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Origin of nonlinear contribution to the shift of the critical temperature in atomic Bose–Einstein condensates

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We discuss a possible origin of the experimentally observed nonlinear contribution to the shift $\Delta T_c = T_c - T_c^0$ of the critical temperature T_c in an atomic Bose–Einstein condensate (BEC) with respect to the critical temperature T_c^0 of an ideal gas. We found that accounting for a nonlinear (quadratic) Zeeman effect (with applied magnetic field closely matching a Feshbach resonance field B_0) in the mean-field approximation results in a rather significant renormalization of the field-free nonlinear contribution b_2, namely $\Delta T_c/T_c^0 \simeq b_2^*(a/\lambda_T)^2$ (where a is the s-wave scattering length, λ_T is the thermal wavelength at T_c^0) with $b_2^* = \gamma^2 b_2$ and $\gamma = \gamma(B_0)$. In particular, we predict $b_2^* \simeq 42.3$ for the $B_0 \simeq 403$ G resonance observed in the ^{39}K BEC.

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Studies of Bose–Einstein condensates (BECs) continue to be an important subject in modern physics (see, e.g., Refs. [1–4] and further references therein). Atomic BECs are produced in the laboratory in laser-cooled, magnetically-trapped ultra-cold bosonic clouds of different atomic species (including ^{87}Rb [5, 6], ^{7}Li [7], ^{23}Na [8], ^{1}H [9], ^{4}He [10], ^{41}K [11], ^{133}Cs [12], ^{174}Yb [13], and ^{52}Cr [14], among others). Also, a discussion of a relativistic BEC has appeared in Ref. [15] and BECs of photons are most recently under investigation [16]. In addition, BECs are successfully utilized in cosmology and astrophysics [17] as they have been shown to constrain quantum gravity models [18].

In the context of atomic BECs interparticle interactions must play a fundamental role since they are necessary to drive the atomic cloud to thermal equilibrium. Thus, they must be carefully taken into account when studying the properties of the condensate. For instance, interatomic interactions change the condensation temperature T_c of a BEC, as was pointed out first by Lee and Yang [19, 20] (see also Refs. [21–30] for more recent works).

The first studies of interactions effects were focused on *uniform* BECs. Here, interactions are irrelevant in the mean field (MF) approximation (see Refs. [25, 28–30]) but they produce a shift in the condensation temperature of uniform BECs with respect to the ideal noninteracting case, which is due to quantum correlations between bosons near the critical point. This effect has been finally quantified in [25, 26] as $\Delta T_c/T_c^0 \simeq 1.8(a/\lambda_T)$, where $\Delta T_c \equiv T_c - T_c^0$ with T_c the critical temperature of the gas of interacting bosons, T_c^0 is the BEC condensation temperature in the ideal noninteracting case, a is the s-wave scattering length used to represent interparticle interactions [1, 3, 4], and $\lambda_T \equiv \sqrt{2\pi\hbar^2/m_a k_{\rm B} T_c^0}$ is the thermal wavelength for temperature T_c^0 with m_a the atomic mass.

But laboratory condensates are not uniform BECs since they are produced in atomic clouds confined in magnetic traps. For trapped BECs, interactions affect the condensation temperature even in the MF approximation, and the shift in T_c in terms of the s-wave scattering length a is given by

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

with $b_1 \simeq -3.4$ [1] and $b_2 \simeq 18.8$ [31].

High precision measurements [32] of the condensation temperature of ^{39}K in the range of parameters $N \simeq (2–8)\cdot 10^5$, $10^{-3} < a/\lambda_T < 6\cdot 10^{-2}$ and $T_c \simeq (180–330)$ nK have detected second-order (nonlinear) effects in $\Delta T_c/T_c^0$ fitted by the expression $\Delta T_c/T_c^0 = b_2^{\rm exp}(a/\lambda_T)^2$ with $b_2^{\rm exp} \simeq 46 \pm 5$. This re-

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sult has been achieved exploiting the high-field 403 G Feshbach resonance in the $|F, m_F\rangle = |1,1\rangle$ hyperfine (HF) state of a ^{39}K condensate where $F \equiv S + I$ is the total spin of the atom with S and I being electron and nuclear spin, respectively, and m_F is the projection quantum number. Thus, the theoretically predicted [31] quadratic-amplitude coefficient b_2 turned out to be in a rather strong disagreement with the available experimental data. There have also been some efforts to theoretically estimate the correct value of b_2 in the MF approximation by considering anharmonic and even temperature-dependent traps [33], which however have not been too successful. Therefore one could expect that a more realistic prediction of the experimental value of $b_2^{\rm exp}$ should take into account some other so far unaccounted effects.

