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Mean-field analysis of Bose–Einstein condensation in general power-law potentials

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Abstract

Mean-field theory is applied to describe the condensation of dilute interacting Bose gases in general power-law potentials. We investigate the behaviour of the critical temperature and derive an analytical approximation which is second order in the atomic scattering length. This result, on the one hand, provides a comparison tool for further, more elaborate, approaches. On the other hand, it also yields qualitative insights into the crossover between homogeneous and inhomogeneous potentials, where different physical mechanisms govern the behaviour of the critical temperature. The connection of the results to previous studies is worked out.

1. Introduction

The study of the critical temperature T_c of dilute interacting Bose gases has recently attracted a significant amount of attention. An interesting result of this research concerns the role of the external trapping potential. It has become clear that the dependence of T_c on the atomic interaction strength is determined by different physical mechanisms in homogeneous and inhomogeneous, e.g., harmonic, potentials, and therefore displays a different behaviour in the two cases. For homogeneous systems, the phase transition is dominated by long-wavelength critical fluctuations which have to be treated nonperturbatively (for overviews, see, e.g., [1–3]), and it was recently shown that in lowest order the shift in T_c increases linearly with the atomic scattering length [4, 5].

For harmonically trapped gases, the inhomogeneity introduces new aspects into the physical picture associated with the condensation phenomenon (see, e.g., [6]). Near the thermodynamic limit, one may assume that the gas is everywhere in local thermal equilibrium. Bose–Einstein condensation sets in near the trap centre and initially affects only a small fraction of the atoms. The remaining atoms are still far away from criticality, and the importance of long-wavelength critical fluctuations is significantly reduced. Essential aspects of the phase transition can thus be described in terms of relatively simple theories, such as mean field [7, 8]. It turns out that, in contrast to the homogeneous case, the shift in T_c is not dominated by critical effects caused by the phase transition, but is mainly due to noncritical modifications of the global density distribution which are induced by the interactions. For fixed particle number N, this leads to a decrease in T_c with the interaction strength instead of an increase.

These observations motivate the problem of examining the crossover between the two limits of homogeneous and inhomogeneous potentials. As a first step in this direction, in the present paper mean-field theory (MFT) is applied to study the condensation, and in particular the critical temperature, of interacting Bose gases in general power-law traps. In this context, one has to be aware of the fact that MFT fails in the homogeneous limit, where it predicts the critical temperature to be independent of the atomic interactions. To obtain a quantitatively accurate description, more elaborate methods necessarily have to be applied. The study of MFT is nevertheless interesting and important for a number of reasons. First, it provides a useful first approximation, against which one can compare more sophisticated theories. We have recently completed a renormalization group (RG) study of condensation in power-law potentials [9], and the good qualitative agreement with MFT even in the quasi-homogeneous regime corroborates the validity of the RG approach. Second, as will be discussed in this paper, MFT also allows us to obtain some qualitative understanding of the crossover process between the limits of homogeneous and inhomogeneous potentials, in particular with regard to the behaviour of the critical temperature. This insight might be more difficult to obtain from other theories. Finally, the study of the MFT approach turns out to be an interesting mathematical problem by itself, for which analytical results can be derived.

The mean-field theory of T_c in general power-law traps has been the subject of several recent studies in the literature [10–13]. In spite of the interest in this topic and the progress made so far, none of these works provides a complete picture of the problem in the sense that it also accurately covers the quasi-homogeneous limit. In fact, some of these references even contain results that appear incorrect in the light of the present work. A further motivation for our study is therefore to extend and clarify these previous works, and also provide a more detailed discussion of the physical contents of the theory.

The paper is organized as follows. In section 2, we summarize some relations regarding ideal Bose gases in power-law traps. In section 3, after outlining the MFT approach, we derive an analytical approximation to the critical temperature which is second order in the atomic scattering length. This result should provide a useful comparison tool for further related studies. We also work out the connection to previous studies. In section 4, we discuss and illustrate the MFT results and their physical contents. In this way, we also obtain some qualitative insights into the problem. In section 5, on the basis of the work of [14, 15], we discuss how effects beyond MFT can be incorporated into the calculation of T_c. This also allows us to better estimate the range of validity of mean-field theory. A short summary is given in section 6.

2. Ideal Bose gases in power-law traps

In this section, we summarize several relations regarding ideal Bose gases in power-law traps. The notation follows [10] and [11]. We consider a system of N ideal bosons of mass m which are trapped in a power-law potential

$$V(\mathbf{r}) = E_1 \left| \frac{x}{L_1} \right|^p + E_2 \left| \frac{y}{L_2} \right|^l + E_3 \left| \frac{z}{L_3} \right|^s, \tag{1}$$

where the constants E_i and L_i set the energy and length scales for the trap in the three spatial dimensions. An important parameter characterizing the potential shape is given by the constant

$$\eta = \frac{1}{p} + \frac{1}{l} + \frac{1}{s} + \frac{1}{2}, \tag{2}$$

which depends on the powers p, l and s appearing in $V(\mathbf{r})$. The characteristic volume

$$V_{\mathrm{char}}^{2(\eta+1)/3} = 8\left(\frac{\hbar^2}{m}\right)^{\eta-\frac{1}{2}} \frac{L_1 L_2 L_3 I(p,l,s)}{E_1^{\frac{1}{p}} E_2^{\frac{1}{l}} E_3^{\frac{1}{s}}}, \tag{3}$$

with $I(p,l,s) = \Gamma(1/p)\Gamma(1/l)\Gamma(1/s)/pls$, provides a rough estimate of the extension of the quantum-mechanical single-particle ground state in the trap. In the homogeneous case, we have $\eta = 1/2$ ($p = l = s = \infty$) and $V_{\mathrm{char}} = 8L_1L_2L_3$, whereas for a harmonic trap $\eta = 2$ ($p = l = s = 2$) and $V_{\mathrm{char}} = (2\pi)^{3/4} a_{ho}^{(1)} a_{ho}^{(2)} a_{ho}^{(3)}$ with $a_{ho}^{(i)} = (L_i\hbar/\sqrt{2mE_i})^{1/2}$ denoting the usual harmonic oscillator length.

