Bosonic and fermionic atomic gases confined on the surface of a sphere

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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).

Quantum particle on the surface of a sphere (I)

Let us consider the single-particle Hamiltonian

$$\hat{H}_0 = -\frac{\hbar^2}{2m}\nabla^2 = -\frac{\hbar^2}{2m}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) - \frac{\hat{L}^2}{\hbar^2 r^2}\right] \quad (1)$$

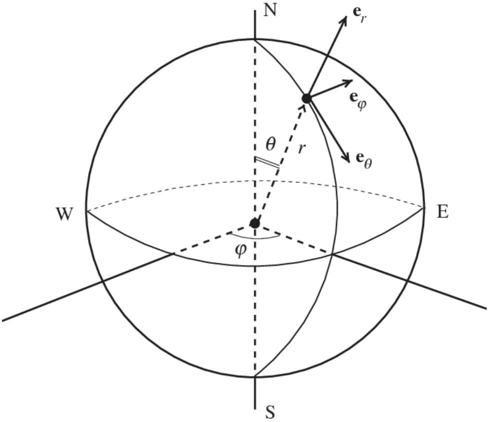
where $\hat{L}^2$ is the square of the orbital angular momentum operator. Under the assumption that the spherical radial coordinate r is fixed and given by

$$r = R \ , \quad (2)$$

the Hamiltonian becomes

$$\hat{H}_0 = \frac{\hat{L}^2}{2mR^2} \ . \quad (3)$$

Quantum particle on the surface of a sphere (II)



Spherical coordinates: radial coordinate $r \in [0, +\infty[$, polar angle $\theta \in [0, \pi]$, azimuthal angle $\phi \in [0, 2\pi]$. If the particle is constrained on the surface of the sphere, $r = R$, with R the radius of the sphere.

Quantum particle on the surface of a sphere (III)

Its eigenvalue problem reads

$$\hat{H}_0|l, m_l\rangle = \epsilon_l \, |l, m_l\rangle \tag{4}$$

because the eigenvalues of $\hat{L}^2$ are $\hbar^2 l(l+1)$ with

$$\epsilon_l = \frac{\hbar^2}{2mR^2} l(l+1) \; . \tag{5}$$

Thus, the energy of a particle of mass m moving on the surface of a sphere of radius R is quantized according to this formula where $l = 0, 1, 2, ...$ 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.

Ideal Bose gas (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

$$N = \sum_{l=0}^{+\infty} \frac{2l+1}{e^{(\epsilon_l - \mu)/(k_B T)} - 1} \,, \tag{6}$$

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

$$N = N_0 + \sum_{l=1}^{+\infty} \frac{2l+1}{e^{\epsilon_l/(k_B T)} - 1} \,, \tag{7}$$

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).

Ideal Bose gas (II)

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

$$n = n_0 + \frac{mk_B T}{2\pi\hbar^2}\left(\frac{\hbar^2}{mR^2 k_B T} - \ln\left(e^{\hbar^2/(mR^2 k_B T)} - 1\right)\right) , \qquad (8)$$

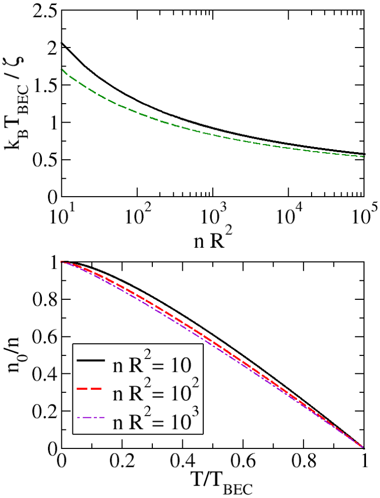
where $n = N/(4\pi R^2)$ is the 2D number density and $n_0 = N_0/(4\pi R^2)$ is the 2D condensate density.
At the critical temperature T_{BEC}, where $n_0 = 0$, one then finds[5]

$$k_B T_{BEC} = \frac{\frac{2\pi\hbar^2}{m} n}{\frac{\hbar^2}{mR^2 k_B T_{BEC}} - \ln\left(e^{\hbar^2/(mR^2 k_B T_{BEC})} - 1\right)} . \qquad (9)$$

As expected, in the limit $R \to +\infty$ one gets $T_{BEC} \to 0$, in agreement with the Mermin-Wagner theorem.[6] However, for any finite value of R the critical temperature T_{BEC} is larger than zero.

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

Ideal Bose gas (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}.

