Beyond mean-field and finite-range effects in ultracold atomic bosons

Luca Salasnich

Dipartimento di Fisica e Astronomia "Galileo Galilei" and CNISM, Università di Padova
INO-CNR, Research Unit of Sesto Fiorentino, Consiglio Nazionale delle Ricerche

Natal, November 14, 2016

Work done in collaboration with
Alberto Cappellaro and Flavio Toigo

Summary

- Partition function of interacting bosons
- Bosons with contact interaction: mean-field
- Bosons with contact interaction: beyond mean-field
- Bosons with finite-range effects: mean-field
- Bosons with finite-range effects: beyond mean-field
- Conclusions

Partition function and functional integration (I)

Let us consider a gas of interacting bosons at temperature T. The grand-canonical partition function $\mathcal{Z}$ is given by[1]

$$\mathcal{Z} = Tr[e^{-\beta(\hat{H}-\mu\hat{N})}] \tag{1}$$

where $\beta = 1/(k_B T)$ with k_B the Boltzmann constant,

$$\begin{aligned} \hat{H} &= \int d^3\mathbf{r}\ \hat{\psi}^+(\mathbf{r})\Big(-\frac{\hbar^2}{2m}\nabla^2 + U(\mathbf{r})\Big)\hat{\psi}(\mathbf{r}) \\ &+ \frac{1}{2}\int d^3\mathbf{r}\ d^3\mathbf{r}'\ \hat{\psi}^+(\mathbf{r})\ \hat{\psi}^+(\mathbf{r}')\ V(\mathbf{r},\mathbf{r}')\ \hat{\psi}(\mathbf{r}')\ \hat{\psi}(\mathbf{r}) \end{aligned} \tag{2}$$

is the Hamiltonian of the bosonic quantum field operator $\hat{\psi}(\mathbf{r})$, with $U(\mathbf{r})$ the confining external potential, $V(\mathbf{r},\mathbf{r}')$ the inter-particle interaction, and the number operator reads

$$\hat{N} = \int d^3\mathbf{r}\ \hat{\psi}^+(\mathbf{r})\hat{\psi}(\mathbf{r})\ . \tag{3}$$

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

Partition function and functional interation (II)

The partition function $\mathcal{Z}$ can be re-written as[2]

$$\mathcal{Z} = \int \mathcal{D}[\psi, \psi^*] \ \exp\left\{ -\frac{S[\psi, \psi^*]}{\hbar} \right\} , \tag{4}$$

where

$$S[\psi, \psi^*] = \int_0^{\hbar\beta} d\tau \int d^3\mathbf{r} \, \mathcal{L}(\psi^*, \psi) \tag{5}$$

is the Euclidean action of the complex classical field $\psi(\mathbf{r}, \tau)$ with Lagrangian density

$$\begin{aligned} \mathcal{L}(\psi^*, \psi) &= \psi^*(\mathbf{r}, \tau)\Big(\hbar \frac{\partial}{\partial \tau} - \frac{\hbar^2}{2m}\nabla^2 + U(\mathbf{r}) - \mu\Big)\psi(\mathbf{r}, \tau) \\ &+ \frac{1}{2}\int d^3\mathbf{r}' \ |\psi(\mathbf{r}', \tau)|^2 \, V(\mathbf{r}, \mathbf{r}') \, |\psi(\mathbf{r}, \tau)|^2 \end{aligned} \tag{6}$$

where $\quad \psi(\mathbf{r}, 0) = \psi(\mathbf{r}, \hbar\beta) \quad$ and $\quad \int \mathcal{D}[\psi, \psi^*] = \prod_{(\mathbf{r},\tau)} \int \frac{d\psi^*(\mathbf{r}, \tau) \, d\psi(\mathbf{r}, \tau)}{2\pi i} .$

$$\tag{7}$$

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

Bosons with contact interaction: mean-field (I)

We consider a D-dimensional ($D = 1, 2, 3$) Bose gas of ultracold and dilute neutral atoms with a contact interaction, namely

$$V(\mathbf{r} - \mathbf{r}') = g\,\delta(\mathbf{r} - \mathbf{r}')\ , \tag{8}$$

where $\delta(x)$ is the Dirac delta function and g the strengh of the intraction. We adopt the path integral formalism, where the atomic bosons are described by the complex field $\psi(\mathbf{r}, \tau)$.

