

Quantum Kinetic Theory of Condensate Growth: Comparison of Experiment and Theory

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In a major extension of our previous model [Phys. Rev. Lett. **79**, 1793 (1997)] of condensate growth, we take account of the evolution of the occupations of lower trap levels, and of the full Bose-Einstein formula for the occupations of higher trap levels. We find good agreement with experiment, especially at higher temperatures. We also confirm the picture of the “kinetic” region of evolution, introduced by Kagan *et al.*, for the time up to the initiation of the condensate. The behavior after initiation essentially follows our original growth equation, but with a substantially increased rate coefficient W^+ . [S0031-9007(98)07849-1]

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Although the first Bose condensed atomic vapor was produced in a magnetic trap only in 1995 [1–3], the kinetics of condensate formation has long been a subject of theoretical study [4,5]. There is now intense theoretical work on Bose-Einstein condensation, which is excellently summarized in [6]. Most theoretical studies of condensate growth either have not treated trapping or have considered only traps which are so broad that the behavior of the vapor is not essentially different from the untrapped situation. Furthermore, they have given only *qualitative* estimates of condensate growth. Our previous paper [7] introduced a simplified formula for the growth of a Bose-Einstein condensate, in which growth resulted from stimulated collisions of atoms in a thermal reservoir, where one of the atoms enters the lowest trap eigenstate, whose occupation thus grows to form a condensate. We thus included the trap eigenfunctions as an essential part of our description, and gave the first *quantitative* formula for the growth of a condensate. The growth rate was of the order of magnitude of that estimated from experiments current at that time.

This direct stimulated effect must be very important once a significant amount of condensate has formed, but in the initial stages there will also be a significant number of transitions to other low lying trap levels whose populations will then also grow. As well as this, there will be interactions between the condensate, the atoms in these low lying levels, and the atomic vapor from which the condensate forms. This paper will extend the description of the condensate growth to include these factors, and will compare the results with experimental data on condensate growth obtained at MIT [8].

As in our previous work, we divide the states in the potential into the *condensate band*, R_C , which consists of the energy levels significantly affected by the presence of a condensate in the ground state, and the *noncondensate band*, R_{NC} , which contains all the remaining energy levels above the condensate band. The division between the

two bands is taken to be at the value, e_{\max} . The situation is illustrated in Fig. 1. The picture we shall use assumes that R_{NC} consists of a large “bath” of atomic vapor, in thermal equilibrium, whose distribution function is given by a time-independent equilibrium Bose-Einstein distribution $\{\exp[(E - \mu)/k_B T] - 1\}^{-1}$ with positive chemical potential μ . The value of e_{\max} will be assumed to be small enough for the majority of atoms to have energies higher than e_{\max} , so that this part of the bath can be treated as being undepleted by the process of condensate growth.

In the following we will use the notation of m as the mass of an atom with s -wave scattering length a , and n_0 for the number of condensate atoms.

The trap levels in R_C must have time-dependent energies due to the effects of the interaction with the growing condensate. The energy of the lowest trap level in R_C is the minimum energy increase when one particle is added to the system; i.e., it is the chemical potential $\mu(n_0)$, for which we use a modified Thomas-Fermi approach $\mu(n_0) = \alpha(n_0 + \nu)^{2/5}$ where $\alpha = (15a\omega_x\omega_y\omega_z m^{1/2}\hbar^2/4\sqrt{2})^{2/5}$ and ν is a constant chosen so that $\mu(0) = \hbar(\omega_x + \omega_y + \omega_z)/2$. As $\mu(n_0)$ rises with an increase in n_0 , the energies of higher energy trap levels must also rise. The exact nature of this

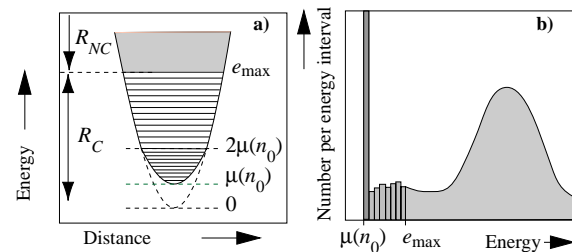


FIG. 1. (a) Representation of the change in the energy spectrum due to the growth of the condensate. (b) Occupations of the levels considered: leftmost is the condensate level, followed by several discrete energy bands, with the constantly occupied R_{NC} at higher energies.