Ideal Fermi gas (I)

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

$$N = 2 \sum_{l=0}^{\infty} \frac{2l+1}{e^{(\epsilon_l - \mu)/(k_B T)} + 1} , \tag{10}$$

where k_B is the Boltzmann constant and μ is the chemical potential. We now use the Euler-MacLaurin formula

$$\sum_{l=0}^{\infty} f(l) = \int_0^{+\infty} dl \, f(l) + \frac{1}{2} f(0) - \frac{1}{12} \frac{df}{dl}(0) + \dots \tag{11}$$

In this way we get the number density

$$n = \frac{N}{4\pi R^2} = \frac{m k_B T}{\pi \hbar^2} \ln\left(1 + e^{\mu/(k_B T)}\right) + \frac{1}{6\pi R^2} \frac{e^{\mu/(k_B T)}}{\left(1 + e^{\mu/(k_B T)}\right)} + \dots \tag{12}$$

that is the familiar result of the 2D flat space plus finite-size corrections which depend on the radius R. As expected, in the thermodynamic limit $R \to +\infty$ only the flat term survives.

Ideal Fermi gas (II)

Notice that in the zero-temperature limit $T \to 0^+$ we have

$$n = \frac{m}{\pi\hbar^2}\mu + \frac{1}{6\pi R^2} + \dots , \tag{13}$$

namely (with $nR^2 \gg 1/(6\pi)$)

$$\mu = \frac{\pi\hbar^2 n}{m} - \frac{\hbar^2}{6mR^2} + \dots . \tag{14}$$

This is the Fermi energy of a two-component ideal Fermi gas with 2D number density n moving a the superface of a sphere of radius R. One can then derive many other thermodynamical quantities. For instance, the internal energy density at zero temperature reads

$$\frac{E}{4\pi R^2} = \int_0^n \mu(\tilde{n})\, d\tilde{n} = \frac{\pi\hbar^2 n^2}{2m} - \frac{\hbar^2 n}{6mR^2} + \dots . \tag{15}$$

Quantum particle near the surface of a sphere (I)

We now consider a quantum particle confined near the surface of a sphere. In particular, we adopt the following single-particle Hamiltonian

$$\hat{H}_0 = -\frac{\hbar^2}{2m}\nabla^2 + \frac{m}{2}\omega_\perp^2 (r - R)^2 \tag{16}$$

which contains an harmonic confinement in the radial direction with frequency $\omega_\perp$. This potential potential has a minimum for $r = R$ and it acts only perpendicularly to the surface of the sphere. As usual, the corresponding characteristic harmonic length is

$$\ell_\perp = \sqrt{\frac{\hbar}{m\omega_\perp}} \, . \tag{17}$$

Assuming that the frequency $\omega_\perp$ is quite large, we write the wavefunction of the quantum particle in spherical coordinates as

$$\Psi(r, \theta, \phi, t) = \chi(r)\,\psi(\theta, \phi, t) \, , \tag{18}$$

where

$$\chi(r) = \mathcal{N}\, e^{-(r-R)^2/(2\ell_\perp^2)} \, . \tag{19}$$

Quantum particle near the surface of a sphere (I)

Imposing that

$$\int_0^{+\infty} dr\, r^2\, |\chi(r)|^2 = 1 \tag{20}$$

we find

$$\mathcal{N} = \frac{1}{\pi^{1/4}\ell_\perp^{1/2} R} \tag{21}$$

in the regime $R \gg \ell_\perp$. Actually, in the same limit we also have

$$\frac{1}{\pi^{1/2}\ell_\perp} e^{-(r-R)^2/\ell_\perp^2} \to \delta(r-R)\ . \tag{22}$$

In other words,

$$|\chi(r)|^2 \to \frac{1}{R^2}\delta(r-R) \tag{23}$$

when $\ell_\perp \to 0^+$. This means that the square modulus of the radial wavefunction reduces to a Dirac delta function centered in $r = R$: in this limit the particle lives on the surface of a sphere.

Quantum particle near the surface of a sphere (II)

Starting from the imaginary-time (Euclidean) Lagrangian density

$$\mathscr{L}_0 = \Psi^*(r,\theta,\phi,\tau)\left(\hbar\frac{\partial}{\partial\tau} - \frac{\hbar^2}{2m}\nabla^2 + \frac{m}{2}\omega_\perp^2(r-R)^2 - \mu\right)\Psi(r,\theta,\phi,\tau) \tag{24}$$

and performing the decomposition described in the previous slides, after integrating over the radial coordinate r we get, in the limit $\ell_\perp \to 0^+$, the effective Lagrangian density on the surface of the sphere

$$\mathcal{L}_0 = \psi^*(\theta,\phi,\tau)\left(\hbar\frac{\partial}{\partial\tau} + \frac{\hat{L}^2}{2mR^2} - \mu_\parallel\right)\psi(\theta,\phi,\tau) \tag{25}$$

with

$$\mu_\parallel = \mu - \frac{\hbar^2}{2m\ell_\perp^2} \; . \tag{26}$$

Interacting bosons (I)