In calculations in the mean-field approximation, we are frequently confronted with spatial integrals that depend on the position $\mathbf{r}$ only through the potential $V(\mathbf{r})$. They can easily be converted into one-dimensional integrals through the transformation $\int \mathrm{d}^3 r f[V(\mathbf{r})] = \int_0^\infty \mathrm{d}\varepsilon \tilde{\rho}(\varepsilon) f(\varepsilon)$. Therein, $\tilde{\rho}(\varepsilon)\,\mathrm{d}\varepsilon$ equals the spatial volume of the equipotential shell of $V(\mathbf{r})$ with width $\mathrm{d}\varepsilon$ at energy ε. The 'density' $\tilde{\rho}(\varepsilon)$ is given by

$$\tilde{\rho}(\varepsilon) = \frac{V_{\mathrm{char}}^{2(\eta+1)/3}}{\Gamma(\eta - 1/2)} \left(\frac{m}{\hbar^2}\right)^{\eta-1/2} \varepsilon^{\eta-3/2}. \tag{4}$$

Note that in the homogeneous case $\tilde{\rho}(\varepsilon) = V_{\mathrm{char}}\delta(\varepsilon)$. The use of $\tilde{\rho}(\varepsilon)$ greatly facilitates the study of general power-law potentials of arbitrary shape. In order to derive equation (4), we consider the Hamiltonian

$$H(\mathbf{p}, \mathbf{r}) = \begin{cases} V(\mathbf{r}) & p < p_0, \\ \infty & p \geqslant p_0, \end{cases}$$

with $p = |\mathbf{p}|$ and p_0 being a constant. The semiclassical number of states for this Hamiltonian is given by [16]

$$\Sigma(\varepsilon) = \frac{1}{6\pi^2\hbar^3} \frac{V_{\mathrm{char}}^{2(\eta+1)/3}}{\Gamma(\eta + 1/2)} p_0^3 \left(\frac{m}{\hbar^2}\right)^{\eta-1/2} \varepsilon^{\eta-1/2}. \tag{5}$$

The number of states $\Sigma(\varepsilon)$ is related to the density $\tilde{\rho}(\varepsilon)$ through $(2\pi\hbar)^3\Sigma(\varepsilon) = \frac{4}{3}\pi p_0^3 \int_{V\leqslant\varepsilon} \mathrm{d}^3 r = \frac{4}{3}\pi p_0^3 \int_0^\varepsilon \mathrm{d}\varepsilon' \tilde{\rho}(\varepsilon')$. Comparing this relation to equation (5), we obtain equation (4).

In the following, we focus on the thermodynamic limit, which is defined by $N V_{\mathrm{char}}^{-2(\eta+1)/3} =$ const, $N, V_{\mathrm{char}} \to \infty$. Above the condensation point, the equation of state for the ideal Bose gas then reads [16, 17]

$$N = \frac{1}{(2\pi)^{3/2}} \left(\frac{m}{\hbar^2\beta}\right)^{\eta+1} V_{\mathrm{char}}^{2(\eta+1)/3} g_{\eta+1}(z), \tag{6}$$

with β being the inverse temperature, μ the chemical potential and $z = \exp(\beta\mu)$ the fugacity. The Bose–Einstein or polylogarithm function g_λ is defined by $g_\lambda(z) = \sum_{k=1}^\infty z^k \big/ k^\lambda$. The spatial density distribution of the gas is given by

$$n(\mathbf{r}) = \lambda_T^{-3} g_{3/2}[\exp(\beta(\mu - V(\mathbf{r})))], \tag{7}$$

with the thermal wavelength $\lambda_T = (2\pi\hbar^2\beta/m)^{1/2}$. By setting $z = 1$ in equation (6) or evaluating $N = \int \mathrm{d}^3 r n(\mathbf{r}, \mu = 0)$ from equation (7), one finds the condition for Bose–Einstein condensation [10]

$$N = \frac{1}{(2\pi)^{3/2}} \left(\frac{m}{\hbar^2\beta_c^0}\right)^{\eta+1} V_{\mathrm{char}}^{2(\eta+1)/3} \zeta(\eta + 1), \tag{8}$$

with $\beta_c^0 = 1\big/k_b T_c^0$ denoting the inverse critical temperature and $\zeta(x)$ the Riemann zeta function.

3. Mean-field description of Bose–Einstein condensation

In mean-field theory, the spatial density of a dilute interacting Bose gas above the condensation point is determined by the relation [18]

$$n_{\mathrm{MF}}(\mathbf{r}) = \frac{1}{\lambda_T^3} g_{3/2}\{\exp[\beta(\mu - V_{\mathrm{eff}}(\mathbf{r}))]\} \tag{9}$$

in the thermodynamic limit. Expression (9) is identical to the one for the ideal gas (7) except for the fact that the atoms now experience an effective potential $V_{\mathrm{eff}}(\mathbf{r}) = V(\mathbf{r}) + 2U_0 n_{\mathrm{MF}}(\mathbf{r})$. In addition to the trapping potential, V_{eff} also contains the mean-field interaction potential $2U_0 n_{\mathrm{MF}}(\mathbf{r})$ that is due to the atomic collisions. The coupling constant is given by $U_0 = 4\pi\hbar^2 a/m$ with a being the s-wave scattering length. In mean-field theory, condensation sets in when the chemical potential reaches the maximum value compatible with equation (9). This critical value is determined by $\mu_{\mathrm{MF}}^{(\mathrm{cr})} = 2U_0 n_{\mathrm{MF}}^{(\mathrm{cr})}(\mathbf{0})$, so that the degeneracy parameter $n_{\mathrm{MF}}^{(\mathrm{cr})}(\mathbf{r} = \mathbf{0})\lambda_T^3$ at the trap centre equals $\zeta(3/2)$ just as in the ideal gas case. To calculate the spatial density $n_{\mathrm{MF}}^{(\mathrm{cr})}(\mathbf{r})$ at criticality, one has to solve equation (9) with $\mu = \mu_{\mathrm{MF}}^{(\mathrm{cr})}$. With the help of $n_{\mathrm{MF}}^{(\mathrm{cr})}(\mathbf{r})$, the critical temperature is then related to the atom number N and the other parameters via

$$N = \int \mathrm{d}^3 r\, n_{\mathrm{MF}}^{(\mathrm{cr})}(\mathbf{r}). \tag{10}$$