The Euclidean Lagrangian density of the free system, i.e. $U(\mathbf{r}) = 0$, in a D-dimensional box of volume L^D and with chemical potential μ is given by

$$\mathcal{L} = \psi^* \left[\hbar\partial_\tau - \frac{\hbar^2}{2m}\nabla^2 - \mu\right]\psi + \frac{1}{2}\,g\,|\psi|^4\ , \tag{9}$$

where g is the strength of the contact inter-atomic coupling.

Bosons with contact interaction: mean-field (II)

In this case one finds immediately the partition function of the uniform and constant order parameter ψ_0 as

$$\mathcal{Z}_0 = \exp\left\{-\frac{S_0}{\hbar}\right\} = \exp\left\{-\beta\,\Omega_0\right\} , \qquad (10)$$

where $S_0 = S[\psi_0]$ and the grand potential Ω_0 reads

$$\frac{\Omega_0}{L^D} = -\mu\,\psi_0^2 + \frac{1}{2}\,g\,\psi_0^4 . \qquad (11)$$

See the figure in the next slide.

Bosons with contact interaction: mean-field (III)

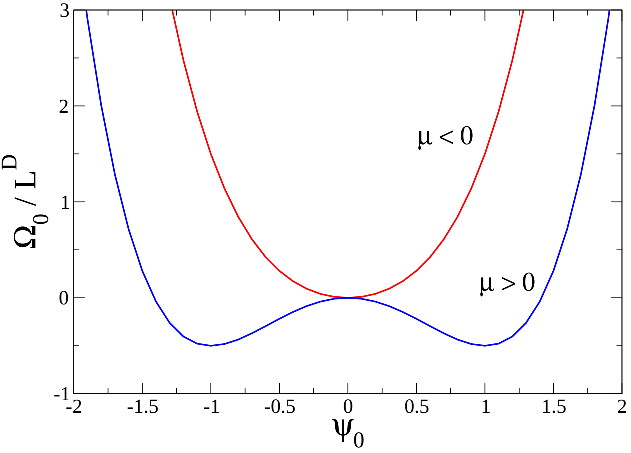

Figure: Mean-field grand potential Ω_0 as a function of the real order parameter ψ_0 for an interacting Bose gas, see Eq. (11). Adapted from LS and F. Toigo, Phys. Rep. **640**, 1 (2016).

Bosons with contact interaction: mean-field (IV)

Again, the constant, uniform and real order parameter ψ_0 is obtained by minimizing Ω_0 as

$$\left(\frac{\partial \Omega_0}{\partial \psi_0}\right)_{\mu,T,L^D} = 0 \; , \tag{12}$$

from which one finds the relation between order parameter and chemical potential

$$\mu = g\,\psi_0^2 \; . \tag{13}$$

showing that in the superfluid broken phase the chemical potential is positive and

$$\psi_0 = \sqrt{\frac{\mu}{g}} \; , \tag{14}$$

Inserting this relation into Eq. (11) we find

$$\frac{\Omega_0}{L^D} = -\frac{\mu^2}{2\,g} \; . \tag{15}$$

Clearly, this mean-field equation of state is lacking important informations encoded in quantum and thermal fluctuations.

Bosons with contact interaction: beyond mean-field (I)

To take into accout quantum and thermal fluctuations we write[3]

$$\psi(\mathbf{r},\tau) = \psi_0 + \eta(\mathbf{r},\tau) \ , \tag{16}$$

$\eta(\mathbf{r},\tau)$ is the complex field of bosonic fluctuations around the order parameter ψ_0 of the system.
We expand the action $S[\psi,\psi^*]$ around ψ_0 up to quadratic (Gaussian) order in $\eta(\mathbf{r},\tau)$ and $\bar{\eta}(\mathbf{r},\tau)$. We find

$$Z = Z_0 \int \mathcal{D}[\eta,\eta^*] \ \exp\left\{ - \frac{S_g[\eta,\eta^*]}{\hbar} \right\} , \tag{17}$$

where

$$S_g[\eta,\eta^*] = \frac{1}{2} \sum_Q (\eta^*_Q, \eta_{-Q}) \ \mathbf{M}_Q \begin{pmatrix} \eta_Q \\ \eta^*_{-Q} \end{pmatrix} \tag{18}$$

is the Gaussian action of fluctuations in reciprocal space with $Q = (\mathbf{q}, i\omega_n)$ the $D+1$ vector denoting the momenta $\mathbf{q}$ and bosonic Matsubara frequencies $\omega_n = 2\pi n/(\beta\hbar)$, and

[3] LS and F. Toigo, Phys. Rep. **640**, 1 (2016).

