Dimensional crossover for the beyond-mean-field correction in Bose gases

Tobias Ilg, Jan Kumlin, Luis Santos, Dmitry S. Petrov, and Hans Peter Büchler

1Institute for Theoretical Physics III and Center for Integrated Quantum Science and Technology, University of Stuttgart, DE-70550 Stuttgart, Germany
2Institut für Theoretische Physik, Leibniz Universität Hannover, Appelstr. 2, DE-30167 Hannover, Germany
3LPTMS, CNRS, Univ. Paris Sud, Université Paris-Saclay, 91405 Orsay, France

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We present a detailed beyond-mean-field analysis of a weakly interacting Bose gas in the crossover from three to low dimensions. We find an analytical solution for the energy and provide a clear qualitative picture of the crossover in the case of a box potential with periodic boundary conditions. We show that the leading contribution of the confinement-induced resonance is of beyond-mean-field order and calculate the leading corrections in the three- and low-dimensional limits. We also characterize the crossover for harmonic potentials in a model system with particularly chosen short- and long-range interactions and show the limitations of the local-density approximation. Our analysis is applicable to Bose-Bose mixtures and gives a starting point for developing the beyond-mean-field theory in inhomogeneous systems with long-range interactions such as dipolar gases or Rydberg-dressed atoms.

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Introduction. Recent experiments have demonstrated the stabilization of quantum droplets with weakly interacting gases with dipolar interactions [1–4], as well as Bose-Bose mixtures [5–7]. The basic ingredient for this remarkable phenomenon is the near cancellation of the mean-field interaction such that the beyond-mean-field corrections become relevant, prevent a collapse of the Bose gas, and eventually lead to the formation of droplets [8]. These quantum droplets have renewed the interest in understanding beyond-mean-field effects [8–10], but although these droplets are inhomogeneous and anisotropic, the theoretical analysis so far has mostly been based on the local-density approximation. In this Rapid Communication, we present the behavior of the beyond-mean-field correction beyond local-density approximation for a dimensional crossover.

The leading correction to the ground-state energy for a weakly interacting Bose gas in three dimensions has been pioneered by Lee, Huang, and Yang (LHY) [11,12], and has been well confirmed experimentally with cold atomic gases [13,14], and the analysis has been extended to dipolar interactions [15]. For lower dimensions, its behavior is well understood from the exactly solvable theory by Lieb and Liniger [16,17] in one dimension, while the behavior in two dimensions has been studied in detail in the past [18–24]. On a theoretical level, the difficulties appear by the proper renormalization of the contact interaction. A natural approach to avoid this problem is the application of the theory developed by Hugenholtz and Pines [25]. This approach is highly suitable for the study of the crossover and has recently been applied for dipolar systems for a qualitative analysis of the crossover [9].

In this Rapid Communication, we calculate the beyond-mean-field correction for a one-component weakly interacting Bose gas with scattering length \(a_s\) in the crossover from three to two and from three to one dimension. We start with a system that is confined along one or two directions by a box potential with length \(l_\perp\) and periodic boundary conditions. This case the ground state is homogeneous and is characterized by the density \(n\). We calculate the LHY correction as a function of the dimensionless parameters \(\lambda = a_s/l_\perp\) and \(\kappa = na_s l_\perp^2\) (see Fig. 1). The result is expressed in terms of known special functions allowing for an analytical description of both limits. In particular, on the low-dimensional side of the crossover (small \(\kappa\)) this method reproduces results obtained for purely low-dimensional models with two-body interactions correctly renormalized by the confinement [26,27]. We extend this crossover analysis to the case of a harmonic confinement by using a particular form of the interaction potential, which guarantees the Gaussian shape of the mean-field ground-state wave function along the crossover, and derive the LHY corrections beyond local-density approximation.