The main goal of this paper is to show that, taking into account the nonlinear (quadratic) Zeeman effect and using the MF approximation, it is quite possible to explain the experimentally observed [32] value of b_2 for the 403 G resonance of the hyperfine $|F, m_F\rangle = |1,1\rangle$ state of ^{39}K with no need to go beyond-MF approximation.

Recall that experimentally the s-wave scattering length parameter a is tuned via the Feshbach-resonance technique based on Zeeman splitting of bosonic atom levels in an applied magnetic field. This means that the interaction constant $g \equiv (4\pi\hbar^2 a/m_a)$ is actually *always* field-dependent. More explicitly, according to the interpretation of the Feshbach resonance [34, 35]

$$a(B) = a_{bg}\left(1 - \frac{\Delta}{B - B_0}\right), \qquad (2)$$

where a_{bg} is a so-called background value of a, B_0 is the resonance peak field, and Δ, the width of the resonance.

Thus, in order to properly address the problem of condensation-temperature shifts (which are always observed under application of a nonzero magnetic field B), one must account for a Zeeman-like contribution. It should be emphasized, however, that a single (free) atom Zeeman effect (induced by either electronic or nuclear spin) $\mu_a B$ is not important for the problem at hand simply because it can be accounted for by an appropriate modification of the chemical potential.

Recall that in the presence of a linear Zeeman effect, the basic properties of an atomic BEC can be understood within the so-called "condensate wave function"approximation [2]

$$\mathcal{H} = \int d^3x H(x), \qquad (3)$$

where $H(x) = gn^2 - E_{\rm Z} n$ with $n(x) = \Psi^+(x)\Psi(x)$ being the local density of the condensate ($\Psi(x)$ is the properly defined wave function of macroscopic condensate), and $E_{\rm Z} = \mu_{\rm B} B$ the Zeeman energy (with $\mu_{\rm B}$ being the Bohr magneton).

Following Bogoliubov's recipe [36], let us consider small deviation of the condensate fraction from the ground state n_0 (the number) by assuming that $n(x) \simeq \simeq n_0 + \delta n(x)$ with $\delta n(x) \ll n_0$. Treating, as usually, n_0 and $\delta n(x)$ independently, we obtain from Eq. (3) that in the presence of the linear Zeeman effect $gn_0 = E_{\rm Z}$ (meaning that $E_{\rm Z}$ is playing a role of the chemical potential [37]) and, as a result, the BEC favors the following energy minimum:

$$\delta H_0(x) = 2gn_0\delta n(x) - E_{\rm Z}\delta n(x) = gn_0\delta n(x), \qquad (4)$$

Thus, we come to the conclusion that at low magnetic fields (where the linear Zeeman effect is valid), in accordance with the available experimental results [37], there is no any tangible change of the BEC properties (including g modification). On the other hand, there is a clear-cut experimental evidence [38, 39] in favor of the so-called Breit–Rabi nonlinear (quadratic) HF-mediated Zeeman effect [40] in BEC. We are going to demonstrate now how this nonlinear phenomenon (which is not a trivial generalization of the linear Zeeman effect) affects the BEC properties (including a feasible condensation temperature shift). Recall that in strong magnetic fields, the magnetic-field energy shift of the sublevel m_F of an alkali-metal-atom ground state can be approximated (with a rather good accuracy) by the following expression [38]

$$E_{\rm NLZ} = A_{\rm HF}\frac{E_{\rm Z}^2}{h\delta\nu_{hf}}, \qquad (5)$$

where $A_{\rm HF} = \left[1 - \frac{4m_F^2}{(2I+1)^2}\right]$ and $\delta\nu_{hf}$ is the so-called hyperfine splitting frequency between two ground states.

Now, by repeating the above-mentioned Bogoliubov's procedure, we obtain a rather nontrivial result for BEC modification. Namely, it can be easily verified that HF-mediated nonlinear Zeeman effect gives rise to the following two *equivalent* options for the energy minimization (based on the previously defined ground state with $E_{\rm Z} = gn_0$): (a) $E_{\rm NLZ} \propto g^2 n_0^2$ or (b) $E_{\rm NLZ} \propto E_{\rm Z} g n_0 = (\mu_{\rm B} B) g n_0$. As a matter of fact, the choice between these two options is quite simple. We have to choose (b) simply because (a) introduces the second order interaction effects ($\propto g^2$) which are neglected in the initial Hamiltonian (3). As a result, the high-field nonlinear Zeeman effect produces the following modification of the local BEC energy:

$$\delta H_{\rm NLZ}(x) \simeq 2gn_0\delta n(x) + A_{\rm HF} g n_0\left(\frac{\mu_{\rm B} B}{h\delta\nu_{hf}}\right)\delta n(x), \qquad (6)$$