Bosons with contact interaction: beyond mean-field (II)

$$\mathbf{M}_Q = \beta \begin{pmatrix} -i\hbar\omega_n + \frac{\hbar^2 q^2}{2m} - \mu + 2g\psi_0^2 & -g\psi_0^2 \\ -g\psi_0^2 & i\hbar\omega_n + \frac{\hbar^2 q^2}{2m} - \mu + 2g\psi_0^2 \end{pmatrix} \quad (19)$$

is the inverse fluctuation propagator.
Integrating over the bosonic fields $\eta(Q)$ and $\bar{\eta}(Q)$ in Eq. (17) one finds the Gaussian grand potential

$$\begin{aligned} \Omega_g &= \frac{1}{2\beta} \sum_Q \ln \mathrm{Det}(\mathbf{M}_Q) \\ &= \frac{1}{2\beta} \sum_{\mathbf{q}} \sum_{n=-\infty}^{+\infty} \ln\left[\beta^2(\hbar^2\omega_n^2 + E_q^2)\right] , \end{aligned} \quad (20)$$

where E_q is given by

$$E_q = \sqrt{\left(\frac{\hbar^2 q^2}{2m} - \mu + 2g\psi_0^2\right)^2 - g^2\psi_0^4} \,. \quad (21)$$

Bosons with contact interaction: beyond mean-field (III)

By using $\psi_0 = \sqrt{\mu/g}$ the spectrum becomes

$$E_q = \sqrt{\frac{\hbar^2 q^2}{2m}\left(\frac{\hbar^2 q^2}{2m} + 2\mu\right)} \simeq c_B\,\hbar q \quad \text{for small } q\ , \tag{22}$$

which is the familiar Bogoliubov spectrum, with $c_B = \sqrt{\mu/m}$.

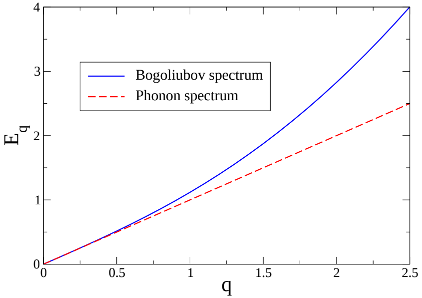

Figure: Bogoliubov spectrum, given by Eq. (22), and its low-momentum phonon spectrum $E_q = c_B\,\hbar q$, where $c_B = \sqrt{\mu/m}$ is the sound velocity. Energy E_q in units of μ and momentum q in units of $\sqrt{m\mu/\hbar^2}$. Adapted from LS and F. Toigo, Phys. Rep. **640**, 1 (2016).

Bosons with contact interaction: beyond mean-field (IV)

Again, the sum over bosonic Matsubara frequencies gives

$$\frac{1}{2\beta}\sum_{n=-\infty}^{+\infty}\ln\left[\beta^2(\hbar^2\omega_n^2+E_q^2)\right]=\frac{E_q}{2}+\frac{1}{\beta}\ln\left(1-e^{-\beta E_q}\right). \tag{23}$$

The total grand potential may then be written as

$$\Omega=\Omega_0+\Omega_g^{(0)}+\Omega_g^{(T)}, \tag{24}$$

where Ω_0 is given by Eq. (15).

$$\Omega_g^{(0)}=\frac{1}{2}\sum_{\mathbf{q}}E_q \tag{25}$$

is the zero-point energy of bosonic collective excitations, i.e. the zero-temperature contribution of quantum Gaussian fluctuations, while

$$\Omega_g^{(T)}=\frac{1}{\beta}\sum_{\mathbf{q}}\ln\left(1-e^{-\beta E_q}\right) \tag{26}$$

takes into account thermal Gaussian fluctuations.

Bosons with contact interaction: beyond mean-field (V)

We notice that the continuum limit of the zero-point energy for the interacting Bose gas

$$\frac{\Omega_g^{(0)}}{L^D} = \frac{1}{2}\frac{S_D}{(2\pi)^D}\int_0^{+\infty} dq\ q^{D-1}\sqrt{\frac{\hbar^2 q^2}{2m}\left(\frac{\hbar^2 q^2}{2m}+2\mu\right)} \tag{27}$$

is ultraviolet divergent at any integer dimension D.
We may rewrite Eq. (27) for the zero point energy of a repulsive Bose gas in dimension D as:

$$\frac{\Omega_g^{(0)}}{L^D} = \frac{S_D(2\mu)^{\frac{D}{2}+1}}{4(2\pi)^D}\left(\frac{2m}{\hbar^2}\right)^{\frac{D}{2}} B\left(\frac{D+1}{2}, -\frac{D+2}{2}\right), \tag{28}$$

where $B(x,y)$ is the Euler Beta function

$$B(x,y) = \int_0^{+\infty} dt \frac{t^{x-1}}{(1+t)^{x+y}}, \qquad Re(x), Re(y) > 0 \tag{29}$$

which may be continued to complex values of x and y as

$$B(x,y) = \frac{\Gamma(x)\,\Gamma(y)}{\Gamma(x+y)}. \tag{30}$$

Bosons with contact interaction: beyond mean-field (VI)

