interaction of strength g.[10]
Adopting functional integration the partition function $\mathcal{Z}$ reads

$$\mathcal{Z} = \int \mathcal{D}[\bar{\psi}, \psi] \; e^{-\frac{S[\bar{\psi},\psi]}{\hbar}}, \tag{6}$$

where, by using $\beta = 1/(k_B T)$ with T the absolute temperature,

$$S[\bar{\psi}, \psi] = \int_0^{\beta\hbar} d\tau \int_0^{2\pi} d\varphi \int_0^{\pi} \sin(\theta) \; d\theta \, R^2 \, \mathcal{L}(\bar{\psi}, \psi) \tag{7}$$

is the Euclidean action and, with $\hat{L}$ is the angular momentum operator,

$$\mathcal{L} = \bar{\psi}(\theta, \varphi, \tau)\left(\hbar\partial_\tau + \frac{\hat{L}^2}{2mR^2} - \mu\right)\psi(\theta, \varphi, \tau) + \frac{g}{2}|\psi(\theta, \varphi, \tau)|^4 \tag{8}$$

is the Euclidean Lagrangian of the bosonic field $\psi(\theta, \phi, \tau)$, which depends on the spherical angles θ and ϕ and on the imaginary time τ.

[10] A. Tononi and LS, Phys. Rev. Lett. **123**, 160403 (2019).

Interacting bosons: path-integral statistical mechanics (II)

The condensate phase is introduced with the Bogoliubov shift

$$\psi(\theta, \varphi, \tau) = \psi_0 + \eta(\theta, \varphi, \tau), \tag{9}$$

where the real field configuration ψ_0 describes the condensate component. By substituting this field parametrization and keeping only second order terms in the field η we rewrite the Lagrangian as

$$\mathcal{L} = \mathcal{L}_0 + \mathcal{L}_g \tag{10}$$

with $\mathcal{L}_0 = -\mu {\psi_0}^2 + g {\psi_0}^4/2$.
We use the following decomposition of the complex fluctuation field $\eta(\theta, \varphi, \tau)$

$$\eta(\theta, \varphi, \tau) = \sum_{\omega_n} \sum_{l=1}^{\infty} \sum_{m_l=-l}^{l} \frac{e^{-i\omega_n \tau}}{R} \mathcal{Y}^l_{m_l}(\theta, \varphi)\, \eta(l, m_l, \omega_n), \tag{11}$$

where $\omega_n = 2\pi n/(\hbar\beta)$ are the Matsubara frequencies, and we introduce the orthonormal basis of the spherical harmonics $\mathcal{Y}^l_{m_l}(\theta, \phi)$.

Interacting bosons: path-integral statistical mechanics (III)

After some analytical calculations, at the Gaussian level the grand potential

$$\Omega = -\frac{1}{\beta}\ln(\mathcal{Z}) \simeq -\frac{1}{\beta}\left(\ln(\mathcal{Z}_0) + \ln(\mathcal{Z}_g)\right) \tag{12}$$

is given by

$$\begin{aligned}\Omega(\mu, {\psi_0}^2) &= 4\pi R^2\left(-\mu{\psi_0}^2 + g{\psi_0}^4/2\right) + \frac{1}{2}\sum_{l=1}^{\infty}\sum_{m_l=-l}^{l} E_l(\mu, {\psi_0}^2) \\ &+ \frac{1}{\beta}\sum_{l=1}^{\infty}\sum_{m_l=-l}^{l} \ln(1 - e^{-\beta E_l(\mu, {\psi_0}^2)})\end{aligned} \tag{13}$$

where

$$E_l(\mu, {\psi_0}^2) = \sqrt{(\epsilon_l - \mu + 2g{\psi_0}^2)^2 - g^2{\psi_0}^4} \tag{14}$$

is the excitation spectrum of the interacting system, with $\epsilon_l = \hbar^2 l(l+1)/(2mR^2)$ the single-particle energy.

Interacting bosons: path-integral statistical mechanics (IV)

The condensate number density n_0 of the system is given by

$$n_0 = {\psi_0}^2 \ , \tag{15}$$

where we fix the value of the order parameter ψ_0 with the condition

$$\frac{\partial \Omega(\mu, {\psi_0}^2)}{\partial \psi_0} = 0 \ . \tag{16}$$

Notice that from this formula we get n_0 as a function of μ.
The total number density of the system is instead given by

$$n = -\frac{1}{4\pi R^2} \frac{\partial \Omega(\mu, n_0(\mu))}{\partial \mu} \ . \tag{17}$$

At the lowest order of a perturbative scheme,[11] where ψ_0 is obtained from the mean-field equation $\frac{\partial \Omega_0(\mu, {\psi_0}^2)}{\partial \psi_0} = 0$, we get $\psi_0 \simeq \sqrt{\mu/g}$ and

$$E_l \simeq E_l^B = \sqrt{\epsilon_l(\epsilon_l + 2\mu)} \ . \tag{18}$$

[11] H. Kleinert, S. Schmidt, and A. Pelster, Phys. Rev. Lett. **93**, 160402 (2004).