For the study of equations (9) and (10), it is useful to note from (9) that $n_{\mathrm{MF}}(\mathbf{r})$ is constant on the equipotential surfaces of $V(\mathbf{r})$, i.e. $n_{\mathrm{MF}}(\mathbf{r}) = n_{\mathrm{MF}}[V(\mathbf{r})] = n_{\mathrm{MF}}(\varepsilon)$. Invoking (4), equation (10) can thus be rewritten as

$$N = \int_0^\infty \mathrm{d}\varepsilon\, \tilde{\rho}(\varepsilon) n_{\mathrm{MF}}^{(\mathrm{cr})}(\varepsilon). \tag{11}$$

We now introduce the dimensionless quantities $z = \exp(\beta\mu), x = \beta\varepsilon, f_{\mathrm{MF}}(x) = \lambda_T^3 n_{\mathrm{MF}}(x), q = a/\lambda_T$ and $\rho(x) = \tilde{\rho}(x/\beta)/\beta$. In these variables, equation (9) reads

$$f_{\mathrm{MF}}(x) = g_{3/2}\{z \exp[-x - 4q f_{\mathrm{MF}}(x)]\} = F_{3/2}[x + 4q f_{\mathrm{MF}}(x) - \ln z], \tag{12}$$

with the Bose function $F_\lambda(x) = g_\lambda[\exp(-x)]$. At criticality, $z = \exp[4q\zeta(3/2)]$.

To calculate the shift in the critical temperature T_c, we insert equation (4) into (11) and derive an expression for $N/(k_B T_\mathrm{c})^{\eta+1}$ in terms of the other system parameters. Comparing this relation to the corresponding one for the ideal gas (cf equation (8)) we find

$$\left(\frac{T_\mathrm{c}^{(\mathrm{MF})}}{T_\mathrm{c}^{(0)}}\right)^{\eta+1} = \frac{\zeta(\eta+1)\Gamma(\eta-1/2)}{\int_0^\infty \mathrm{d}x\, x^{\eta-3/2} f_{\mathrm{MF}}^{(\mathrm{cr})}(x)} \equiv \frac{\zeta(\eta+1)\Gamma(\eta-1/2)}{I_0^\infty(q,\eta)}, \tag{13}$$

where we have set

$$I_a^b(q,\eta) = \int_a^b \mathrm{d}x\, x^{\eta-3/2} f_{\mathrm{MF}}^{(\mathrm{cr})}(x). \tag{14}$$

Note that equation (13) would yield the exact critical temperature (within the local-density approximation), if $f_{\mathrm{MF}}^{(\mathrm{cr})}(x)$ were replaced by the exact scaled density distribution.

In general, the mean-field critical temperature for a given set of system parameters can only be determined numerically by calculating $f_{\mathrm{MF}}^{(\mathrm{cr})}(x)$ from equation (12) and evaluating the integral $I_0^\infty(q,\eta)$. For small $q = a/\lambda_T$, however, an analytic approximation can be derived. To this end, we first examine the behaviour of $f_{\mathrm{MF}}^{(\mathrm{cr})}$ at small x with the help of the series expansion [19]

$$F_\lambda(x) = \Gamma(1-\lambda)x^{\lambda-1} + \sum_{n=0}^\infty \frac{(-1)^n}{n!}\zeta(\lambda-n)x^n, \tag{15}$$

which is absolutely convergent for $|x| < 2\pi$. Using (15) to expand the Bose function $F_{3/2}$, that appears on the right-hand side of equation (12), up to order $\frac{1}{2}$ in its argument, we obtain the approximation

$$f_{\rm MF}^{\rm (cr)}(x) \approx \zeta(3/2) + 8\pi q - \sqrt{(8\pi q)^2 + 4\pi x}. \tag{16}$$

Continuing the expansion up to linear order, one finds

$$f_{\rm MF}^{\rm (cr)}(x) \approx \zeta(3/2) + \frac{8\pi q - \zeta(1/2)Qx}{Q^2} - \frac{1}{Q^2}\sqrt{(8\pi q)^2 + 4\pi Qx}, \tag{17}$$

with $Q = 1 + 4q\zeta(1/2)$. It should be noted that the approximation (17) is rather accurate; e.g., for $x \leqslant 0.01$ the relative deviation from the numerically determined exact value is always less than 5×10^{-6} and it decreases rapidly with growing q. We now discuss the small-x contributions to the integral $I_0^\infty(q,\eta)$ of equation (13). To this end, we evaluate $I_0^u(q,\eta)$ with the upper integration limit u chosen such that $u \gg q^2$, but still small enough that the approximations (16) and (17) are applicable. From the first expansion we obtain

$$\begin{aligned} I_0^u(q,\eta) &\approx \int_0^u \mathrm{d}x\, x^{\eta-3/2}\left[\zeta(3/2) + 8\pi q - \sqrt{(8\pi q)^2 + 4\pi x}\right] \\ &= [\zeta(3/2) + 8\pi q]\frac{u^{\eta-1/2}}{\eta - 1/2} + \frac{8\pi q u^{\eta-1/2}}{\eta - 1/2}\,{}_2F_1\left(-\frac{1}{2}, -\frac{1}{2}+\eta, \frac{1}{2}+\eta; -\frac{u}{16\pi q^2}\right) \\ &= -\frac{2\sqrt{\pi}u^\eta}{\eta} + \frac{\zeta(3/2)u^{\eta-1/2}}{\eta - 1/2} + q\frac{8\pi u^{\eta-1/2}}{\eta - 1/2} - q^2\frac{16\pi^{3/2}u^{\eta-1}}{\eta - 1} \\ &\quad + q^{2\eta}(16\pi)^\eta\frac{\Gamma(\eta+1/2)\Gamma(-\eta)}{\eta - 1/2} + O(q^3). \end{aligned} \tag{18}$$

