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Weakly interacting Bose–Einstein condensates in temperature-dependent generic traps

Dedicated to the loving memory father El'ias Castellanos de Luna

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We study the shift ΔT_c in the condensation temperature of an atomic Bose–Einstein condensate trapped in a temperature-dependent three-dimensional generic potential. With no assumptions other than the mean-field approach and the semiclassical approximation, it is shown that the inclusion of a T-dependent trap improves upon the pure semiclassical result giving better agreement between the predicted ΔT_c and its experimental value. However, despite this improvement, the effect of a T-dependent trap is not sufficient to fully reduce the discrepancy between theoretical prediction and data.

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I. Introduction. Since its theoretical prediction by Bose and Einstein [1, 2] in the 1920s until its laboratory observation with magneto-optical traps [3–6] from 1995 onwards Bose–Einstein condensation (BEC) of dilute atomic gases has stimulated enormous efforts of related work. Among the issues addressed one finds, e.g., rigorous mathematical questions related to BEC [7], diverse theoretical and heuristic aspects [8, 9], and is now even viewed as a viable tool for precision tests in gravitational physics [10–20].

The study of its associated thermodynamic properties is naturally also a pertinent aspect of BECs [21–25]. Indeed, the condensation temperature T_c, i.e., the critical temperature below which a macroscopic quantum state of matter appears, has been the subject of considerable discussion, see Ref. [8, 26] and Refs. therein. In particular, the influence of interparticle interactions on T_c turns out to be a deep nontrivial matter, see e.g. Refs. [27–29].

Interboson interactions produce a shift $\Delta T_c/T_c^0 \equiv (T_c-T_c^0)/T_c^0$ in the condensation temperature T_c with respect to that of the ideal noninteracting case T_c^0 in the thermodynamic limit. For instance, the contributions to $\Delta T_c/T_c^0$ due to interactions in a uniform dilute gas originate in the fact that the associated many-body system is affected by long-range critical fluctuations rather than from purely mean-field (MF) considerations [26, 30, 31]. However, it is generally accepted that $\Delta T_c/T_c^0$ for this system behaves like $c_1\delta+(c_2'\ln\delta+c_2'')\delta^2$, with the dimensionless variable $\delta\equiv\rho^{1/3}a$ where ρ is the corresponding boson number density, a the S-wave two-body scattering length [30] related to the pair interaction, and the c_i's are dimensionless constants. A good fit [27] gives $c_1\simeq 1.32$, $c_2'\simeq 19.75$, and $c_2''\simeq 75.7$.

It is noteworthy that these ideas can be extended to more general traps [32–34] in which the relative shift $\Delta T_c/T_c^0$ on the condensation temperature explicitly exhibits a sensitive trap-dependence. This extension to *generic* traps allows summarizing the corrections on $\Delta T_c/T_c^0$ as function of a simple index parameter describing the trap *shape*.

On the other hand, when interactions are considered for the more common *harmonic* traps one finds a shift in T_c up to second order in the S-wave scattering length a within the MF approach given by [28, 29]

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$$\frac{\Delta T_c}{T_c^0} \simeq b_1(a/\lambda_{T_c^0}) + b_2(a/\lambda_{T_c^0})^2, \tag{1}$$

where

$$k_{\rm B}T_c^0 = \hbar\omega[N/\zeta(3)]^{1/3} \tag{2}$$

(with $\zeta(3) \simeq 1.202$) is the condensation temperature associated with the ideal system ($a = 0$) in the thermodynamic limit [22], and $b_1 \simeq -3.426$ [35] while $b_2 \simeq 11.7$ [29], together with $\lambda_{T_c^0} \equiv (2\pi\hbar^2/mkT_c^0)^{1/2}$ the thermal wavelength. Furthermore, these results seem to contrast with the results reported, e.g., in Refs. [36, 37] since, as mentioned in Ref. [28], the well-known logarithmic corrections to (1) are not discernible within the error bars.