Therefore, accounting for nonlinear Zeeman contribution will directly result in a renormalization of the high-field scattering length

$$a^* = a\left(1 + \frac{1}{2}A_{\rm HF}\frac{\mu_{\rm B}B}{h\delta\nu_{hf}}\right). \tag{7}$$

Now, by inverting (2) and expanding the resulting $B(a)$ dependence into the Taylor series (under the experimentally satisfied conditions $a_{bg} \ll a$ and $\Delta \ll B_0$)

$$B(a) \simeq B_0\left\{1 - \frac{\Delta}{B_0}\left[\left(\frac{a_{bg}}{a}\right) + \left(\frac{a_{bg}}{a}\right)^2 + ...\right]\right\} \tag{8}$$

one obtains

$$a^* \simeq \gamma a + O(a_{bg}/a, \Delta/B_0) \tag{9}$$

for an explicit form of the renormalized scattering length due to Breit–Rabi–Zeeman splitting with

$$\gamma \equiv 1 + \frac{1}{2}A_{\rm HF}\left(\frac{\mu_{\rm B}B_0}{h\delta\nu_{hf}}\right). \tag{10}$$

To find the change in b_2 in the presence of the quadratic Zeeman effect one simply replaces the original (Zeeman-free) scattering length a in (1) with its renormalized form a^* given by (9), which results in a nonlinear contribution to the shift of the critical temperature, specifically

$$\frac{\Delta T_c}{T_c^0} \simeq b_2\left(\frac{a^*}{\lambda_T}\right)^2. \tag{11}$$

Furthermore, by using (9), one can rewrite (11) in terms of the original scattering length a and renormalized amplitude b_2^* as follows

$$\frac{\Delta T_c}{T_c^0} \simeq b_2^*\left(\frac{a}{\lambda_T}\right)^2, \tag{12}$$

where the coefficient due to the Breit–Rabi–Zeeman contribution is

$$b_2^* \simeq \gamma^2 b_2 \tag{13}$$

with γ defined earlier.

Let us consider the particular case of the $B_0 \simeq 403$ G resonance of the hyperfine $|F, m_F\rangle = |1,1\rangle$ state of ^{39}K. For this case [41], $S = 1/2$, $m_F = 1$, $I = 3/2$, and $\delta\nu_{hf} \simeq 468$ MHz. These parameters produce $A_{\rm HF} = 3/4$ and $\gamma \simeq 1.5$ which readily leads to the following estimate of the quadratic amplitude contribution due to the HF mediated Breit–Rabi–Zeeman effect, $b_2^* \simeq 2.25 b_2 \simeq 42.3$ (using the mean-field value $b_2 \simeq 18.8$ [31]), in a good agreement with the observations [32]. It is interesting to point out that the obtained value of γ for ^{39}K BEC is a result of a practically perfect match between the two participating energies: Zeeman contribution at the Feshbach resonance field, $\mu_{\rm B}B_0 \simeq 4\cdot 10^{-25}$ J, and the contribution due to Breit–Rabi hyperfine splitting between two ground states, $h\delta\nu_{hf} \simeq 3\cdot 10^{-25}$ J.

And finally, an important comment is in order regarding the applicability of the present approach (based on the Taylor expansion of (2)) to the field-induced modification of the linear contribution (defined via the amplitude b_1 in (1)) to the shift in T_c. According to the experimental curve depicting ΔT_c vs a/λ_T behavior, the linear contribution is limited by $10^{-3} \le a/\lambda_T \le 5\cdot 10^{-3}$. Within the Feshbach-resonance interpretation, this corresponds to a low-field ratio $a/a_{bg} \simeq 1$ which invalidates the Taylor expansion scenario based on using a small parameter $a_{bg}/a \ll 1$ applicable in high fields only. Besides, as we have demonstrated earlier, the linear Zeeman effect (valid at low fields only) is not responsible for any tangible changes of BEC properties. Therefore, another approach is needed to properly address the field-induced variation (if any) of the linear contribution b_1.

To conclude, it was shown that accounting for a hyperfine-interaction induced Breit–Rabi nonlinear (quadratic) Zeeman term in the mean-field approximation can explain the experimentally observed shift in the critical temperature T_c for the ^{39}K condensate. It would be interesting to subject the predicted universal relation (13) to a further experimental test to verify whether or not it can also explain the shift in other bosonic-atom condensates.

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