In (18), ${}_2F_1(a,b,c;x)$ denotes the hypergeometric function [20], and the relation

$$\begin{aligned} {}_2F_1\left(-\frac{1}{2}, -\frac{1}{2}+\eta, \frac{1}{2}+\eta; z\right) &= \frac{\eta - 1/2}{\eta}(-z)^{1/2}\,{}_2F_1\left(-\frac{1}{2}, -\eta, 1-\eta; 1/z\right) \\ &\quad - \frac{\Gamma(\eta+1/2)\Gamma(-\eta)}{2\sqrt{\pi}}(-z)^{1/2-\eta}, \end{aligned} \tag{19}$$

as well as the series expansion of ${}_2F_1$ were used. Evaluating $I_0^u(q,\eta)$ in the same way with the approximation (17), one finds

$$\begin{aligned} I_0^u(q,\eta) \approx &-\frac{2\sqrt{\pi}u^\eta}{\eta} + \frac{\zeta(3/2)u^{\eta-1/2}}{\eta - 1/2} - \frac{\zeta(1/2)u^{\eta+1/2}}{\eta + 1/2} \\ &+ q\left(\frac{8\pi u^{\eta-1/2}}{\eta - 1/2} + \frac{12\sqrt{\pi}\zeta(1/2)u^\eta}{\eta} + \frac{4\zeta^2(1/2)u^{\eta+1/2}}{\eta + 1/2}\right) + q^2\left(-\frac{16\pi^{3/2}u^{\eta-1}}{\eta - 1}\right. \\ &\left. - \frac{64\pi\zeta(1/2)u^{\eta-1/2}}{\eta - 1/2} - \frac{60\sqrt{\pi}\zeta^2(1/2)u^\eta}{\eta} - \frac{16\zeta^3(1/2)u^{\eta+1/2}}{\eta + 1/2}\right) \\ &+ q^{2\eta}(16\pi)^\eta\frac{\Gamma(\eta+1/2)\Gamma(-\eta)}{\eta - 1/2}[1 + 4q\zeta(1/2)]^{-(\eta+3/2)} + O(q^3). \end{aligned} \tag{20}$$

Comparing relations (18) and (20), which are of increasing accuracy, we conclude that $I_0^u(q,\eta)$ can be written as a power series in q that has the form

$$I_0^u(q,\eta) = A_0(u,\eta) + A_1(u,\eta)q + A_2(u,\eta)q^2 + (16\pi)^\eta\frac{\Gamma(\eta+1/2)\Gamma(-\eta)}{\eta - 1/2}q^{2\eta} + o(q^2). \tag{21}$$

From (21), we can distinguish two different kinds of contributions to $I_0^u(q,\eta)$. On the one hand, we have a nonanalytic term proportional to $q^{2\eta}$, which, for $u \gg q^2$, no longer depends on u. This contribution is thus completely determined by the behaviour of $f_{\rm MF}^{(\rm cr)}(x)$ at small x or, in physical terms, near the trap centre. On the other hand, we find terms that are proportional to integer powers of q and have u-dependent coefficients $A_i(u,\eta)$. The two approximations (18) and (20) provide power series expansions for these coefficients that are of increasing order in u.

Let us now consider equation (12) in the limit of large x. If $x \gg 4q\big[\zeta(3/2) - f_{\rm MF}^{(\rm cr)}(x)\big]$, we can perform a Taylor expansion of the right-hand side around x, i.e.

$$y = F_{3/2}(x) + F_{1/2}(x)4q[\zeta(3/2) - y] + \tfrac{1}{2}F_{-1/2}(x)\{4q[\zeta(3/2) - y]\}^2 + O(q^3), \tag{22}$$

where $y \equiv f_{\rm MF}^{(\rm cr)}(x)$. The iterative solution of (22) yields

$$\begin{aligned} f_{\rm MF}^{(\rm cr)}(x) &= F_{3/2}(x) + 4F_{1/2}(x)[\zeta(3/2) - F_{3/2}(x)]q \\ &\quad + \big\{8F_{-1/2}(x)[\zeta(3/2) - F_{3/2}(x)]^2 - 16F_{1/2}^2(x)[\zeta(3/2) - F_{3/2}(x)]\big\}\, q^2 + O(q^3) \\ &= b_0(x) + b_1(x)q + b_2(x)q^2 + O(q^3). \end{aligned} \tag{23}$$

For sufficiently large u it thus follows that

$$I_u^\infty(q,\eta) = B_0(u,\eta) + B_1(u,\eta)q + B_2(u,\eta)q^2 + O(q^3), \tag{24}$$

with $B_i(u,\eta) = \int_u^\infty {\rm d}x\, x^{\eta-3/2} b_i(x)$.

It now remains to combine the two results (21) and (24) and relate the coefficients A_i and B_i to each other. To this end, we turn again to the expansion (23). It is only applicable for sufficiently large x and clearly becomes invalid for $x \to 0$ as $b_2(x)$ diverges (as well as the omitted higher-order terms). This is consistent with the fact that in this limit, the small-x approximations (16) and (17) cannot be expanded as Taylor series in q. Nevertheless, it turns out that the functions $b_i(x)$ can directly be used to calculate the coefficients $A_i(u,\eta)$ of equation (21). To see this, we expand the b_i as power series in x with the help of relation (15) and use these series to evaluate the integrals $\int_0^u {\rm d}x\, x^{\eta-3/2} b_i(x)$ (which appear after inserting equation (23) into (14)). In the expressions resulting in this way from $b_0(x)$ and $b_1(x)$, it turns out that the first few terms exactly reproduce the respective terms in equations (18) and (20). For $b_2(x)$, the first three terms match exactly with equation (20) whereas the fourth term, which is proportional to $x^{\eta+1/2}$, has a prefactor of $[-16\zeta(1/2) + 96\pi\zeta(-1/2)]/(\eta + 1/2)$ instead of $-16\zeta(1/2)/(\eta + 1/2)$ as in equation (20). We assume that this discrepancy would disappear if the expansion leading to equations (16) and (17) were carried out to the next order. We also have to take into account the fact that the integral $\int_0^u {\rm d}x\, x^{\eta-3/2} b_2(x)$ diverges at the lower limit as soon as $\eta \leqslant 1$ (compare with first term in expansion of $A_2(u,\eta)$). To cure this deficiency and bring the result in accordance with equation (20), we have to regularize the integral by subtracting the diverging contribution, i.e. we define

$$\mathcal{R}\int_0^u {\rm d}x\, x^{\eta-3/2} b_2(x) \equiv \lim_{\varepsilon\to 0}\left[\int_\varepsilon^u {\rm d}x\, x^{\eta-3/2} b_2(x) - \frac{16\pi^{3/2}\varepsilon^{\eta-1}}{\eta - 1}\right], \tag{25}$$

(for the special case $\eta = 1$ see below).