Note that from (1) ΔT_c is negative for repulsive interactions, i.e., $a > 0$ since b_1 is negative. The result (1) is in excellent agreement with laboratory measurements of $\Delta T_c/T_c^0$ [29, 38–40] to first order in $(a/\lambda_{T_c^0})$ but differs somewhat with data to second order $(a/\lambda_{T_c^0})^2$. In Ref. [28], high precision measurements of the condensation temperature of the bosonic atom ^{39}K vapor in the range of parameters $N \simeq (2{-}8)\cdot 10^5$, $\omega \simeq (75{-}85)$ Hz, $10^{-3} < a/\lambda_{T_c^0} < 6\cdot 10^{-2}$ and $T_c \simeq (180{-}330)$ nK have detected second-order effects in $\Delta T_c/T_c^0$. The measured $\Delta T_c/T_c^0$ is well fitted by a quadratic polynomial (1) with best-fit parameters $b_1^{\rm exp} \simeq -3.5 \pm 0.3$ and $b_2^{\rm exp} \simeq 46 \pm 5$ so that the value $b_2 \simeq 11.7$ [29] is strongly excluded by data. This discrepancy between (1) and data may be due to beyond-MF effects (see Ref. [29]). Beyond-MF effects are expected to be important near criticality, where the physics is often nonperturbative. It would therefore seems reasonable that a beyond-MF treatment might give a correct estimation of b_2. However, this is not certain since beyond-MF effects have been calculated in the case of *uniform* condensates [37, 41] but are still poorly understood for *trapped* BECs [36, 42, 43–45]. It thus seems that it is currently not possible to ascertained whether the discrepancy between b_2 and $b_2^{\rm exp}$ can be explained in the MF context or arises from beyond-MF effects.

Nevertheless, the effect of interactions on the condensation temperature T_c of a Bose–Einstein condensate trapped in a harmonic potential was recently discussed [35]. In the latter paper it was shown that, within the MF Hartree–Fock (HF) and semiclassical approximations, interactions among the particles produce a shift $\Delta T_c/T_c^0 \simeq b_1(a/\lambda_{T_c^0}) + b_2(a/\lambda_{T_c^0})^2 + \psi\left[a/\lambda_{T_c^0}\right]$ with $\lambda_{T_c^0} \equiv (2\pi\hbar^2/mkT_c^0)^{1/2}$ the thermal wavelength, and $\psi\left[a/\lambda_{T_c^0}\right]$ a non-analytic function such that $\psi[0] = \psi'[0] = \psi''[0] = 0$ but $|\psi'''[0]| = \infty$. Therefore, with only the usual assumptions of the HF and semiclassical approximations, interaction effects are perturbative to second order in $a/\lambda_{T_c^0}$ and the expected nonperturbativity of physical quantities at the critical temperature emerges only at third order. Indeed, in Ref. [35] an analytical estimation for $b_2 \simeq 18.8$ was obtained which improves the previous numerical fit-parameter value of $b_2 \simeq 11.7$ obtained in Ref. [29]. Even so, the value for b_2 obtained in Ref. [35] still differs substantially from the empirical value $b_2^{\rm exp} \simeq 46 \pm 5$ [28].

We mention that the temperature shift $\Delta T_c/T_c^0$ induced by interparticle interactions obtained in Ref. [35] seems to contradict, for instance, the result reported in Ref. [36] where the interaction induced temperature shift is estimated as

$$\frac{\Delta T_c}{T_c^0} = b_1(a/\lambda_{T_c^0}) + \left[b_2' + b_2'' \ln(a/\lambda_{T_c^0})\right](a/\lambda_{T_c^0})^2 \tag{3}$$

with $b_1 \simeq -3.426$, $b_2' \simeq -45.86$, and $b_2'' \simeq -155.0$ [37] (see also Ref. [27] for a discussion). This result has been obtained using lattice simulations and a technique based on a scalar field analogy, but is questionable (see discussion in Ref. [35]) besides being in striking contradiction to the data. It is thus clear that these results differ substantially from the estimations obtained in Ref. [35] and the results obtained here (see below), but also conflict with the results obtained in Ref. [29] as well as experiment [28].