We rewrite Eq. (27) using Eq. (30) to get

$$\frac{\Omega_g^{(0)}}{L^D} = \frac{S_D (2\mu)^{\frac{D}{2}+1}}{4(2\pi)^D} \left(\frac{2m}{\hbar^2}\right)^{\frac{D}{2}} \frac{\Gamma(\frac{D+1}{2})\,\Gamma(-\frac{D+2}{2})}{\Gamma(-\frac{1}{2})} \; . \tag{31}$$

This expression is now finite when $D = 1$ or $D = 3$, while it is still divergent if $D = 2$ since $\Gamma(p)$ diverges for integers $p \leq 0$. In particular, setting $D = 3$ in Eq. (31) we get

$$\frac{\Omega_g^{(0)}}{L^3} = \frac{8}{15\pi^2} (\frac{m}{\hbar^2})^{3/2} \mu^{5/2} \; . \tag{32}$$

In conclusion, the total grand potential of the three-dimensional Bose gas is then given by[4]

$$\frac{\Omega}{L^3} = -\frac{\mu^2}{2\,g} + \frac{8}{15\pi^2} (\frac{m}{\hbar^2})^{3/2} \mu^{5/2} + \frac{1}{\beta L^3} \sum_{\mathbf{q}} \ln\left(1 - e^{-\beta E_q}\right) \; . \tag{33}$$

[4] LS and F. Toigo, Phys. Rep. **640**, 1 (2016).

Bosons with contact interaction: beyond mean-field (VII)

At zero temperature the beyond-mean-field pressure P is then[5]

$$P = -\frac{\Omega}{L^3} = \frac{\mu^2}{2\,g} - \frac{8}{15\pi^2}(\frac{m}{\hbar^2})^{3/2}\mu^{5/2} \, . \tag{34}$$

Remarkaly, P becomes unphysical ($P < 0$) at very large μ. The corresponding zero-temperature number density n reads

$$n = \frac{\partial P}{\partial \mu} = \frac{\mu}{g} - \frac{4}{3\pi^2}(\frac{m}{\hbar^2})^{3/2}\mu^{3/2} \, . \tag{35}$$

This formula can be inverted perturbatively giving

$$\mu = gn \left(1 + \frac{4}{3\pi^2}(\frac{m}{\hbar^2})^{3/2} g (gn)^{1/2} \right) \, , \tag{36}$$

that is the familiar beyond-mean-field equation of state.[6]

---

[5] T.D. Lee and C.N. Yang, Phys. Rev. **117**, 12 (1960).

[6] Lee D.T., K. Huang and C.N. Yang, Phys. Rev. **106**, 1135 (1957).

Bosons with contact interaction: beyond mean-field (VIII)

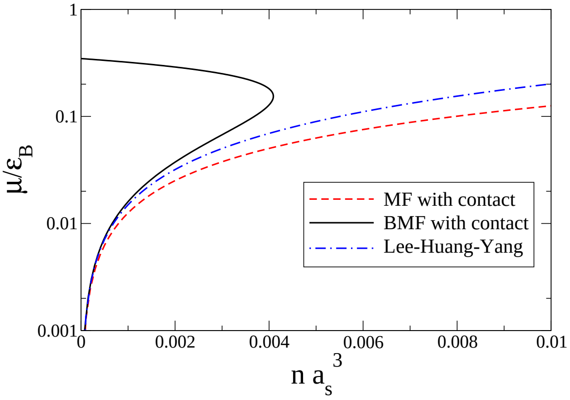

Figure: Chemical potential μ vs gas parameter na_s^3 for a 3D Bose gas with contact repulsive interaction $g = 4\pi\hbar^2 a_s/m$, with a_s is the s-wave scattering length. Solid line is the result of our zero-temperature Gaussian theory. Dot-dashed line is the Lee-Huang-Yang formula, that is a perturbative approximation of the Gaussian theory. Here $\epsilon_B = \hbar^2/(ma_s^2)$ is the characteristic energy of the interacting Bose gas and n is the number density.

