Beyond-mean-field functional integration for Bose-Einstein condensates

Andrea Tononi

Dipartimento di Fisica e Astronomia "Galileo Galilei" and CNISM, Universitá di Padova, Via Marzolo 8, I-35131 Padova, Italy

Abstract

Functional integration of a nonrelativistic scalar field is an elegant formulation of Quantum Field Theory to study the Thermodynamics of Bose-Einstein condensates, made with dilute ultracold atomic gases. In a beyond-mean-field approach one can derive the static and dynamical properties of a condensate confined in different geometries and with D-spatial dimensions. In particular, we have applied this method recently to calculate the condensate fraction and the superfluid one of a dilute Bose-Einstein condensate in three and in two dimensions. In another work, we have studied the condensation of an interacting Bose gas confined on a thin spherical shell, a work triggered by the forthcoming experiments with bubble traps in microgravity settings.

Contact informations

Andrea Tononi

andrea.tononi@phd.unipd.it

www.andreatononi.com

FUNCTIONAL INTEGRATION IN SHORT

The partition function $\mathcal{Z}$ represents the sum over all possible configurations of a system. If the system is described by a field $\psi(\vec{r}, t)$, we can "sum" over all the possible field configurations, defined for every $\vec{r}$ and t. Quantum mechanics emerges from the superposition of all possible field configurations, each one with its probability amplitude.

The method

Functional integration is a formulation of **Quantum Field Theory** which, within a beyond-mean-field approximation, allows us to calculate the **grand canonical partition function** $\mathcal{Z}$.

These are the main steps of our method:

1) Write $\mathcal{L}$
- Nonrelativistic field $\psi(\vec{r}, \tau)$
- Kinetic energy, chemical potential
  - Choose $V(\vec{r})$

2) SSB + BMF
- Spontaneous Symmetry Breaking of $U(1)$
  - Keep quadratic terms in fluctuation field

3) Calculate $\mathcal{Z}$
- Plane waves, spherical harmonics
  - Integrate quadratic fluctuation field

4) Thermodynamics
- Grand Potential Ω
- Pressure P
- Number density n
  - Condensate and superfluid densities n_0, n_s

Our aim is to investigate condensation (i.e. macroscopic occupation of the same single-particle state), and superfluidity (dissipationless flow) in ultracold atomic systems.

Functional integration

We consider a uniform D-dimensional Bose gas of identical cold atoms with mass m, described by the complex field $\psi(\vec{r}, \tau)$. The grand canonical partition function is [1]

$$\mathcal{Z} = \int D(\bar{\psi}, \psi) e^{-\frac{S[\bar{\psi},\psi]}{\hbar}}, \quad S[\bar{\psi}, \psi] = \int_0^{\beta\hbar} d\tau \int_{L^D} d^D r \mathcal{L},$$

$$\mathcal{L} = \bar{\psi}(\vec{r}, \tau)\left(\hbar\partial_\tau - \frac{\hbar^2\nabla^2}{2m} - \mu\right)\psi(\vec{r}, \tau) + \frac{1}{2}\int d^D r' \, |\psi(\vec{r}, \tau)|^2 \, V(\vec{r} - \vec{r}') \, |\psi(\vec{r}', \tau)|^2.$$

The superposition of a normal fluid current with velocity $\vec{v}_n$ and a superfluid current with velocity $\vec{v}_s$ can be introduced through

$$\partial_\tau \to \partial_\tau - i\vec{v}_n \cdot \vec{\nabla}, \qquad \psi(\vec{r}, \tau) \to e^{i\frac{m\vec{v}_s \cdot \vec{r}}{\hbar}}\psi(\vec{r}, \tau), \qquad (1)$$

and $\vec{v}_n = \vec{v}_s = \mathbf{0}$ recovers the description of static properties. The mean-field plus Gaussian approximation is given by

$$\psi(\vec{r}, \tau) = \psi_0 + \eta(\vec{r}, \tau) \qquad (2)$$

Performing the functional integration, we obtain the grand potential $\Omega = -\beta^{-1}\ln(\mathcal{Z})$ as