The small parameter ensuring the weakly interacting regime for a three-dimensional Bose gas is \(\sqrt{na_s^2} \ll 1\). This condition can either be satisfied by small scattering lengths or in the dilute regime. With decreasing the density in the presence of a transverse confinement, the system crosses over into the low-dimensional regime signaled by the condition that the transverse level spacing \(E_\perp = \hbar^2/2ml_\perp^2\) is comparable to the chemical potential \(\mu = 4\pi\hbar^2 a_n n/m\) giving rise to a dimensionless parameter \(\kappa = na_s l_\perp^2 / \mu / E_\perp\). The regime \(\kappa \gg 1\) describes a three-dimensional setup, while for \(\kappa \ll 1\) the system is effectively lower dimensional (see Fig. 1). Furthermore in one dimension, it is well established that the strongly correlated Tonks-Girardeau regime is reached in the low-density limit, while weakly interacting bosons appear for high densities \(n_{\text{int}}a_s^2 \gg 1\); here, \(n_{\text{int}} = nl_\perp^2\) is the one-dimensional density and the 1D scattering length \(a_{\text{int}} = -l_\perp^2/2\pi a_s\). Therefore, the proper small parameter controlling the weakly interacting regime in the full crossover regime is given by \(\lambda = a_s/l_\perp \ll 1\), and \(\kappa\) is restricted to stay in the interval \(\lambda^2 \ll \kappa \ll 1/\lambda^2\) (see Fig. 1). By contrast, there...
ultraviolet divergencies. One can understand this behavior as the chemical potential. The beyond-mean-field predictions are valid it is convenient to express the ground-state energy $E_1$ for three dimensions, $1/\sqrt{n_{\text{a.u.}}} \ll 1$ for one dimension, and $1/\ln n_{\text{a.u.}} \ll 1$ for two dimensions. These requirements translate to the conditions $\lambda^2 \ll \kappa \ll 1/\lambda^2$ for the 3D-1D crossover and $\kappa \ll 1/\lambda^2$ for the 2D-2D crossover, where $\lambda = a_d/L_1$. Furthermore, it shows that $\lambda$ is our small parameter and we require $\lambda \ll 1$ for the validity of our results.

is no lower-density limit for the weakly interacting regime in two dimensions and one requires $\kappa \ll 1/\lambda^2$. Written in terms of $\lambda$ and $\kappa$, the beyond-mean-field correction in the three-dimensional regime takes the form [11,12]

$$E_{\text{3D}} = \frac{2\pi \hbar^2 V}{m} \left( \kappa^2 + \frac{128}{15\sqrt{\pi}} \kappa^{5/2} + \frac{32\sqrt{\pi}}{\pi \kappa} \int_0^1 dq q^2 \sqrt{1-q^2} \cot(\pi w) \right)$$

where $V$ denotes the volume of the system. In the following, it is convenient to express the ground-state energy $E[\kappa, \lambda]$ in the crossover in terms of the energy scale $E_0 = \frac{2\pi \hbar^2 V}{m} \frac{\lambda^2}{\sqrt{n_{\text{a.u.}}}}$.

Our approach for the determination of the beyond-mean-field correction in the crossover is based on the theory developed by Hugenholtz and Pines [25]. This method is equivalent to the conventional approach based on the Bogoliubov theory [28], but naturally avoids difficulties with ultraviolet divergencies. One can understand this behavior as the divergencies in the Bogoliubov theory only provide a correction to the mean-field term proportional to $n^2$. In the approach of Hugenholtz and Pines the ground-state energy is determined by a differential equation, that does not determine this mean-field term. From the differential equation and fixing the correct mean-field behavior in three dimensions, we obtain the ground-state energy (see Supplemental Material [29])

$$E = E_{\text{3D}} + \kappa^2 \lambda E_0 \int_{\kappa_0}^{\kappa} \frac{dk'}{k'} [h(k') - h_{\text{3D}}(k')]$$

The first term in the integral accounts for the correction to the beyond-mean-field contribution in the crossover and takes the form

$$h(k) = \frac{1}{k^3} \sum_{\ell=1}^{3} \left[ \frac{2e^2 + 3\kappa \epsilon}{\sqrt{e^2 + 2\kappa \epsilon}} - 2e - \kappa \right]$$

Here, $\epsilon = \pi (\epsilon u^2 + \epsilon v^2 + \epsilon w^2)/2$ is the single-particle excitation spectrum for periodic boundary conditions with $u$, $v$, and $w$ the three components of the single-particle momentum in dimensionless units. Furthermore, the notation $\sum$ describes a summation over the transversal confined degrees of freedom, and an integration over the unconfined dimensions. The last term in the integral in Eq. (2) guarantees that the integral is convergent and vanishes for $\kappa \to \infty$. It takes the form $h_{\text{3D}}(\kappa) = -\frac{64}{15\sqrt{\pi \kappa}}$, and is the corresponding expression to $h(\kappa)$ for a three-dimensional system.