Based on the agreement between the power series expansions, we conclude that the integrals $\int_0^u {\rm d}x\, x^{\eta-3/2} b_i(x)$ permit an accurate evaluation of the coefficients $A_i(u,\eta)$ of equation (21). As the 'small-x' and 'large-x' coefficients A_i and B_i are thus represented by the same type of integral, we can readily combine results (21) and (24) to arrive at the final expression for the complete integral

$$I_0^\infty(q,\eta) = \Gamma(\eta - 1/2)\zeta(\eta + 1) + C_1(\eta)q + C'(\eta)q^{2\eta} + C_2(\eta)q^2 + o(q^2), \tag{26}$$

where

$$C_1(\eta) = 4\int_0^\infty \mathrm{d}x\, x^{\eta-3/2} F_{1/2}(x)[\zeta(3/2) - F_{3/2}(x)], \tag{27}$$

$$C'(\eta) = (16\pi)^\eta \frac{\Gamma(\eta+1/2)\Gamma(-\eta)}{\eta - 1/2}, \tag{28}$$

$$C_2(\eta) = \mathcal{R}\int_0^\infty \mathrm{d}x\, x^{\eta-3/2}\big\{8F_{-1/2}(x)[\zeta(3/2) - F_{3/2}(x)]^2 - 16F_{1/2}^2(x)[\zeta(3/2) - F_{3/2}(x)]\big\}, \tag{29}$$

and we have used that $\int_0^\infty \mathrm{d}x\, x^{\eta-3/2} b_0(x) = \Gamma(\eta - 1/2)\zeta(\eta+1)$. Using equations (13) and (26), the shift in the critical temperature $t_{\mathrm{MF}} = 1 - T_{\mathrm{c}}^{(\mathrm{MF})}\big/T_{\mathrm{c}}^0$ is determined as

$$\begin{aligned} t_{\mathrm{MF}} &= -\frac{C_1(\eta)}{c(\eta)}q - \frac{C'(\eta)}{c(\eta)}q^{2\eta} + \left(\frac{\eta+2}{2c^2(\eta)}C_1^2(\eta) - \frac{C_2(\eta)}{c(\eta)}\right)q^2 + o(q^2) \\ &= D_1(\eta)q + D'(\eta)q^{2\eta} + D_2(\eta)q^2 + o(q^2), \end{aligned} \tag{30}$$

with $c(\eta) = (\eta+1)\Gamma(\eta - 1/2)\zeta(\eta+1)$. Equations (26) and (30) are the main results of this section.

Let us emphasize that our deduction of equation (26) does not constitute an exact mathematical proof. However, instead of attempting a rigorous derivation, we turn to consistency checks and numerical studies for establishing the validity of (26). Regarding the consistency checks, it is instructive to investigate the cases $\eta = 1/2$ and $\eta = 1$ where we have to deal with divergences in the coefficients C_i and C'. As to $\eta = 1/2$, it is known that there is no mean-field shift in the critical temperature, so we see from equation (13) that $I_0^\infty(q,\eta)$ has to diverge like $\Gamma(\eta - 1/2)\zeta(\eta+1)$ in the limit $\eta \to 1/2$. This means that all q-dependent contributions in (26) have to remain finite for $\eta \to 1/2$. One can show that in this limit $C_1(\eta)$ behaves like $8\pi/(\eta - 1/2) + O(1)$ whereas $C'(\eta) \sim -8\pi/(\eta - 1/2) + O(1)$, so that the combination of the q- and $q^{2\eta}$-contributions remains finite. The coefficient $C_2(\eta)$ behaves like $-64\pi\zeta(1/2)/(\eta - 1/2) + O(1)$. If we go back to equation (20) and expand the factor $[1 + 4q\zeta(1/2)]^{-3/2-\eta}$ in the term containing $q^{2\eta}$, we obtain a contribution that behaves like $[64\pi\zeta(1/2)/(\eta - 1/2) + O(1)]q^{2\eta+1}$ and thus cancels the divergence of the q^2 term. Apart from this observation, however, we have not studied the $q^{2\eta+1}$ term further and therefore do not include it in equation (26).

At $\eta = 1$, the coefficients $C'(\eta)$ and $C_2(\eta)$ diverge. One finds that $C'(\eta) \sim 16\pi^{3/2}/(\eta - 1) + 136.404 + O(\eta - 1)$, whereas $C_2(\eta) \sim -16\pi^{3/2}/(\eta - 1) + 395.4 + o(\eta - 1)$ with the constant term determined numerically. Invoking L'Hopital's rule we obtain the result

$$I_0^\infty(q, \eta = 1) = \Gamma(1/2)\zeta(3/2) + C_1(1)q + 32\pi^{3/2}q^2\log q + 531.4q^2 + o(q^2), \tag{31}$$

for $\eta = 1$ which is free of divergences.

Besides these consistency checks, we have also carefully compared equation (26) with numerical calculations of $I_0^\infty(q,\eta)$ to verify its validity. Some illustrative results are displayed in the next section. Apart from the calculations shown there, we have, e.g., confirmed equation (31) with the help of fits to the numerical data. We have also reproduced the second-order coefficient for $\eta = 2$, and, finally, verified that the regularization procedure of equation (25) leads to results consistent with numerics. In conclusion, we have thus found strong support for the validity of equations (26)–(29).