$$\Omega(\mu_e, \psi_0^2, T) = \underbrace{L^D\left(-\mu_e\psi_0^2 + \frac{1}{2}g_0\psi_0^4\right)}_{\Omega_0} + \underbrace{\frac{1}{2}\sum_{\vec{k}} E_{\vec{k}}(\psi_0^2)}_{\Omega_g^{(0)}} + \underbrace{\beta^{-1}\sum_{\vec{k}} \ln\left(1 - e^{-\beta(E_{\vec{k}}(\psi_0^2) + \hbar(\vec{v}_n - \vec{v}_s)\cdot\vec{k})}\right)}_{\Omega_g^{(T)}} \qquad (3)$$

where, using $\varepsilon_k = \hbar^2 k^2/(2m)$, we define the excitation spectrum

$$E_{\vec{k}}(\psi_0^2) = \sqrt{\left(\varepsilon_k - \mu_e + g_0\psi_0^2 + \psi_0^2 \, V(\vec{k})\right)^2 - (\psi_0^2 \, V(\vec{k}))^2} \qquad (4)$$

and the effective chemical potential $\mu_e = \mu - \frac{1}{2}m\vec{v}_s \cdot (\vec{v}_s - 2\vec{v}_n)$.

Two-dimensional equation of state

The zero-temperature equation of state connects the pressure $P = -\Omega/L^D$ and the chemical potential μ. In Ref. [3], we study the finite range interaction $V(k) = g_0 + g_2 k^2$ (in momentum space). With the superfluid parametrization $\psi = \sqrt{\rho_0 + \delta\rho}\, e^{i\theta}$, equivalent to Eq. 2, we derive the zero-temperature equation of state for a 2D homogeneous Bose gas

$$P(\mu, T=0) = \frac{m\mu^2}{8\pi\hbar^2\lambda^{3/2}}\left[\ln\left(\frac{\epsilon_0}{\mu}\lambda\right) - \frac{1}{2}\right], \qquad \text{with} \quad \lambda = 1 + \frac{4m\,\mu}{\hbar^2\, g_0}g_2,$$

which is obtained through a dimensional regularization procedure of the diverging grand potential $\Omega_g^{(0)}$. Here g_0 and g_2 can be linked with experimentally tunable parameters: the s-wave scattering length a_s, and the characteristic range of the interaction R_{ch}.

Finite-range corrections to the zero-temperature equation of state in 2D.

Bose-Einstein condensation on the surface of a sphere

The investigation of condensation on a 2D spherical surface is triggered by the experimental possibility to confine the atoms on a thin spherically-symmetric bubble trap. In Ref. [4], we write $\mathcal{L}$ for a Bose gas on the surface of a sphere with radius R. The fluctuation field η in Eq. (2) is decomposed in terms of spherical harmonics $\mathcal{Y}_{m_l}^l$, with the condensate state represented by the $l = 0$ term. The grand potential is formally the same of Eq. (3), with $\epsilon_k \to \epsilon_l = \hbar^2 l(l+1)/(2mR^2)$ in the excitation spectrum, and we consider the zero-range interaction $V(r) = g\delta(r)$. We calculate the critical temperature T_{BEC} for interacting bosons confined on a thin spherical shell

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

and the condensate fraction n_0/n

$$\frac{n_0}{n} = 1 - \frac{mg}{4\pi\hbar^2} - \frac{1}{4\pi R^2 n}\left[1 + \sqrt{1 + \frac{2gmnR^2}{\hbar^2}}\right] + \frac{mk_B T}{2\pi\hbar^2 n}\ln\left(e^{\frac{\hbar^2}{mR^2 k_B T}\sqrt{1+\frac{2gmnR^2}{\hbar^2}}} - 1\right).$$

We also investigate the Berezinski-Kosterlitz-Thouless (BKT) transition driven by vortical configurations on the surface of the sphere. The finite-size phase diagram of the transition is represented in Fig. 1.