Crossover to two dimensions. We start with the dimensional crossover from a three-dimensional setup toward a two-dimensional slab with just a single transverse dimension confined. The ground-state energy in the crossover is denoted as $E_{\text{2D}}$. Then, $\sum = \int du dv$ and the integrations $\int du dv$ can be performed analytically leading to

$$h(\kappa) = \frac{1}{k^3} \left[ g(0) + 2 \sum_{w=1}^{\infty} \frac{\pi w^2}{2} \right]$$

with $g(q^2) = 2q^2(q^2 + \kappa - q\sqrt{q^2 + 2\kappa^2}) - \kappa^2$. The summation can be performed by introducing a contour integral $\sum_{w=1}^{\infty} = -\frac{1}{2\pi} \int_0^\infty dq q \cot(\pi w)$ with the contour $\gamma$ surrounding the positive real axis. Then, only the integration along the branch cut of $\sqrt{q^2 + 2\kappa^2}$ contributes, while the pole at $w = 0$ cancels $g(0)$ in the summation. By this procedure, we obtain

$$h(\kappa) = -\frac{32}{\sqrt{\pi \kappa}} \int_0^1 dq q^2 \sqrt{1-q^2} \coth(\sqrt{4\pi \kappa} q)$$

As a consequence, the ground-state energy $E_{\text{2D}}$ in the crossover from three to two dimensions takes the form

$$E_{\text{2D}} = \frac{E_{\text{3D}}}{E_0} = \kappa^2 + \lambda + \frac{128}{15\sqrt{\pi}} \kappa^{5/2} + \frac{32\sqrt{\pi}}{\pi \kappa} \int_0^1 dq q^2 \sqrt{1-q^2} \ln(1 - e^{-\sqrt{16\pi \kappa}/q})$$

and is shown in Fig. 2; note that it is most convenient to show only the beyond-mean-field corrections $\Delta E_{\text{2D}} = (E_{\text{2D}}/E_0 - \kappa^2)/\lambda$. In the three-dimensional regime with $\kappa \gg 1$, the transverse confinement leads to an attractive correction to the ground-state energy,

$$\frac{E_{\text{2D}} - E_{\text{3D}}}{E_0} \ll \frac{\pi^{3/2}}{90} \lambda \sqrt{\kappa} + O(\lambda \kappa^{-1/2})$$

which is nonvanishing even for $\kappa \to \infty$. For the quasi-two-dimensional Bose gas with $\kappa \ll 1$, the ground-state energy behaves as

$$\frac{E_{\text{2D}}(\kappa)}{E_0} \approx \frac{\kappa^2 + \lambda \kappa^2 \ln(k^4 \sqrt{e}) + \frac{2\pi}{3} \lambda \kappa^3 + O(\lambda \kappa^4)}{E_0}$$

This expression accounts for the negative beyond-mean-field correction to the ground-state energy as well as the zero crossing [see Fig. 2(a)]. The third term describes an effective three-body interaction due to quantum fluctuations, while the first two terms provide the ground-state energy of a purely two-dimensional Bose gas. In order to establish the latter connection, we note that the ground-state energy of a two-dimensional Bose gas takes the form [20-24]

$$\frac{E}{\hbar^2 \Lambda^2} = \ln \left( \frac{1}{\tilde{r}_{\text{a.u.}}} \right) + \ln \left( \frac{\ln \left( \frac{1}{\tilde{r}_{\text{a.u.}}} \right)}{\ln \left( \frac{\ln \left( \frac{1}{\tilde{r}_{\text{a.u.}}} \right)}{\ln \left( \frac{1}{\tilde{r}_{\text{a.u.}}} \right)} \right)} \right) = \ln(e^{2\pi^2 \sqrt{e}})$$

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with the two-dimensional density $n_{2D} = nL$ and the two-dimensional scattering length $a_{2D}$. The connection between the $s$-wave scattering length $a_s$ and $a_{2D}$ in confined systems has been derived for a harmonic trapping potential [27, 30]; its generalization to periodic boundary conditions is straightforward $a_{2D} = 2L_e^{-1/2}e^{-\gamma}$ (see Supplemental Material [29]) and was first obtained in [31]. Inserting this $a_{2D}$ into the ground-state energy of the two-dimensional Bose gas Eq. (8) and performing an expansion in the small parameter $\lambda = a_s/L$, we reproduce the first two terms in Eq. (7). Note that the expansion (7) implies $\kappa \gtrsim \lambda e^{-1/\lambda}$. Otherwise, for exponentially low densities, the two-dimensional small parameter $1/|\ln n_{2D}|^2 = 1/|\ln(\kappa/\lambda) - 1/\lambda| \ll 1$ [18] is no longer dominated by $\lambda$ but rather by the logarithm of the densities.