Let us now relate our results to previous mean-field studies of Bose–Einstein condensation in general power-law potentials. The first relevant work appears to be [10]. Its equation (24) leads in lowest order to a proportionality between the shift $t_{\rm MF}$ and the interaction parameter q (as in our equation (30)). However, the calculation of [10] does not yield the correct value for the proportionality constant $D_1(\eta)$. For $\eta = 2$, e.g., one finds $-4/3$ instead of -3.43. In addition, mean-field theory is predicted to lead to a nonvanishing shift for the homogeneous case. The first correct derivation of $D_1(\eta)$ for harmonic potentials was provided in [7], and this result was subsequently generalized to arbitrary power-law potentials by Shi and Zheng [11]. The equivalence of their formula

$$D_1(\eta) = -\frac{4}{(\eta+1)\zeta(\eta+1)}\left[\zeta(3/2)\zeta(\eta) - \sum_{i,j=1}^{\infty}\frac{1}{i^{3/2}j^{1/2}(i+j)^{\eta-1/2}}\right], \quad (32)$$

to our expression can be shown by evaluating the integral (27) with the help of the relation $F_\lambda(x) = \sum_{k=1}^{\infty}\exp(-kx)/k^\lambda$.

Relation (32) was later rederived in [12]. This work, however, reports incorrect numerical values for $D_1(\eta)$; in particular, it predicts D_1 to diverge at $\eta = 1$ and to vanish for $\eta \to 1/2$. These problems indicate that equation (32) is not well suited for numerical studies; our expression (27), in contrast, can be evaluated without difficulties with standard numerical routines. In this context, it is interesting to note that an alternative sum representation for $D_1(\eta)$ can be derived by expressing the term $\zeta(3/2) - F_{3/2}(x)$ in equation (27) with the help of equation (15) and performing the integration. This yields

$$D_1(\eta) = \frac{4}{(\eta+1)\Gamma(\eta-1/2)\zeta(\eta+1)}\left[\Gamma(-1/2)\Gamma(\eta)\zeta(\eta+1/2) + \sum_{n=1}^{\infty}\frac{(-1)^n}{n!}\zeta(3/2-n)\zeta(\eta+n)\Gamma(\eta+n-1/2)\right]. \quad (33)$$

As the series (15) converges absolutely only for $x < 2\pi$, the sum (33) constitutes an asymptotic series. However, for η not too far from 1/2, one obtains accurate values by truncating the sum at $n = 7$.

Another recent mean-field study of condensation in power-law potentials was provided in [13]. There it is claimed that the result for $D_1(\eta)$ only holds for $\eta > 1$, whereas for $\eta \leqslant 1$ it is argued that the standard mean-field approach leads to inconsistencies and unphysical results. This is seen as an indication that it is necessary to modify the standard approach. In contrast, the present work shows the consistency of the normal mean-field equations and the validity of the result for $D_1(\eta)$ for any value of η.

Compared with these previous studies, the main theoretical progress of the current work consists in extending the analytical calculation of the mean-field condensation temperature to higher orders in the interaction parameter. This extension is indispensable for studying the quasi-homogeneous limit $\eta \to 1/2$. Furthermore, in the next section we also provide for the first time a qualitative discussion of the physical contents of the mean-field results and, in particular, investigate the transition between homogeneous and inhomogeneous traps.

4. Discussion of mean-field results

In this section, we discuss and interpret the results derived above. To this end, we display in figure 1 the behaviour of the mean-field critical temperature. The diagrams show the relative shift $t_{\rm MF} = 1 - T_{\rm c}^{\rm (MF)}\big/T_{\rm c}^0$ as a function of the potential parameter η for various values of the scaled interaction strength $q = a/\lambda_T$. The evaluation of $t_{\rm MF}$ by numerically solving equation (12) (full curve) is compared to the analytical approximation (26). The dashed curves

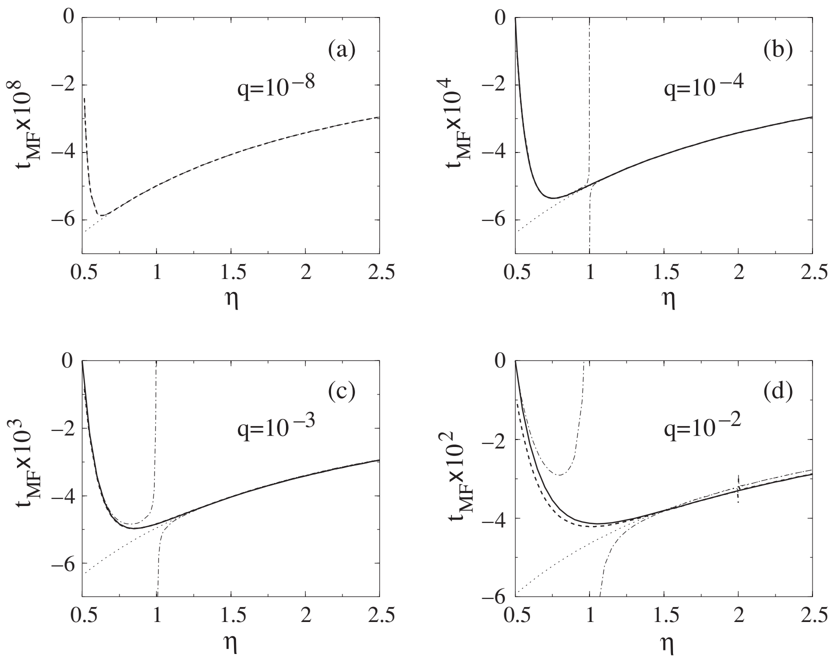

Figure 1. Mean-field calculation of critical temperature according to equation (13). Diagrams show the relative shift t_{MF} as a function of η for fixed $q = 10^{-8}$ (a), 10^{-4} (b), 10^{-3} (c) and 10^{-2} (d). Equation (13) was evaluated by numerically solving (12) (full curves), use of approximation (26) (dashed), use of term linear in q in (26) (dotted), use of linear and $q^{2\eta}$ term (dash-dotted).

are calculated with the full expression (26), whereas the other curves only take into account the term linear in q (dotted) or the sum of the linear and $q^{2\eta}$ terms (dash-dotted). To relate the values for q shown in the diagrams to current experiments with ultracold atoms, we note that the recent measurements of T_{c} in a harmonic trap were carried out for interaction strengths of the order of $q \approx 10^{-2}$ [21].