Also, it was recently proposed [46] that accounting for a nonlinear quadratic Zeeman effect gives a value of b_2 which depends on the properties of the atomic species of the condensate, which for a ^{39}K condensate gives a value $b_2 \simeq 42.3$ in much better agreement with measurements obtained in Ref. [28]. But this result is based on a physical mechanism completely different from the one considered here. Furthermore, to confirm whether that the quadratic Zeeman effect actually plays such an important role in the physics of atomic condensates, one should repeat the measurements performed in Ref. [28] for different atomic species and compare the results with the predictions obtained in Ref. [46]. However, to our knowledge, Ref. [28] is the only reported measurement of the nonlinear coefficient b_2.

We therefore propose that before addressing beyond-MF effects these facts suggest that MF effects might still be well-understood and deserve further analysis.

In fact, in a recent paper [47] the use of an effective *temperature-dependent trapping potential* was suggested in order to calculate the condensation temperature of noninteracting systems; see also Ref. [48] for a wide-ranging justification of T-dependent Hamiltonians. Hence, it might be useful to explore this idea in the context of the effects on the condensation temperature caused by interparticle interactions.

These considerations drove us into the novel terrain of T-dependent Hamiltonians, and more specifically to T-dependent trapping potentials. We note that this it is not the first time that such a terrain has been reached, e.g., we find the successful use of T-dependent dynamics in: a) superconductivity in the work of Bogoliubov, Zubarev, and Tserkovnikov, as mentioned by Blatt [49]; b) an explanation [50] of the empirical law in superconductors $H_c(T) = H_c(0)[1 - (T/T_c)^2]$ where $H_c(T)$ is the critical magnetic field at T; c) finite-T behavior [24, 25, 51–54] of a class of relativistic field theories (RFTs) to address the question of restoration of a symmetry which at $T = 0$ is broken either dynamically or spontaneously; d) the Wick–Cutkosky model [55] in a RFT; 5) numerous unidentified solar-emission lines [56]; e) QCD to explain [57, 58] the masses of different quarkonium families and their deconfinement temperatures; and most recently, as mentioned above, f) in a comparative study [47] of the experimental features of the Bose–Einstein condensates in several species of bosonic atomic gases.

We thus examine the possibility of such T-dependent generic potentials in order to analyze (and hopefully even improve upon) the value $b_2 \simeq 18.8$ obtained in Ref. [35] within the HF MF theory, and also to explore its discrepancy with the empirical value $b_2^{\rm exp} \simeq 46 \pm 5$. Our conclusion is that, even though the inclusion of a temperature dependence in the trapping potential might improve the predicted value of b_2, this is not sufficient to obtain full agreement with data. We stress that we consider T-dependent effective potentials from a phenomenological point of view. In other words, the inclusion of such external potentials is of theoretical and/or mathematical interest, in order to analyze, for instance, the shift in the condensation temperature caused by interactions. For all this we now entertain T-dependent generic traps $V(r, T)$.

II. Mean field Hartree–Fock approximation. Following Ref. [35] we define the following semiclassical energy spectrum in the MF HF approximation (see, e.g., [8, 22])

$$E(p, r, g) = \epsilon(p, r) + 2g\, n(r, g), \tag{4}$$

where $\epsilon(p, r) \equiv p^2/2m + V(r)$ with $V(r)$ the external potential, $n(r, g)$ the spatial density of bosons, and $g \equiv 4\pi\hbar^2 a/m$ the parameter describing the interaction.

Moreover, the semiclassical condition allows approximating summations over energy states by integrals, namely $\sum_{\mathbf{k},\mathbf{r}} \to \int d^3r d^3p/(2\pi\hbar)^3$. Therefore, the number of particles N in three-dimensional space obeys the normalization condition [8, 22]

$$N = N_0 + \int \frac{d^3r d^3p}{(2\pi\hbar)^3} \left\{ \exp\left[\frac{E(p, r, g) - \mu}{k_{\rm B} T} \right] - 1 \right\}^{-1}, \tag{5}$$

where N_0 is the number of particles in the ground state, μ – the corresponding chemical potential, and $k_{\rm B}$ – the Boltzmann constant.