**Crossover to one dimension.** Next we focus on the dimensional crossover from a three-dimensional setup toward a one-dimensional tube with two transverse dimensions confined. Like the Bogoliubov theory, the method used here relies on the existence of a condensate, which is absent in one dimension. In the weakly interacting regime, however, the ground-state energy is well described within the Bogoliubov theory, as the system still exhibits quasi-long-range order [32]. The ground-state energy in the crossover is denoted as $E_{1D}(\kappa)$, and the evaluation of $h(\kappa)$ requires $\sum_{v, w} f(\epsilon)$. In contrast to the 2D situation, we first perform the integration over $\kappa'$. Then, the expression for the beyond-mean-field correction reduces to

$$E_{1D} - E_{in} \approx \lambda \int_{v, w} f(\epsilon) - \int_{v, w} dv dw f(\epsilon),$$

where $f(\epsilon) = \sqrt{\epsilon^2 + 2\epsilon \epsilon - \epsilon - \kappa}$. Again, it is possible to derive an expression in well-known functions by performing the double sum (see Supplemental Material [29])

$$E_{1D}/E_0 = \kappa^2(1 + \lambda C_{1D}) - \lambda \frac{8}{3\sqrt{\pi}} \kappa^{3/2} + \lambda \kappa^2 \int_0^\infty \frac{d\tau}{\sqrt{\pi} \tau}$$

$$\times \left[ \theta_3(0, e^{-\tau})^2 - 1 \right] \left[ 1 - e^{-2\kappa/\tau} \right] \frac{I_1(2\kappa/\tau)}{\tau \kappa}. \quad (9)$$

Here, $\theta_3(z, q) = \sum q^{n^2} \cos(2nz)$ denotes the Jacobi theta function, while $I_1(z)$ is the modified Bessel function. The term involving $C_{1D}$ is a shift to the mean-field energy due to the confinement defined as

$$C_{1D} = \int dv dw \frac{1}{\sqrt{v^2 + w^2}} - \sum_{v, w} f(\epsilon) \approx 3.899,$$

where the summation $\sum$ omits the term $v = w = 0$. The beyond-mean-field correction $\Delta E_{1D} = (E_{in}/E_0 - \kappa^2)/\lambda$ along the crossover is shown in Fig. 2(b).

Using the properties of Bessel functions, we expand Eq. (9) for small values of $\kappa \ll 1$ and we obtain the leading corrections for the one-dimensional regime

$$E_{1D}/E_0 \approx (1 + \lambda C_{1D}) - \frac{8}{3\sqrt{\pi}} \kappa^{3/2} + \lambda B_{2D} \kappa^3 + O(\kappa^4) \quad (10)$$

with $B_{2D} = (1/\pi \sum v, w v^2 + w^2)^{3/2} \approx 2.88$. These terms account for the attractive part of the beyond-mean-field correction as well as the zero crossing [see Fig. 2(b)]. Again, we have a very clear interpretation of these results: the term with $\kappa^3$ provides an effective three-body interaction, while the other terms account for the ground-state energy of a one-dimensional Bose gas. The latter is well established to take the form [16]

$$E/L = -\frac{\hbar^2}{m_{1D}} n_{1D}^2 \left( 1 - \frac{4\sqrt{2}}{3\pi} \frac{1}{\sqrt{\tau_{1D}}} \right). \quad (11)$$