We now investigate a system of interacting bosons on the surface of a sphere of radius R and contact interaction of strength.
Adopting functional integration the grand canonical partition function $\mathcal{Z}$ reads

$$\mathcal{Z} = \int \mathcal{D}[\psi^*, \psi] \, e^{-\frac{S[\psi^*, \psi]}{\hbar}}, \tag{27}$$

where

$$S[\psi^*, \psi] = \int_0^{\hbar/(k_B T)} d\tau \int_0^{2\pi} d\varphi \int_0^{\pi} \sin(\theta) \, d\theta \, \mathcal{L}(\psi^*, \psi) \tag{28}$$

is the Euclidean action functional,

$$\mathcal{L} = \mathcal{L}_0 + \frac{g_{\parallel}}{2} |\psi(\theta, \varphi, \tau)|^4 \tag{29}$$

is the Euclidean Lagrangian density, with $\mathcal{L}_0$ given by Eq. (25) and

$$g_{\parallel} = \frac{g_{3D}}{\sqrt{2}\pi \ell_{\perp} R^2} \tag{30}$$

being g_{3D} the 3D contact interaction strength.

Interacting bosons (II)

By considering the bosonic partition function, within a perturbative scheme[7] one obtains[8] the following BEC critical temperature

$$k_B T_{BEC} = \frac{\frac{2\pi\hbar^2 n}{m} - \frac{g_{2D} n}{2}}{\frac{\hbar^2}{2mR^2 k_B T_{BEC}}\left(1+\sqrt{1+\frac{2g_{2D} mnR^2}{\hbar^2}}\right) - \ln\left(e^{\frac{\hbar^2}{mR^2 k_B T_{BEC}}\sqrt{1+\frac{2g_{2D} mnR^2}{\hbar^2}}} - 1\right)} \tag{31}$$

with

$$g_{2D} = g_{\parallel} R^2 = \frac{g_{3D}}{\sqrt{2}\pi\ell_{\perp}} \,. \tag{32}$$

This formula is a meaningful generalization of the one we have previously seen in the case of ideal bosons on the surface of a sphere, namely

$$k_B T_{BEC} = \frac{\frac{2\pi\hbar^2}{m} n}{\frac{\hbar^2}{mR^2 k_B T_{BEC}} - \ln\left(e^{\hbar^2/(mR^2 k_B T_{BEC})} - 1\right)} \,. \tag{33}$$

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

Interacting bosons (III)

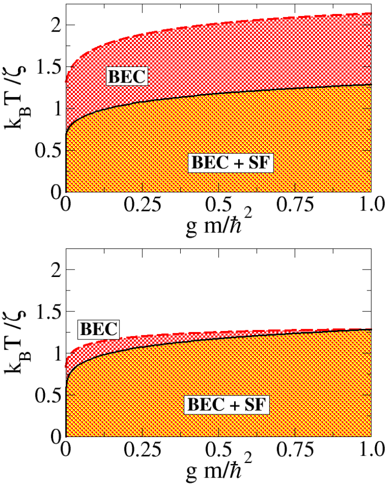
For the sake of completeness, we discuss the phase diagram[9] of the gas of bosons on the surface of a sphere by using the plane $(gm/\hbar^2, k_B T/\zeta)$, where $gm/\hbar^2$ is the adimensional interaction strength of bosons and $k_B T/\zeta$ is the adimensional temperature with $\zeta = \hbar^2 n/m$. Here $g = g_{2D}$.

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.

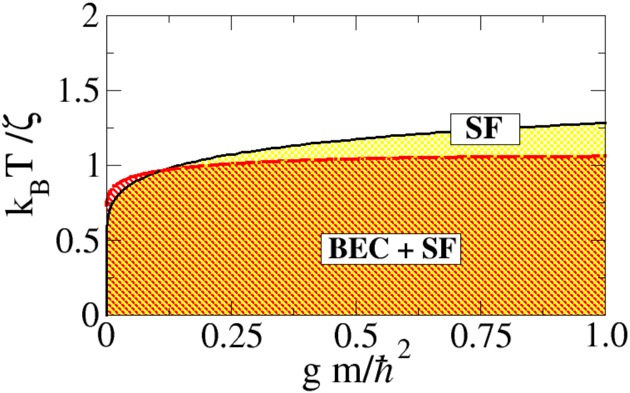
[9] A. Tononi and LS, Phys. Rev. Lett. **123**, 160403 (2019)

Interacting bosons (IV)



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). Here $g = g_{2D}$.