Bosons with finite-range effects: mean-field (I)

Let us now consider again a generic finite-range inter-atomic potential between bosons. The Lagrangian density can be written as

$$\mathcal{L}(\psi^*,\psi) = \psi^*(\mathbf{r},\tau)\Big(\hbar\frac{\partial}{\partial\tau} - \frac{\hbar^2}{2m}\nabla^2 + U(\mathbf{r}) + \frac{1}{2}U_{NL}(\mathbf{r},\tau) - \mu\Big)\psi(\mathbf{r},\tau)\ , \quad (37)$$

where

$$U_{NL}(\mathbf{r},\tau) = \int d^3\mathbf{r}'\, |\psi(\mathbf{r}',\tau)|^2\, V(|\mathbf{r}-\mathbf{r}'|)\ . \quad (38)$$

By substituting $\mathbf{r}' = \mathbf{r} + \mathbf{s}$ and developing $\psi(\mathbf{r}+\mathbf{s},\tau)$ in powers of $\mathbf{s}$ one gets at the second order

$$|\psi(\mathbf{r}',\tau)|^2 = |\psi(\mathbf{r},\tau)|^2 + \sum_{i=x,y,z} s_i\partial_i|\psi(\mathbf{r},\tau)|^2 + \frac{1}{2}\sum_{i,j=x,y,z} s_i s_j \partial^2_{ij}|\psi(\mathbf{r},\tau)|^2$$

and consequently

$$U_{NL}(\mathbf{r},\tau) = g|\psi(\mathbf{r},\tau)|^2 - g_2\nabla^2|\psi(\mathbf{r},\tau)|^2\ , \quad (39)$$

where

$$g = \int d^3\mathbf{s}\, V(|\mathbf{s}|) \qquad \text{and} \qquad g_2 = -\frac{1}{2}\int d^3\mathbf{s}\, s^2\, V(|\mathbf{s}|)\ , \quad (40)$$

because $\int d^3\mathbf{s}\ s_i s_j V(|\mathbf{s}|)$ is different from zero only if $i = j$.

Bosons with finite-range effects: mean-field (II)

Thus, the local Lagrangian density of our effective field theory reads

$$\begin{aligned}\mathcal{L} &= \psi^*(\mathbf{r},\tau)\left[\hbar\partial_\tau - \frac{\hbar^2}{2m}\nabla^2 + U(\mathbf{r}) - \mu\right]\psi(\mathbf{r},\tau) \\ &+ \frac{g}{2}|\psi(\mathbf{r},\tau)|^4 - \frac{g_2}{2}|\psi(\mathbf{r},\tau)|^2\left(\nabla^2|\psi(\mathbf{r},\tau)|^2\right) .\end{aligned} \tag{41}$$

Clearly, setting $g_2 = 0$ one recovers the theory with contact interaction. It is well know that, in three dimensions,

$$g = \frac{4\pi\hbar^2}{m} a_s \tag{42}$$

with a_s the s-wave scattering length. Moreover, the parameter g_2 is ralated to s-wave scattering length a_s and to effective range r_s of the true inter-atomic potential by[7]

$$g_2 = \frac{2\pi\hbar^2}{m} a_s^2\ r_s\ . \tag{43}$$

[7] E. Braaten and A. Nieto, Phys. Rev. B **55**, 8090 (1997).

Bosons with finite-range effects: mean-field (III)

Mean-field results are obtained performing the saddle-point approximation, namely by considering the mean-field partition function

$$\mathcal{Z}_0 = \exp\left\{ -\frac{S[\psi_0, \psi_0^*]}{\hbar} \right\} , \tag{44}$$

where the stationary field $\psi_0(\mathbf{r})$ is obtained from

$$\delta S[\psi_0, \psi_0^*] = 0 , \tag{45}$$

which gives the Euler-Lagrange equation

$$\Big[-\frac{\hbar^2}{2m}\nabla^2 + g|\psi_0(\mathbf{r})|^2 - g_2 \left(\nabla^2|\psi_0(\mathbf{r})|^2\right)\Big]\psi_0(\mathbf{r}) = \mu\ \psi_0(\mathbf{r}) . \tag{46}$$

This is the so-called modified Gross-Pitaevskii equation,[8] which contains a gradient correction proportional to g_2 with respect to the familiar Gross-Pitaevskii equation.

[8] H. Fu, Y. Wang, and B. Gao, Phys. Rev. A **67**, 053612 (2003); H. Veksler, S. Fishman, and W. Ketterle, Phys. Rev. A **90**, 023620 (2014).