Including the effect of the confinement-induced resonance [26], the relation between $a_{1D}$ and the $s$-wave scattering length $a_s$ takes the form $a_{1D} = -\frac{1}{2\pi} \frac{\hbar^2}{m_{1D}} n_{1D}^2 (1 - C_{1D} a_s)$ (see Supplemental Material [29]). Note, that the parameter $C_{1D}$ is modified for periodic boundary conditions compared to a harmonic trapping [26]. Expanding the ground-state energy of a 1D Bose gas in the small parameter $\lambda = a_s/L$, therefore provides the first two terms in Eq. (10), i.e., it naturally includes the leading contribution of the confinement-induced resonance. Finally, it is also possible to provide an analytical expansion in the three-dimensional (3D) regime for $\kappa \gg 1$, and the leading
correction is attractive:
\[
\frac{E_{1D} - E_{\text{lo}}}{E_0} \approx -\sqrt{E_0} \frac{A_{1D}}{2\pi^{3/2}} + O(\kappa^{-1/2})
\]  \hspace{1cm} (12)
with the constant \(A_{1D} = \sum_{v,w} (v^2 + w^2)^{-2} \approx 6.0268\).

Harmonic confinement. Finally, we apply our understanding of the crossover to a system with harmonic confinement in the transverse directions; the trapping frequency is related to the transverse confinement length via \(\omega_\perp = h/m\ell_\perp^2\). We are not interested in mean-field modifications of the ground-state wave function due to interactions, which was studied previously [33–35], but rather on beyond-mean-field corrections for a setup, where the condensate remains in the lowest state of the harmonic confinement. Experimentally, this goal can be achieved for bosonic mixtures [8].

On the theoretical level, this goal is conveniently achieved by adding an attractive interaction potential, which is dominated by a large range \(r_0 \gg L_\perp, L_\perp/\sqrt{K}\) within the tube elongated along \(x\), e.g., \(-4\pi \hbar^2 a_s/(r_0^2 \pi m)\delta(|x|/\sqrt{2})\delta(z)\delta(z)\delta(x)/(2\Gamma_\perp^2)\). Note, that such a potential does not contribute to the beyond-mean-field corrections due to its large range, but guarantees that the condensate remains in the lowest energy state of the transverse confinement within mean-field theory.

We start with the analysis of the dimensional crossover from three to one dimension with harmonic confinement. Then, it is convenient to define \(\kappa = n_{a}\sqrt{a_s}\), while the single-particle excitation spectrum in dimensionless units is modified to \(E = \pi/2u^2 + (v + w)/2u^2\) with \(v, w \in \{0, 1, 2, \ldots\}\), i.e., \(v\) and \(w\) denote the quantum numbers for the harmonic oscillator modes of the transverse confinement. The interaction potential will lead to mixing of different transverse modes, and therefore, the Bogoliubov transformation in general involves many transverse modes, i.e., \(a_{\alpha\beta} = \sum_{\alpha\beta} \left[ a_{\alpha\beta}^{\text{bog}} b_{\alpha\beta}^{\text{bog}} - a_{\beta\alpha}^{\text{bog}} b_{\beta\alpha}^{\text{bog}} \right] / a_{\alpha\beta}^{\text{bog}}\) the new bosonic operators, and \(\bar{a}_{\alpha\beta}^{\text{bog}} (v_{\alpha\beta}^{\text{bog}})\) the factors of the Bogoliubov transformation. Then, the term \(h(\kappa)\) within the approach by Hugenholtz and Pines takes the form (see Supplemental Material [29])
\[
h(\kappa) = \frac{4\pi}{\kappa} \int du \sum_{\alpha\beta} \sum_{vw} [E - E_{\alpha\beta}] |v_{\alpha\beta}^{\text{bog}}|^2
\]  \hspace{1cm} (13)
with \(E_{\alpha\beta}\) the Bogoliubov excitation energy in dimensionless units. In general, the determination of the Bogoliubov excitation spectrum \(E_{\alpha\beta}\) and the factors \(v_{\alpha\beta}^{\text{bog}}\) requires a numerical analysis. The beyond-mean-field correction to the ground-state energy is determined by fixing the correct mean-field term \(\propto \kappa^2\). In the previous analysis, we observed that the beyond-mean-field correction includes the modification of the mean-field term by the confinement-induced resonance. This allows us to fix the mean-field term in the one-dimensional regime \(\kappa \ll 1\). Alternatively, one would expect that for a very shallow trapping potential the local-density approximation is well justified, which in turn allows us to fix the mean-field term for \(\kappa \gg 1\); our numerical analysis shows that both approaches coincide. The result of this numerical analysis in the full crossover from three to one dimension is shown in Fig. 2(c). In the three-dimensional regime with \(\kappa \gg 1\), we find excellent agreement between the numerical analysis and the prediction within the local-density approach. The latter is obtained by integrating the 3D LHY result in Eq. (1) over the transversal density profile of the condensate, i.e., \(E_{1D} = \frac{3v_s^2}{r_0^2 \pi m} \kappa^{3/2} E_0\) for \(\kappa \gg 1\) with \(E_0 = \hbar \omega_\perp L/a_s\). Note, that the term \(\kappa^2\) is missing due to our special choice of the interaction potential. In turn, for \(\kappa \ll 1\) it is possible to derive the leading corrections to the ground-state energy by determining the Bogoliubov energy \(E_{\alpha\beta}\) and the factors \(v_{\alpha\beta}^{\text{bog}}\) within perturbation theory. It is required to perform the analysis up to second-order perturbation theory for \(E_{\alpha\beta}\) and first order for \(v_{\alpha\beta}^{\text{bog}}\) (see Supplemental Material [29]). Then, the beyond-mean-field correction takes the form
\[
\frac{E_{1D}^h - E_{1D}^<}{E_0} \approx \frac{\kappa^3 C_{10}^h}{\sqrt{2} \sqrt{3\pi}} - \frac{4\sqrt{2}}{3\pi} \kappa^3/2 + \frac{4\sqrt{2} \ln(4/3)}{\pi} \kappa^5/2 + O(\kappa^5).
\]  \hspace{1cm} (14)