At the condensation temperature T_c we assume within MF theory that the chemical potential μ is given by [35]

$$\mu_c(g) = 2g\, n(r = 0, g). \tag{6}$$

Further assuming just above T_c that in the ground state N_0 is negligible it follows that

$$N\pi\hbar^3/2 = \int dr dp r^2 p^2 \times \\ \times \left\{ \exp\left[\frac{E(p, r, g) - \mu_c(g)}{k_{\rm B} T_c(g)} \right] - 1 \right\}^{-1} \equiv \int d\Omega \Lambda\left[\theta\right], \tag{7}$$

where

$$d\Omega \equiv dr dp r^2 p^2, \quad \Lambda\left[\theta\right] \equiv \left[\exp\theta - 1\right]^{-1},$$

$$\theta \equiv \frac{\epsilon(p, r) + 2\bar{n}(r, g)}{k_{\rm B} T_c(g)}, \quad \bar{n}(r, g) \equiv n(r, g) - n(0, g). \tag{8}$$

From (7) we are able to extract, in principle, T_c as a function of the parameter g describing interactions. Note that the scattering length a can be positive or negative, its sign and magnitude depending crucially on the details of the atom-atom potential [8]. However, a negative scattering length could lead to instabilities within the system [22], and finite-size effects could be important in this situation due to the number of particles N not being large enough [8]. Here, we restrict ourselves, as usual, to positive values of the interaction parameter g in order to compare our results with the reported [28] experimental data.

On the other hand, if ΔT_c is analytic in g one can express the relative shift in T_c for small values of g as follows

$$\frac{\Delta T_c}{T_c^0} = \sum_{h=1}^{\infty} \frac{g^h}{h!} \frac{\partial_g^h T_c(g)}{T_c(g)} \bigg|_{g=0}. \tag{9}$$

Note that $T_c(g = 0) = T_c^0$ is by definition the T_c for the noninteracting system, given by (2). Additionally, the expansion coefficients can be expressed as

$$\frac{\partial_g^h T_c(g)}{T_c(g)} \bigg|_{g=0} \equiv \frac{I_h}{\left(k_{\rm B} T_c^0 \lambda_{T_c^0}^3\right)^h}, \tag{10}$$

where the numerical factors I_h depend on the external potential under consideration and can be calculated explicitly.

This enables one to reexpress (9) as a power series in the dimensionless interaction-dependent variable $a/\lambda_{T_c^0}$

$$\frac{\Delta T_c}{T_c^0} = \sum_{h=1}^{\infty} \frac{2^h I_h}{h!} \left(a/\lambda_{T_c^0}\right)^h \equiv \sum_{h=1}^{\infty} b_h \left(a/\lambda_{T_c^0}\right)^h \qquad (11)$$

which defines the coefficients b_h. For an isotropic harmonic potential $V(r) \sim r^2$ the first two factors I_1 and I_2 are given respectively by [35]

$$I_1 = 2\frac{\displaystyle\int d\Sigma\, \Lambda' \left[u^2+v^2\right] Q\left[v^2\right]}{\displaystyle\int d\Sigma\, \left(u^2+v^2\right) \Lambda' \left[u^2+v^2\right]}, \qquad (12)$$

$$I_2 = 4\int d\Sigma \Big\{\Lambda' \left[u^2+v^2\right] S\left[v^2\right] + \Lambda'' \left[u^2+v^2\right] \times \qquad (13)$$
$$\times \left[Q[v^2] - \frac{1}{2}[u^2+v^2]I_1\right]^2\Big\} \Big/ \int d\Sigma (u^2+v^2)\Lambda'[u^2+v^2],$$

where $d\Sigma \equiv dudvu^2v^2$, $Q[\alpha] \equiv g_{3/2}\left[\exp(-\alpha)\right] - g_{3/2}\left[1\right]$, and $g_\alpha[z] = \sum_{k=1}^{\infty} z^k/k^\alpha$ is the so-called Bose–Einstein function [59]. Thus $S[\alpha] \equiv \frac{3}{2}I_1 Q[\alpha] + (\alpha I_1 - 2Q[\alpha])\, g_{1/2}\left[\exp(-\alpha)\right]$ with $\alpha \equiv \left[V(r) + 2g\bar{n}(r,g)\right]/k_{\rm B}T_c(g)$, see Ref. [35] for details.