Interacting bosons: path-integral statistical mechanics (V)

Within this perturbative scheme[12] from the previous equations we obtain[13] the BEC critical temperature

$$k_B T_{BEC} = \frac{\frac{2\pi\hbar^2 n}{m} - \frac{gn}{2}}{\frac{\hbar^2}{2mR^2 k_B T_{BEC}}\left(1+\sqrt{1+\frac{2gmnR^2}{\hbar^2}}\right) - \ln\left(e^{\frac{\hbar^2}{mR^2 k_B T_{BEC}}\sqrt{1+\frac{2gmnR^2}{\hbar^2}}} - 1\right)}, \tag{19}$$

where the condensate density n_0 is zero.

[12] H. Kleinert, S. Schmidt, and A. Pelster, Phys. Rev. Lett. **93**, 160402 (2004).
[13] A. Tononi and LS, Phys. Rev. Lett. **123**, 160403 (2019).

Superfluid density and BKT critical temperature (I)

Adopting the Landau formula for the normal density in a superfluid,[14] we calculate the bare superfluid density $n_s^{(0)}(T)$ as

$$n_s^{(0)} = n - \frac{1}{k_B T} \int_1^{+\infty} \frac{dl\,(2l+1)}{4\pi R^2} \, \frac{\hbar^2 (l^2 + l)}{2mR^2} \, \frac{e^{E_l^B/(k_B T)}}{(e^{E_l^B/(k_B T)} - 1)^2} \, . \qquad (20)$$

Moreover, applying the Kosterlitz-Nelson criterion[15] we evaluate numerically the Berezinskii-Kosterlitz-Thouless critical temperature T_{BKT} of the superfluid-normal transition induced by the proliferation of quantized vortices.[16]

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[14] L. Landau, Phys. Rev. **60**, 356 (1941); E.M. Lifshitz and L. P. Pitaevskii, Statistical Physics: Theory of the Condensed State, Course of Theoretical Physics, Vol. 9 (Butterworth-Heinemann, 1980).

[15] D. R. Nelson and J. M. Kosterlitz, Phys. Rev. Lett. **39**, 1201 (1977).

[16] V.L. Berezinskii, Sov. Phys. JETP **34** 610 (1971); J.M. Kosterlitz and D.J. Thouless, Journal of Physics C: Solid State Physics **6** 1181 (1973).

Superfluid density and BKT critical temperature (II)

In our problem of interacting bosons on the surface of a sphere, we determine the critical temperature T_{BKT} by using the exact Nelson-Kosterlitz criterion[17]:

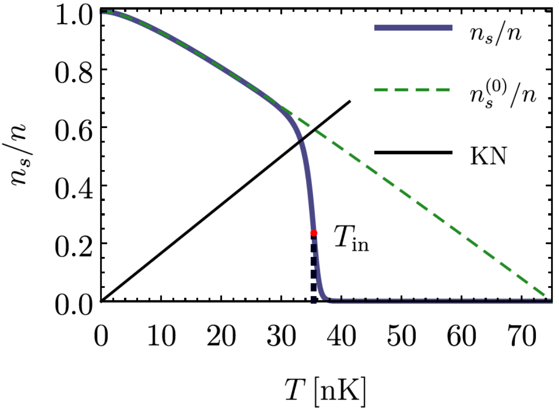
$$k_B T_{BKT} = \frac{\pi}{2} \frac{\hbar^2}{m} n_s(T_{BKT}^-) \, . \tag{21}$$

However, for the sake of simplicity, often one uses the bare superfluid density $n_s^{(0)}(T)$ instead of the renormalized one $n_s(T)$, that is an approximated Nelson-Kosterlitz criterion.

In a recent paper[18] we have analyzed in detail the use of the renormalized superfluid density $n_s(T)$ to determine T_{BKT} by solving the Kosterlitz-Thouless renormalization group equations.

[17] D. R. Nelson and J. M. Kosterlitz, Phys. Rev. Lett. **39**, 1201 (1977).
[18] A. Tononi, A. Pelster, and LS, Phys. Rev. Research **4**, 013122 (2022).

Superfluid density and BKT critical temperature (III)



The bare superfluid density $n_s^{(0)}$ overestimates the renormalized one n_s. However, the renormalized superfluid fraction n_s/n of a shell-shaped superfluid does not display an abrupt jump, but vanishes smoothly around the temperature T_{in} of the inflection point. Adapted from A. Tononi, A. Pelster, and LS, Phys. Rev. Research **4**, 013122 (2022).

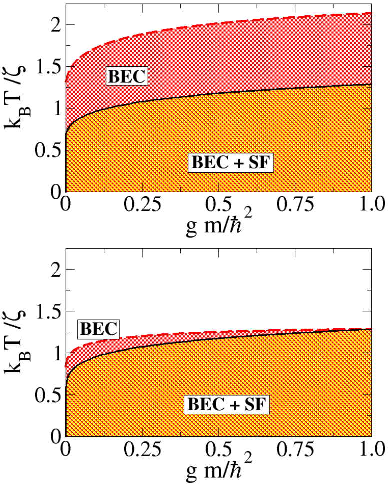
Phase diagram for bosons on the surface of a sphere (I)

We now study the phase diagram of the gas of bosons on the surface of a sphere by using the plane $(gm/\hbar^2, k_B T/\zeta)$, where $gm/\hbar^2$ is the adimensional interaction strength of bosons and $k_B T/\zeta$ is the adimensional temperature with $\zeta = \hbar^2 n/m$.