Bosons with finite-range effects: mean-field (IV)

We consider a uniform and real scalar field ψ_0. Under this condition we find immediately

$$\mu = g\,\psi_0^2 \tag{47}$$

and

$$\frac{\Omega_0}{L^3} = -\mu\,\psi_0^2 + \frac{1}{2} g\,\psi_0^4 \tag{48}$$

with L^3 the volume of the uniform system. Inserting Eq. (47) into Eq. (48) we find

$$\frac{\Omega_0}{L^3} = -\frac{\mu^2}{2g}\ . \tag{49}$$

Clearly this mean-field equation of state does not depend only on g_2. Effective-range effects are absent in the uniform system at the mean-field level.

Bosons with finite-range effects: beyond mean-field (I)

The mean-field (saddle-point) approximation lacks important informations encoded in quantum and thermal fluctuations. As previously pointed out, the main goal of this paper is to take into account nonlocal effect in these fluctuations. To this end we set

$$\psi(\mathbf{r},\tau) = \psi_0(\mathbf{r}) + \eta(\mathbf{r},\tau) \tag{50}$$

and expand the action $S[\psi,\psi^*]$ of Eq. (5) around $\psi_0(\mathbf{r})$ up to quadratic (Gaussian) order in $\eta(\mathbf{r},\tau)$ and $\eta^*(\mathbf{r},\tau)$. This is the so-called one-loop approximation. We find

$$Z = Z_0 \int \mathcal{D}[\tilde{\eta},\tilde{\eta}^*] \ \exp\left\{-\frac{S_g[\tilde{\eta},\tilde{\eta}^*]}{\hbar}\right\}, \tag{51}$$

where

$$S_g[\tilde{\eta},\tilde{\eta}^*] = \frac{1}{2}\sum_Q (\tilde{\eta}^*(Q),\tilde{\eta}(-Q)) \ \mathbf{M}(Q) \begin{pmatrix} \tilde{\eta}(Q) \\ \tilde{\eta}^*(-Q) \end{pmatrix} \tag{52}$$

is the Gaussian action of fluctuations in reciprocal space and $\mathbf{M}(Q)$ is the inverse fluctuation propagator.

Bosons with finite-range effects: beyond mean-field (II)

The matrix $\mathbf{M}(Q)$ is strongly simplified if $U(\mathbf{r}) = 0$ and ψ_0 is uniform. In this case, taking into account Eq. (47), the matrix reads

$$\mathbf{M}(Q) = \beta \begin{pmatrix} -i\hbar\omega_n + \frac{\hbar^2 q^2}{2m} - \mu + A & \psi_0^2 \, \tilde{V}_{EFT}(q) \\ \psi_0^2 \, \tilde{V}_{EFT}(q) & i\hbar\omega_n + \frac{\hbar^2 q^2}{2m} - \mu + A \end{pmatrix} \tag{53}$$

where $A = \psi_0^2 (g + \tilde{V}_{EFT}(q))$ and $\tilde{V}_{EFT}(q)$ given by

$$\tilde{V}_{EFT}(q) = g + g_2 \, q^2 \; . \tag{54}$$

Clearly the term proportional to g_2 gives a finite-range correction of the contact term proportional to g.

Bosons with finite-range effects: beyond mean-field (III)

Integrating over the bosonic fields $\tilde{\eta}(Q)$ and $\tilde{\eta}^*(Q)$ we obtain the Gaussian grand potential

$$\Omega_g = \frac{1}{2\beta}\sum_Q \ln \mathrm{Det}(\mathbf{M}(Q)) = \frac{1}{2\beta}\sum_{\mathbf{q}}\sum_{n=-\infty}^{+\infty} \ln\left[\beta^2(\hbar^2\omega_n^2 + E_{\mathbf{q}}^2)\right] , \quad (55)$$

where $E_{\mathbf{q}}$ is the Bogoliubov spectrum

$$E_{\mathbf{q}} = \sqrt{\left(\frac{\hbar^2 q^2}{2m} - \mu + \psi_0^2\left(g + \tilde{V}_{EFT}(q)\right)\right)^2 - \psi_0^4\tilde{V}_{EFT}(q)^2} . \quad (56)$$

By using $\mu = g\psi_0^2$ (order-parameter equation) one obtains a familiar form for the Bogoliubov spectrum, i.e.

$$E_{\mathbf{q}} = \sqrt{\frac{\hbar^2 q^2}{2m}\left(\frac{\hbar^2 q^2}{2m} + 2\frac{\mu}{g}\tilde{V}_{EFT}(q)\right)} . \quad (57)$$