Interacting bosons (V)



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). Here $g = g_{2D}$.

Interacting fermions (I)

Currently we are studying the problem of two-spin-component interacting fermions moving on the surface of a sphere of radius R. The Euclidean action is given by

$$S[\bar{\psi}_\sigma, \psi_\sigma] = \int_0^{\hbar/(k_B T)} d\tau \int_0^{2\pi} d\varphi \int_0^{\pi} d\theta \, \sin(\theta) \, \mathcal{L}(\bar{\psi}_\sigma, \psi_\sigma) \tag{34}$$

where

$$\mathcal{L} = \sum_{\sigma=\uparrow,\downarrow} \bar{\psi}_\sigma \left(\hbar \frac{\partial}{\partial \tau} + \frac{\hat{L}^2}{2mR^2} - \mu_{\|} \right) \psi_\sigma + g_{\|} \bar{\psi}_\uparrow \bar{\psi}_\downarrow \psi_\downarrow \psi_\uparrow \tag{35}$$

with $\psi_\sigma(\theta, \phi, \tau)$ the Grassman field, which depends on the angular variables θ and ϕ, and also on the imaginary time τ.

Interacting fermions (II)

As in the case of bosons, also for fermions the grand canonical partition function $\mathcal{Z}$ can be written in the framework of functional integration as follows

$$\mathcal{Z} = \int \mathcal{D}[\bar{\psi}_\sigma, \psi_\sigma] \, e^{-\frac{S[\bar{\psi}_\sigma, \psi_\sigma]}{\hbar}} \tag{36}$$

where the functional integration involves the Berezin integral of Grassmann fields.

The grand potential is then given by

$$\Omega = -k_B T \, \ln(\mathcal{Z}) \,, \tag{37}$$

while the average number of fermions reads

$$N = -\left(\frac{\partial \Omega}{\partial \mu}\right)_{T,R} \,. \tag{38}$$

Interacting fermions (III)

Repulsive fermions can be investigated by using the Hartree-Fock approximation:

$$\bar{\psi}_{\uparrow}\bar{\psi}_{\downarrow}\psi_{\downarrow}\psi_{\uparrow} \simeq \frac{\tilde{n}}{2}\bar{\psi}_{\uparrow}\psi_{\uparrow} + \frac{\tilde{n}}{2}\bar{\psi}_{\downarrow}\psi_{\downarrow} - \frac{\tilde{n}^2}{4} \ , \tag{39}$$

assuming a balanced configuration

$$\frac{\tilde{n}}{2} = \tilde{n}_{\uparrow} = \tilde{n}_{\downarrow} \tag{40}$$

with

$$\tilde{n}_{\sigma} = \langle \bar{\psi}_{\sigma}\psi_{\sigma} \rangle \ . \tag{41}$$

In this way the Hartre-Fock Lagrangian Euclidean density is quadratic with respect to the fermionic fields

$$\mathcal{L}_{\rm HF} = \sum_{\sigma=\uparrow,\downarrow} \bar{\psi}_{\sigma} \left(\hbar \frac{\partial}{\partial \tau} + \frac{\hat{L}^2}{2mR^2} - \mu_{\parallel} + g_{\parallel}\frac{\tilde{n}}{2} \right) \psi_{\sigma} - g_{\parallel}\frac{\tilde{n}^2}{4} \tag{42}$$

and the corresponding Gaussian functional integrals can be exactly calculated. Notice that $n = \tilde{n}/R^2$.

Conclusions

- We have analyzed a quantum particle on (and near) the surface of a sphere[10].
- We have discussed the critical temperature T_{BEC} of Bose-Einstein condensation for **ideal bosons**, and also for **repulsive bosons** with contact interaction.
- We have investigated the thermodynamics of the **ideal Fermi** gas on the surface of a sphere, finding finite-size corrections which depend on the radius R of the sphere.
- For the sake of completeness we have illustrated[11] the phase diagram of the **interacting Bose** gas, characterized by Bose-Einstein condensation with or without superfluidity.
- We have also shown the Euclidean action functional of **interacting fermions** confined on the surface of a sphere.

[10] A. Tononi and LS, Nature Rev. Phys. **5**, 398 (2023).
[11] A. Tononi and LS, Phys. Reports **1072**, 1 (2024).

Acknowledgements

Thank you for your attention!