From the figures, we find the numerical results and the full approximation (26) to be almost indistinguishable for $q \leqslant 10^{-3}$. At $q = 10^{-2}$, there are small discrepancies for $\eta < 1$. Our approximation contains divergences at $\eta = 1/2$ due to the q^2 term and at $\eta = 2$ due to the $q^{2\eta}$ term, which would have to be balanced by higher-order terms in the expansion. However, these divergences become relevant only in very small regions around the critical values of η that are not resolved in our plots except for the singularity at $\eta = 2, q = 10^{-2}$ (compare figure 1(d)). On the other hand, we see how the divergences of the q^2 and $q^{2\eta}$ terms cancel each other around $\eta = 1$ (compare dashed and dash-dotted curves). For the smallest value of q, i.e. 10^{-8} in figure 1(a), the numerical calculation becomes unreliable, so that we only show the approximation whose accuracy is established by the agreement with the exact results at larger q.

For $q \lesssim 10^{-3}$, the exact solution is very well approximated by the sum of the linear and the $q^{2\eta}$ term, whereas the second-order term is only relevant for compensating the narrow divergence at $\eta = 1$. To interpret the results, we thus focus on the contributions proportional to q and $q^{2\eta}$. The corresponding coefficients $C_1(\eta)$ and $C'(\eta)$ have different physical origins. From equation (27), we see that $C_1(\eta)$ is given by an integral over the variable x with an integration range extending from 0 to ∞. As $x = \beta_c \varepsilon$ with ε representing the energy of the equipotential surfaces of the trapping potential $V(\mathbf{r})$, this amounts to an integration over the whole configuration space available to the Bose gas. The integral itself is over the mean-field density corrections due to the atomic interactions (represented by the combination of Bose functions) weighted by the equipotential shell volume $\rho(x)\,\mathrm{d}x$. The function $\rho(x)$, which was defined in equation (4), characterizes the influence of the trapping potential shape.

We thus conclude that $C_1(\eta)$ describes the large-scale potential shape effects on the critical temperature. These effects are due to the fact that the atomic interactions change the atomic density distribution—and effectively the critical atom number—in comparison to an ideal gas condensing at the same temperature, but they are not directly related to the actual phase transition process at the trap centre. The weight function $\rho(x) \sim x^{\eta-3/2}$ shows that for growing η, i.e. increasingly inhomogeneous traps, the contributions of the trap centre are more and more suppressed in favour of the regions of large x. It is in this area away from the phase transition regime where the mean field description is expected to be more and more accurate.

The coefficient $C'(\eta)$, on the other hand, has a very different physical origin. As we have seen in the previous section, it is determined by the behaviour of $f_{\mathrm{MF}}^{(\mathrm{cr})}(x)$ near the trap centre, where this function can no longer be represented as a simple power series in q. Of course, in this region mean-field theory can only provide a rough approximation to the true behaviour of the Bose gas, and an accurate description would have to take into account the influence of critical fluctuations. Nevertheless, let us consider $f_{\mathrm{MF}}^{(\mathrm{cr})}(x)$ as a crude, simplified representation of the actual behaviour. The two contributions $C_1(\eta)q$ and $C'(\eta)q^{2\eta}$ to $T_{\mathrm{c}}^{(\mathrm{MF})}$ then allow us to separate the influence of large-scale mean-field effects, which are dominant in inhomogeneous traps, and the (critical) effects near the trap centre, which play an important role for quasi-homogeneous potentials. In figure 1, we can clearly identify the crossover between the quasi-homogeneous regime of small η, where the contributions from $C'(\eta)$ are relevant, and the inhomogeneous regime, where $T_{\mathrm{c}}^{(\mathrm{MF})}$ is well approximated through the term $C_1(\eta)q$ alone. With growing interaction parameter q the size of the quasi-homogeneous regime increases, as expected. At this point let us emphasize again that mean-field theory cannot provide accurate quantitative results for T_{c}, but, as we have seen, it helps us work out and interpret the qualitative behaviour. In fact, more sophisticated renormalization group calculations [9] confirm the picture obtained in this way.

5. Beyond mean-field theory

After studying mean-field theory for the critical temperature of Bose gases in power-law potentials, there arises the question of whether it is possible to also take into account effects beyond mean-field in a simple way. In [14, 15] it was proposed that for sufficiently inhomogeneous, for example harmonic, potentials these effects can be incorporated by replacing the mean-field condensation condition $(\beta\mu)_c = 4q\zeta(3/2)$ by the exact relation for the homogeneous gas. This approach is expected to provide a more accurate description of the critical atomic density distribution $n^{(\mathrm{cr})}(\mathbf{r})$ in regions sufficiently far away from the trap centre so that equation (9) is applicable. The additional 'large-scale' changes in $n^{(\mathrm{cr})}(\mathbf{r})$ or $f^{(\mathrm{cr})}(\mathbf{r})$, respectively, that are introduced in this way, are assumed to contribute more to the shift in T_{c} than effects directly related to the phase transition at the trap centre. In [14], the improved condensation condition is obtained from a renormalization group calculation, whereas in [15] the analytical approximation

$$(\beta\mu)_c \simeq 4q\zeta(3/2) + (c_2' \ln q + c_2'')q^2 = 4q\zeta(3/2) + \delta(\beta\mu)_c, \tag{34}$$

with $c_2' = 32\pi$ and $c_2'' \approx 386.7$ is derived.