Within the approximations adopted, depending on the values of $gm/\hbar^2$, $k_B T/\zeta$, but also nR^2, the system can show:
– coexistence of condensation and superfluidity (BEC+SF);
– superfluidity in the absence of condensation (SF);
– Bose-Einstein condensation in the absence of superfluidity (BEC).

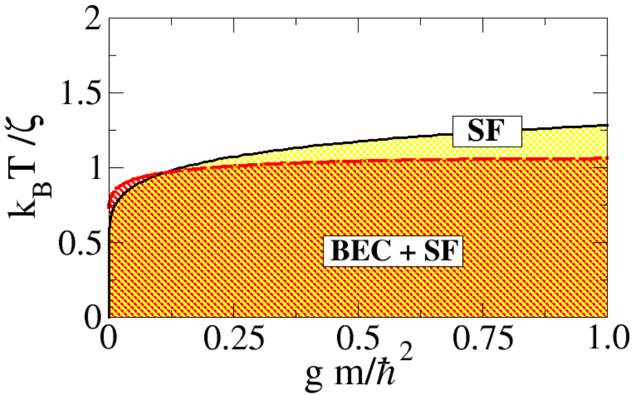
In the thermodynamic limit, i.e. $nR^2 \to +\infty$, the BEC region shrinks to zero.

Phase diagram for bosons on the surface of a sphere (II)



Phase diagram of the bosonic system for $nR^2 = 10^2$ (**upper panel**) and $nR^2 = 10^4$ (**lower panel**). Here $\zeta = \hbar^2 n/m$. Adapted from A. Tononi and LS, Phys. Rev. Lett. **123**, 160403 (2019).

Phase diagram for bosons on the surface of a sphere (III)



Phase diagram of the bosonic system for $nR^2 = 10^5$. Here $\zeta = \hbar^2 n/m$.
Adapted from A. Tononi and LS, Phys. Rev. Lett. **123**, 160403 (2019).

Conclusions (I)

- Triggered by recent achievements of space-based BECs under microgravity, which confine atoms on a thin shell, we have investigated[19] BEC on the surface of a sphere finding:
  – BEC critical temperature for non-interacting bosons;
  – BEC thermodynamcs, superfluid density, and BEC and BKT critical temperatures for interacting bosons.
- In another paper[20], we instead analyzed BEC on the surface of an ellipsoid for realistic bubble-trap parameters calculating:
  – BEC critical temperature both non-interacting and interacting bosons;
  – the free expansion of the hollow Bose condensate.

[19] A. Tononi and LS, Phys. Rev. Lett. **123**, 160403 (2019).
[20] A. Tononi, F. Cinti, and LS, Phys. Rev. Lett. **125**, 010402 (2020).

Conclusions (II)

- In a recent paper[21] we have studied in detail the BKT phase transition for a BEC on the surface of a sphere calculating the renormalized superfluid density of the system by deriving and solving generalized Kosterlitz-Thouless renormalization group equations.
- In 2022 Andrea Tononi has further investigated the 2D equation of state and the relationship between the 2D interaction strength g and the 2D s-wave scattering length a_s.[22]
- Finally, in a recent perspective review paper[23], we have discussed the state of the art on low-dimensional quantum gases in curved geometries.

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[21] A. Tononi, A. Pelster, and LS, Phys. Rev. Research **4**, 013122 (2022).
[22] A. Tononi, Phys. Rev. A **105**, 023324 (2022).
[23] A. Tononi and LS, Nat. Rev. Phys. **5**, 398 (2023).

Open problems

- The surface of a sphere has a constant curvature while the surface of an ellipsoid does not have a constant curvature. Does a locally-varying curvature affect the quantum-thermal properties of a Bose gas constrained to move on the surface of an ellipsoid?
- For a particle constrained on a curve it appears a quantum-curvature potential[24]

$$U_{QC}(s) = -\frac{\hbar^2 \kappa(s)^2}{8m} ,$$

  where $\kappa(s)$ is the local geodesic curvature of the curve and s is the curvilinar abscissa (arclength) along the curve.
- Similarly, also for a particle constrained on a surface it appears a quantum-curvature potential.[25] In the case of the surface of an ellipsoid this quantum-curvature potential could strongly affect the quantum-thermal properties of a Bose gas.

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[24] LS, Bose-Einstein condensate in an elliptical waveguide, SciPost Phys. Core **5**, 015 (2022); Y. Nikolaieva, LS, and A. Yakimenko, arXiv:2306.11873.

[25] N.S. Moller, F.E.A. dos Santos, V.S. Bagnato, and A. Pelster, New. J. Phys. **22**, 063059 (2020).

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