The first term on the right side accounts for the correction to the mean-field term due to the confinement-induced resonance with \(C_{10}^h \approx 1.4603\) [26], while the second term describes the beyond-mean-field contribution of a purely one-dimensional system. Finally, the term with \(\kappa^5/2\) provides the leading correction in the crossover. It is highly remarkable that for harmonic confinement a term \(\kappa^5/2\) appears, which was absent in the previous analysis with periodic boundary conditions. These predictions are fully confirmed with the numerical approach [see Fig. 2(e)]. However, for a correct description of the zero crossing it is also important to include the next term \(B_{10}^h \kappa^3\) in the expansion. The prefactor \(B_{10}^h\) is determined by a fitting procedure to the numerical evaluation, which predicts \(B_{10}^h \approx 0.1\).

An analogous calculation can also be performed for the 3D-2D crossover within a harmonic confinement \(\kappa = n_{a}\sqrt{a_s} L_\perp\). Again, we expect the prediction by local-density approximation for \(\kappa \gg 1\), while for \(\kappa \ll 1\) the ground-state energy reduces to the two-dimensional result \(E_{1D}^h = \hbar \omega_\perp \ln|\kappa C_{10}^h| L^2 / \ell_\perp^2\) with \(C_{10}^h \approx 28.69\) [27,29,30] including the renormalized scattering length. The next term due to the crossover can again be derived within perturbation theory and provides a correction \(\propto \kappa^3 \ln \kappa\).

Conclusion. We present a detailed study of the beyond-mean-field corrections for a weakly interacting Bose gas in the dimensional crossover. While for a transverse confinement with periodic boundary conditions the analysis can be performed analytically, for a realistic setup with harmonic confinement a numerical analysis is required, and we find excellent agreement with the predictions from local-density approximation for \(\kappa \gg 1\). Furthermore, we find that the correction to the local-density approximation lowers the ground-state energy. This phenomenon might explain the recently observed systematic shift in the scattering length determined by the stability of self-bound droplets [2]: the finite extent of the droplets in transverse direction naturally introduces a confinement of the underlying gas and hence a correction to the local-density approximation. In addition, our results show that the full crossover is excellently described by the combination of the leading contribution for \(\kappa \ll 1\) and \(\kappa \gg 1\), which in general is sufficient to describe the qualitative behavior throughout the crossover. Our results are immediately
applicable to Bose-Bose mixtures of equal masses, as the treatment of the beyond-mean-field effects in the vicinity of the collapse reduces to that of a scalar gas with an effective interaction. Moreover, the results give a starting point for developing the beyond-mean-field theory in inhomogeneous systems with long-range interactions such as dipolar particles or Rydberg-dressed atoms.

Note added. Recently, we became aware of very related results by Zin et al. [36].

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