Note that the assumptions used above lead to $b_1 \simeq -3.426$ in agreement with the experimental $b_1 \simeq -3.5 \pm 0.3$ obtained in Ref. [28]. Also, one gets $b_2 \simeq 18.8$ which improves upon the estimation of $b_2 \simeq 11.7$ in Ref. [29]. However, this value still remains much smaller than the experimental estimation $b_2^{\rm exp} \simeq 46 \pm 5$ reported in Ref. [28].

III. ***T*-dependent generic potentials and T_c.** Here we consider the following T-dependent generic potentials

$$V(r,T) = \frac{m\omega^2 r^2}{2}\left[1 + d\left(\frac{m\omega^2 r^2}{2k_{\rm B}T}\right)^{\beta/2}\right], \qquad (14)$$

$$V(r,T) = \frac{m\omega^2 r^2}{2}\left(\frac{m\omega^2 r^2}{2k_{\rm B}T}\right)^{\delta/2} \qquad (15)$$

for $T = T_c$ and with d, β, and δ dimensionless parameters.

A. T-dependent generic potential with free parameters d and β. Here we use the potential (14) and find $b_1(d,\beta)$ from (10) for $h = 1$ as a function of d and β, which reads

$$\left.\frac{\partial_g T_c(g)}{T_c(g)}\right|_{g=0} = \frac{I_1(d,\beta)}{k_{\rm B}T_c^0 \lambda_{T_c^0}^3}, \qquad (16)$$

where

$$I_1 = 2\frac{\int d\Sigma \Lambda' \left[u^2+v^2(1+dv^\beta)\right] Q\left[v^2(1+dv^\beta)\right]}{\int d\Sigma \left[u^2+v^2(1+dv^\beta)\right] \Lambda' \left[u^2+v^2(1+dv^\beta)\right]}. \qquad (17)$$

This integral can be evaluated numerically for b_1 which gives

$$b_1(d,\beta) = 2I_1(d,\beta). \qquad (18)$$

Therefore one can find a range of values of d and β which are in agreement with the empirical value $b_1 \simeq -3.5 \pm 0.3$ found in Ref. [28]. On the other hand, we may calculate $b_2(d,\beta)$ from for the parameters under consideration from

Table 1

Values of $b_1(\beta,d)$, $b_2(\beta,d)$ obtained from the parameters d and β

β	d	$b_1(d,\beta)$	$b_2(d,\beta)$
−1	0.01	−3.41931	18.6006
−1	0.1	−3.36182	17.3356
−1	10	−2.36313	6.64378
0	0	−3.42603	18.7765
0	0.1	−3.42603	18.7765
0	1	−3.42603	18.7765
0	10	−3.42603	18.7765
1	0.1	−3.51504	20.2565
1	1	−3.76418	25.2715
1	10	−3.97423	31.7773
2	0.1	−3.63134	22.0627
2	1	−3.98266	29.4989
2	10	−4.26837	39.7218

$$I_2(d,\beta) = 4\int d\Sigma \Big(\Lambda'\left[u^2+v^2(1+dv^\beta)\right] \times$$
$$\times S\left[v^2(1+dv^\beta)\right] + \Lambda''\left[u^2+v^2(1+dv^\beta)\right] \times$$
$$\times \left\{Q[v^2(1+dv^\beta)] - \frac{1}{2}[u^2+v^2(1+dv^\beta)]I_1(d,\beta)\right\}^2\Big)$$
$$\times \left\{\int d\Sigma[u^2+v^2(1+dv^\beta)\Lambda'[u^2+v^2(1+dv^\beta)]\right\}^{-1}, \qquad (19)$$

where

$$S[\alpha] \equiv \frac{3}{2}I_1(d,\beta)Q[\alpha] + \{\alpha I_1(d,\beta) - 2Q[\alpha]\}\, g_{1/2}\exp(-\alpha). \qquad (20)$$

From this one obtains

$$b_2(d,\beta) = 2I_2(d,\beta). \qquad (21)$$

We remark that the case $\beta = -1$ corresponds to the potential suggested in Ref. [47]. Table 1 shows the results obtained for b_1 and b_2 from different values of parameters d and β. We found that for $\beta = 1$ and $d = 1$, $b_1 \simeq -3.764$ which is in agreement with the experimental value $b_1^{\exp} \simeq -3.5 \pm 0.3$ obtained in Ref. [28]. We also obtain $b_2 \simeq 25.27$ which improves upon the result $b_2 \simeq 18.8$ obtained in Ref. [35]. However, our estimation for the parameter b_2 still remains smaller than the experimental estimation $b_2^{\exp} \simeq 46 \pm 5$ reported in Ref. [28].