Bosons with finite-range effects: beyond mean-field (IV)

The sum over bosonic Matsubara frequencies gives

$$\frac{1}{2\beta}\sum_{n=-\infty}^{+\infty}\ln\left[\beta^2(\hbar^2\omega_n^2+E_{\mathbf{q}}^2)\right]=\frac{E_{\mathbf{q}}}{2}+\frac{1}{\beta}\ln\left(1-e^{-\beta E_{\mathbf{q}}}\right)\,, \tag{58}$$

and the total grand potential may then be written as

$$\Omega=-\frac{\mu^2}{2g}+\Omega_g^{(0)}+\Omega_g^{(T)}\,, \tag{59}$$

where

$$\Omega_g^{(0)}=\frac{1}{2}\sum_{\mathbf{q}}E_{\mathbf{q}} \tag{60}$$

is the zero-point energy of bosonic collective excitations, i.e. the zero-temperature contribution of quantum Gaussian fluctuations, while

$$\Omega_g^{(T)}=\frac{1}{\beta}\sum_{\mathbf{q}}\ln\left(1-e^{-\beta E_{\mathbf{q}}}\right) \tag{61}$$

takes into account thermal Gaussian fluctuations.

Bosons with finite-range effects: beyond mean-field (V)

Taking into account explicitly that $\tilde{V}_{EFT}(q) = g + g_2\, q^2$ the Bogoliubov spectrum can be written

$$E_q = \sqrt{\frac{\hbar^2 q^2}{2m}\left((1+\chi\mu)\frac{\hbar^2 q^2}{2m} + 2\mu\right)}\,, \tag{62}$$

where

$$\chi = \frac{4m}{\hbar^2}\frac{g_2}{g} \tag{63}$$

takes into account finite-range effects of the inter-atomic potential.
The zero-temperature Gaussian grand potential

$$\frac{\Omega_g^{(0)}}{L^3} = \frac{1}{4\pi^2}\int_0^\infty dq\, q^2\, E_q \tag{64}$$

is ultraviolet divergent with E_q given by Eq. (62). Performing, as before, dimensional regularization, we get the regularized grand potential

$$\frac{\Omega_g^{(0)}}{L^3} = \frac{8}{15\pi^2}\left(\frac{m}{\hbar^2}\right)^{3/2}\frac{\mu^{5/2}}{(1+\chi\mu)^2}\,. \tag{65}$$

Bosons with finite-range effects: beyond mean-field (VI)

At zero temperature the beyond-mean-field pressure P is then

$$P = -\frac{\Omega}{L^3} = \frac{\mu^2}{2\,g} - \frac{8}{15\pi^2}(\frac{m}{\hbar^2})^{3/2}\frac{\mu^{5/2}}{(1+\chi\mu)^2} \ . \tag{66}$$

The corresponding zero-temperature number density n reads

$$n = \frac{\partial P}{\partial \mu} = \frac{\mu}{g} - \frac{4}{3\pi^2}\left(\frac{m}{\hbar^2}\right)^{3/2}\frac{\mu^{3/2}}{(1+\chi\mu)^2} + \frac{64}{15\pi^2}\left(\frac{m}{\hbar^2}\right)^{5/2}\frac{g_2}{g}\frac{\mu^{5/2}}{(1+\chi\mu)^3} \ . \tag{67}$$

This formula can be inverted perturbatively giving

$$\mu = gn\left(1 + \frac{4}{3\pi^2}\left(\frac{m}{\hbar^2}\right)^{3/2} g(gn)^{1/2} - \frac{64}{15\pi^2}\left(\frac{m}{\hbar^2}\right)^{5/2} g_2(gn)^{3/2}\right) \ . \tag{68}$$

Bosons with finite-range effects: beyond mean-field (VII)