It is instructive to generalize the result for harmonic traps obtained in [15] to arbitrary power-law potentials. Using the mean-field framework described in section 3, one finds that the 'modified' critical temperature $T_c^{(\mathrm{mod})}$ obeys the relation

$$\left(\frac{T_c^{(\mathrm{mod})}}{T_c^{(0)}}\right)^{\eta+1} = \frac{\zeta(\eta+1)\Gamma(\eta-1/2)}{\int_0^\infty \mathrm{d}x\, x^{\eta-3/2} f_{\mathrm{mod}}^{(\mathrm{cr})}(x)}, \tag{35}$$

where $f_{\mathrm{mod}}^{(\mathrm{cr})}(x)$ is determined by

$$f_{\mathrm{mod}}^{(\mathrm{cr})}(x) = F_{3/2}\big[x + 4q\big(f_{\mathrm{mod}}^{(\mathrm{cr})}(x) - \zeta(3/2)\big) - \delta(\beta\mu)_c\big], \tag{36}$$

i.e. $f_{\mathrm{mod}}^{(\mathrm{cr})}(x) = f_{\mathrm{MF}}^{(\mathrm{cr})}(x - \delta(\beta\mu)_c)$. In the same way as in section 3, we can derive the expansion

$$\begin{aligned}\int_0^\infty \mathrm{d}x\, x^{\eta-3/2} f_{\mathrm{mod}}^{(\mathrm{cr})}(x) &= \Gamma(\eta-1/2)\zeta(\eta+1) + C_1(\eta)q + \Gamma(\eta-1/2)\zeta(\eta)(c_2'\ln q + c_2'')q^2 \\ &\quad + (16\pi)^\eta \frac{\Gamma(\eta+1/2)\Gamma(-\eta)}{\eta-1/2} q^{2\eta}\left[1 - \frac{c_2'\ln q + c_2''}{16\pi}\right]^\eta + C_2(\eta)q^2 + o(q^2), \end{aligned} \tag{37}$$

where we have used that $\mathcal{R}\int_0^\infty x^{\eta-3/2}F_{1/2}(x)\,\mathrm{d}x = \Gamma(\eta-1/2)\zeta(\eta)$. For $\eta = 2$, where the term containing $q^{2\eta}$ is negligible, this result reproduces the main correction $\Gamma(3/2)\zeta(2)(c_2'\ln q + c_2'')q^2$ to mean-field theory found in [15]. This contribution is introduced through the first-order term in a Taylor series expansion of equation (36) analogously to equation (22).

It should be noted, however, that [15] uses the perturbative result of [22] instead of mean-field theory in order to calculate the function $f^{(\mathrm{cr})}$. Perturbation theory yields the same first-order approximation to $f^{(\mathrm{cr})}$ as mean-field—which is why we obtain the same main correction term—, but leads to a somewhat different second-order contribution. For this reason, our result differs from [15] with regard to the term $C_2(\eta)q^2$. As seen in section 4, however, this term is of only small qualitative significance. More important in the present context is the fact that perturbation theory cannot be used to continue $f^{(\mathrm{cr})}$ to the trap centre due to infrared divergences. The mean-field expression for $f^{(\mathrm{cr})}$, on the other hand, is well defined for all x. It thus allows us to obtain at least an estimate for the transition temperature even for quasi-homogeneous potentials where the main contributions to the integral $\int_0^\infty \mathrm{d}x\, x^{\eta-3/2} f^{(\mathrm{cr})}(x)$ come from the region of small x.

From equation (37) we can draw the following conclusions. (i) Although the modified result has a slightly different analytical structure, it does not lead to essential qualitative changes in the behaviour of the critical temperature. The main qualitative results of the discussion in section 4 still remain valid. (ii) The corrections change the mean-field expression (26) beyond linear order in q. A necessary—although obviously not sufficient—condition for the *quantitative* validity of mean-field theory is thus the requirement that the linear approximation to (26) (i.e. negligence of the terms of higher order in q) describes the exact mean-field result well. If this condition is not fulfilled, the mean-field result also contains contributions from the inaccurate higher-order terms. Using this criterion, one can immediately infer the areas in figure 1 where mean-field theory can be valid quantitatively. For example, for $q = 10^{-8}$ (figure 1(a)), the exact mean-field result and the linear approximation agree for $\eta \gtrsim 0.7$, whereas for $q = 10^{-4}$ and $q = 10^{-3}$ (figures 1(b) and (c)), agreement is shifted to $\eta \gtrsim 0.9$ and $\eta \gtrsim 1.2$, respectively. In these regions, the necessary condition for the quantitative validity of mean-field theory is fulfilled. (iii) The most prominent differences between the mean-field and the modified result arise in the limit $\eta \to 0.5$. Whereas for the homogeneous Bose gas, mean-field predicts a critical temperature independent of the atomic interactions, the modified result yields a positive shift in T_c proportional to $q|\ln q|^{1/2}$. However, this is still in disagreement with current theories [4, 5] which predict a linear increase with q. Using the numerical values for c_2' and c_2'' given above, the shift also turns out to be too large.

6. Summary

In this paper, mean-field theory was applied to study the condensation, and in particular the critical temperature, of interacting Bose gases in general power-law potentials. Compared to previous studies of this subject [10–13], progress has been made in several aspects of the problem. First, the use of the density function $\tilde{\rho}(\varepsilon)$ of equation (4) allows us to write the general mean-field expression (13) for T_c in terms of a one-dimensional (instead of 3D) integral even for arbitrary anisotropic power-law potentials. This greatly simplifies the further analytical and numerical work.

The previous studies considered the dependence of the critical temperature on the interaction parameter $q = a/\lambda_T$ only up to first order. This is justified for the study of sufficiently inhomogeneous, e.g. harmonic, potentials. However, it turns out that the consideration of higher-order contributions is indispensable for understanding the general behaviour of the mean-field result, especially when turning towards the quasi-homogeneous regime. We have therefore derived an analytical approximation to T_c, which is of second order in q, and verified its validity by comparing it to numerical calculations. Besides terms linear and quadratic in q, the resulting expression (30) also contains a term proportional to $q^{2\eta}$ with η being the potential shape parameter (2). The approximation describes the exact mean-field result well for all types of potentials and can thus serve as a comparison tool for further treatment of the problem with more accurate methods.

Using the mean-field results, we have worked out main qualitative aspects of how the critical temperature depends on the shape of the trapping potential. It is known that the behaviour of T_c is governed by different physical mechanisms in the homogeneous and inhomogeneous regimes. With the help of the derived approximation, we have been able to identify the crossover between these limits, as different terms can be associated with contributions characteristic for the two regimes. Certainly, the mean-field approach cannot provide a quantitatively accurate description of the problem. Nevertheless, the emerging qualitative picture has been confirmed by a recent renormalization group study [9].

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