B. Temperature-dependent generic potential with free parameter δ. On the other hand, for the potential (15) Eq. (10) is only a function of δ since

$$\left.\frac{\partial_g T_c(g)}{T_c(g)}\right|_{g=0} = \frac{I_1(\delta)}{k_B T_c^0 \lambda_{T_c^0}^3}, \tag{22}$$

where now

$$I_1 = 2\frac{\int d\Sigma \Lambda' \left[u^2 + v^{2+\delta}\right] Q\left[v^{2+\delta}\right]}{\int d\Sigma \left(u^2 + v^{2+\delta}\right) \Lambda' \left[u^2 + v^{2+\delta}\right]}. \tag{23}$$

This integral must also be evaluated numerically in order to obtain the value of b_1

$$b_1(\delta) = 2I_1(\delta). \tag{24}$$

Thus, one can find a range of values of δ which are in agreement with the empirical value $b_1 \simeq -3.5 \pm 0.3$. Table 2 shows the results obtained for $b_1(\delta)$ and $b_2(\delta)$ from different values of the parameter δ, we found that, for $\delta = 0.5$, $b_1 \simeq -3.7862$ which is in agreement with the experimental value $b_1^{\exp} \simeq -3.5 \pm 0.3$ obtained in Ref. [28], and consequently we select $b_2 \simeq 25.986$:

Table 2

Values of $b_1(\delta)$ and $b_2(\delta)$ obtained from the parameter δ

δ	$b_1(\delta)$	$b_2(\delta)$
−0.1	−3.34203	17.3782
0	−3.42603	18.7765
0.1	−3.50564	20.1912
0.2	−3.58118	21.621
0.3	−3.65295	23.0644
0.5	−3.78626	25.986
1	−4.06981	33.3811

$$b_2(\delta) = 2I_2(\delta). \tag{25}$$

A similar procedure leads to

$$I_2(\delta) = 4\int d\Sigma(\Lambda'[u^2 + v^{2+\delta}]S\left[v^{2+\delta}\right] +$$
$$+\Lambda''[u^2 + v^{2+\delta}]\{Q[v^{2+\delta}] - \frac{1}{2}(u^2 + v^{2+\delta})I_1(\delta)^2\}) \times$$
$$\times \left\{\int d\Sigma \left(u^2 + v^{2+\delta}\right) \Lambda' \left[u^2 + v^{2+\delta}\right]\right\}^{-1}, \tag{26}$$

where

$$S[\alpha] \equiv \frac{3}{2} I_1(\delta) Q[\alpha] + [\alpha I_1(\delta) - 2Q[\alpha]]\, g_{1/2} \exp(-\alpha) \tag{27}$$

from which one obtains $b_2(\delta)$ (see Table 2). Note that, even though the potential (15) contains only one parameter, it gives better agreement with data than the potential (14) which contains two parameters.

IV. Conclusions. We have explored the shift in the condensation temperature up to second order in the S-wave scattering length, for a Bose–Einstein condensate trapped in a temperature-dependent generic potential, with no further assumptions than the semiclassical and Hartree–Fock approximations. Thus, we have recovered the usual value for the parameter b_1, and consequently, were able to improve the numerical value associated with the second parameter b_2 up to 25.271 for the corresponding potential (14), and 25.986 for the second potential (15) compared to the value obtained in Ref. [35] under typical laboratory conditions. However, the corresponding values for b_2 obtained here remain smaller than the experimental value reported in Ref. [28]. Such disagreement might be related to effects beyond the HF MF framework. Finally, we stress here that the use of temperature-dependent traps open up a very interesting line of research for other relevant properties associated with Bose–Einstein condensates.

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