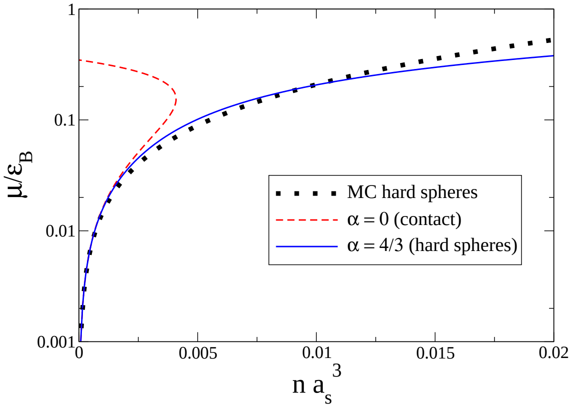

Figure: Chemical potential μ vs gas parameter na_s^3 for a 3D Bose gas of hard spheres. Filled squares are Monte Carlo (MC) data [M. Rossi and LS, Phys. Rev. A **88**, 053617 (2013)]. Solid line and dashed line are results of our zero-temperature Gaussian theory with effective-range adimensional parameter $\alpha = 4(g_2/g_0)/a_s^2$. Dot-dashed line is the Lee-Huang-Yang formula. Here $\epsilon_B = \hbar^2/(ma_s^2)$ is the characteristic energy of the interacting Bose gas, a_s is the s-wave scattering length and n is the number density.

Bosons with finite-range effects: beyond mean-field (VIII)

The zero-temperature condensate density n_0 can be related to the number density n keeping ψ_0 and μ as independent variables. We use the formula

$$n = - \left(\frac{\partial \Omega(\mu, \psi_0, T=0)}{\partial \mu} \right)_{\substack{\mu = g\psi_0^2 \\ \psi_0^2 = n_0}} , \qquad (69)$$

where $\Omega(\mu, \psi_0, T=0)$ is the grand potential calculated by using the Bogoliubov spectrum

$$E_{\mathbf{q}} = \sqrt{\left(\frac{\hbar^2 q^2}{2m} - \mu + \psi_0^2 \left(g + \tilde{V}_{EFT}(q) \right) \right)^2 - \psi_0^4 \tilde{V}_{EFT}(q)^2} \, . \qquad (70)$$

with $\tilde{V}_{EFT}(q)$ given by

$$\tilde{V}_{EFT}(q) = g + g_2 \; q^2 \, . \qquad (71)$$

Bosons with finite-range effects: beyond mean-field (IX)

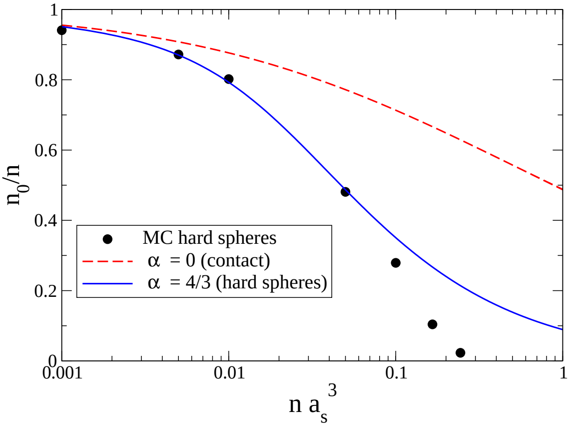

Figure: Condensate fraction n_0/n vs gas parameter na_s^3 for a Bose gas of hard spheres. Filled squares are Monte Carlo (MC) data [M. Rossi and LS, Phys. Rev. A **88**, 053617 (2013)]. Solid line and dashed line are results of our Gaussian theory with effective-range adimensional parameter $\alpha = 4(g_2/g_0)/a_s^2$. Dot-dashed line is the familiar Bogoliubov formula.

Bosons with finite-range effects: beyond mean-field (X)

The finite-temperature Gaussian contribution to the equation of state is obtained from $\Omega_g^{(T)}$, which can be written as

$$\frac{\Omega_g^{(T)}}{L^3} = -\frac{1}{6\pi}\int_0^\infty dq\, q^3\, \frac{dE_q}{dq}\frac{1}{e^{\beta E_q}-1}\ . \tag{72}$$

Expanding this expression at low temperature T we find

$$\frac{\Omega_g^{(T)}}{L^3} = -\frac{\pi^2}{90}\left(\frac{m}{\hbar^2}\right)^{3/2}\frac{(k_B T)^4}{\mu^{3/2}}\left(1-\frac{5\pi^2}{7}(k_B T)^2\frac{1+\chi\mu}{\mu^2}\right)\ . \tag{73}$$

Conclusions

- The regularization of zero-point energy[9] gives remarkable beyond-mean-field effects for repulsive bosons at zero temperature.
- Also finite-range effects become relevant at the Gaussian level:
  – equation of state
  – condensate fraction
- All these results can be extended at finite temperature.

[9] For a very recent comprehensive review see:
LS and F. Toigo, Zero-Point Energy of Ultracold Atoms, Physics Reports 640, 1 (2016).

Acknowledgements

Thank you for your attention!

Main sponsors: PRIN-MIUR, UNIPD.