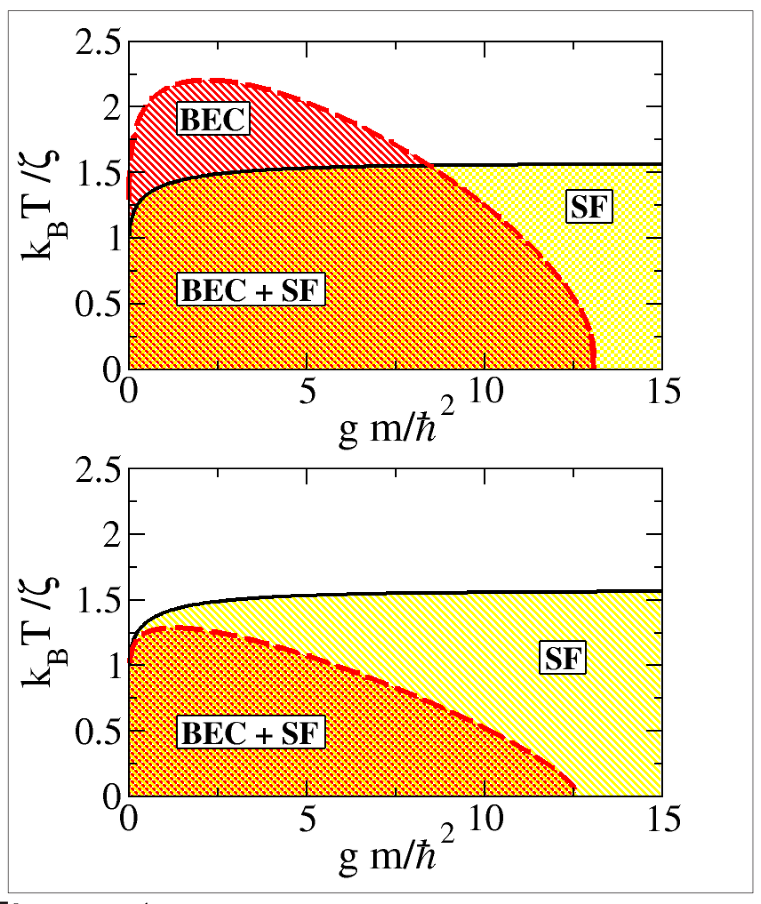

Figure 1. Phase diagram of a shell-shaped condensate with $nR^2 = 10^2$ (upper panel), and $nR^2 = 10^4$ (lower panel). The black curve represents the critical temperature for BKT transition: notice the interplay of Bose-Einstein condensation (BEC) and superfluidity (SF).

These results are of interest for the experiments with bubble traps in the thin-shell limit on the Cold Atom Laboratory in the ISS.

Condensation and superfluidity in D dimensions

We calculate the number density n as a function of condensate density n_0 and T as

$$n(n_0, T) = -\frac{1}{L^D}\frac{\partial\Omega(\mu_e, \psi_0, T)}{\partial\mu_e}\bigg|_{\mu_e = g_0 n_0} = n_0 + f_g^{(0)}(n_0) + f_g^{(T)}(n_0)$$

while the superfluid density $n_s = n(n_0, T) - n_n(n_0, T)$, with n_n the normal density, is obtained from the momentum density of the fluid

$$\vec{\mathcal{P}} = -\frac{1}{L^D}\frac{\partial\Omega(\mu_e, \psi_0)}{\partial\vec{v}_n}\bigg|_{\mu_e = g_0 n_0} = n_s(n_0, T)\, m\vec{v}_s + n_n(n_0, T)\, m\vec{v}_n$$

For the finite-range effective interaction $V(k) = g_0 + g_2 k^2$ we calculate [2] in 3D and in 2D:

Finite-range corrections to n_0/n

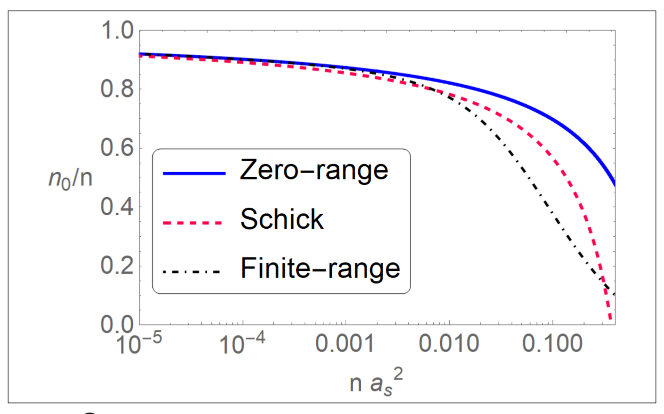

Figure 2. 2D condensate fraction n_0/n at $T = 0$ and $R_{ch} = 2a_s$, in terms of the gas parameter na_s^2.

Finite-range corrections to n_s/n

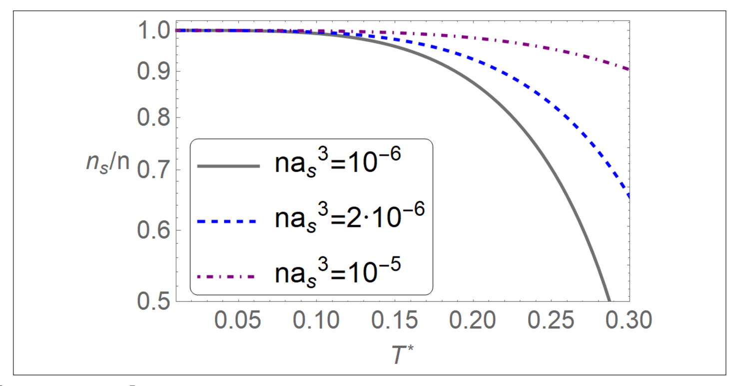

Figure 4. 3D superfluid fraction n_s/n for $r_{eff} = a_s$, as a function of the rescaled temperature $T^* = k_B T/E_r$, where $E_r = \hbar^2 n^{2/3}/m$.

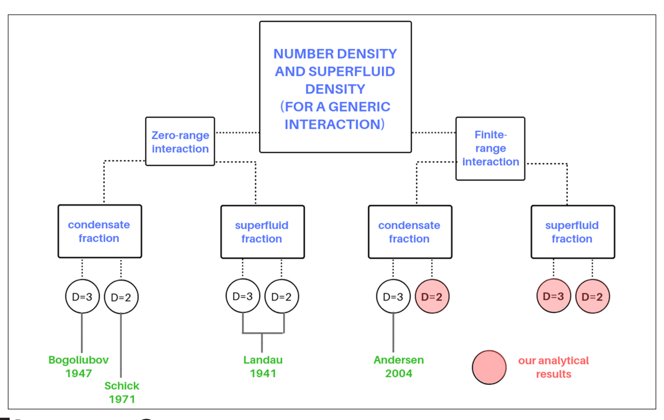

Figure 3. Flowchart diagram of our results.

The finite-range corrections to the condensate fraction n_0/n and to the superfluid fraction n_s/n can be detected in $D = 3$ in the regime $a_s/r_e \leq 1$ and in $D = 2$ for $a_s/R_{ch} \leq 1$ but not where they are much lower than 1. In that case, the higher order terms which we are neglecting in the gradient expansion of the interaction potential become relevant.

Bibliography

[1] N. Nagaosa, *Quantum Field Theory in Condensed Matter Physics* (Springer 1999).

[2] A. Tononi, A. Cappellaro, L. Salasnich, Condensation and superfluidity of dilute Bose gases with finite-range interaction, New Journal of Physics, **20**, 125007 (2018).

[3] A. Tononi, Zero-Temperature Equation of State of a Two-Dimensional Bosonic Quantum Fluid with Finite-Range Interaction, Condensed Matter **4**, 20 (2019).

[4] A. Tononi, L. Salasnich, Bose-Einstein condensation on the surface of a sphere, arXiv:1903.08453 (2019).