rise does not affect the results greatly. An approximate treatment arises by leaving the levels with energies above $2\mu(n_0)$ unchanged (including all levels in R_{NC}), and compressing the spacing of the levels under $2\mu(n_0)$, so that the energies are given by

$$e_m = e_m^0 + \theta[2\mu(n_0) - e_m^0][2\mu(n_0) - e_m^0 - \mu(0)]/2, \quad (1)$$

where e_m^0 are the noninteracting harmonic potential energy levels, and $\theta(x)$ is the step function. Note that $e_0^0 = \mu(0)$, and thus $e_0 = \mu(n_0)$. The levels used in this model are represented graphically in Fig. 1. To simplify the equations we also group the levels in narrow bands of mean energy e_k , g_k levels per group, and n_k particles per group—the $k = 0$ group contains only one level, the condensate, so that $g_0 = 1$, and n_0 is the number of atoms in the condensate. This corresponds to the *ergodic* assumption used in [5,9,10]. As a result of this procedure there are two different kinds of dynamics, *scattering* and *growth*, as illustrated in Fig. 2. The evolution for the population of the m th level in R_C is then

$$\frac{\partial n_m}{\partial \tau} = \dot{n}_m = \dot{n}_m|_{\text{growth}} + \dot{n}_m|_{\text{scatt}}. \quad (2)$$

Equations of motion then follow from quantum kinetic theory [11], and full derivation will be given elsewhere. Heuristically the result amounts to modifying the quantum Boltzmann (QBE) equation as follows.

(i) We use the QBE in an approximated ergodic form, where $e_{\min} = \min(e_m, e_n, e_p, e_q)$ [9],

$$g_n \frac{\partial f(e_n)}{\partial \tau} = \sum_{e_m, e_p, e_q} \delta(e_m + e_n - e_p - e_q) g(e_{\min}) \times \{f(e_p)f(e_q)[1 + f(e_m)][1 + f(e_n)] - f(e_m)f(e_n)[1 + f(e_p)][1 + f(e_q)]\}, \quad (3)$$

where $n_k = g_k f(e_k)$ is the number of particles with energy e_k , and $\tau = (8ma^2\omega^2/\pi\hbar) \times t$. Here we take the form for an *isotropic* 3-dimensional harmonic oscillator, with frequency $\omega = (\omega_x\omega_y\omega_z)^{1/3}$.

(ii) We use the modified energy levels as given above, but otherwise do not change the QBE.

(iii) We sum out over all levels in R_{NC} which is assumed time independent.

(iv) We omit any scattering between atoms which both have energies less than e_{\max} , which is reasonable if the number of atoms in the bath is almost 100% of the total number of atoms.

(v) The wave function of the condensate satisfies the Gross-Pitaevskii equation with chemical potential $\mu(n_0)$.

We emphasize, however, that these are not simply *ad hoc* modifications, but can all be derived using

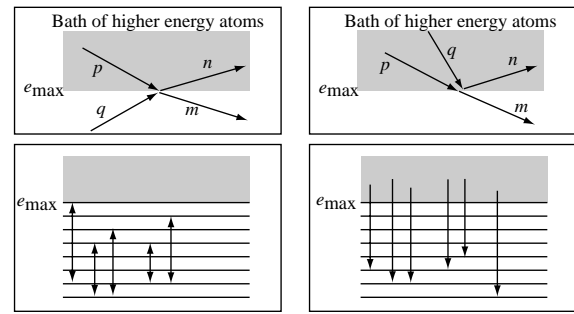


FIG. 2. The transitions being considered: Left, scattering; right, growth.

quantum kinetic theory as in [11], and some reasonable approximations.

The individual terms are as follows.

Scattering.—A collision between an atom initially in an energy level below e_{\max} and a bath atom transfers the first atom to another energy level below e_{\max} . This is described by

$$\dot{n}_m|_{\text{scatt}} = e^{\mu/k_B T} \Gamma(T) \times \left\{ \sum_{k < m} \frac{1}{g_m} [n_k(g_m + n_m) e^{-\hbar\omega_{mk}/k_B T} - n_m(g_k + n_k)] + \sum_{k > m} \frac{1}{g_k} [n_k(g_m + n_m) - n_m(g_k + n_k) e^{-\hbar\omega_{km}/k_B T}] \right\}, \quad (4)$$

where $\omega_{km} = e_k - e_m$. The value of $\Gamma(T) = \sum_{e_m > e_{\max}} e^{-e_m/k_B T}$ depends on the energy spectrum. We use the value for an *isotropic* 3-dimensional harmonic oscillator with frequency $\omega = (\omega_x\omega_y\omega_z)^{1/3}$. Thus $e_n = (n + 3/2)\hbar\omega$, so that we find

$$\Gamma(T) = \frac{e^{-e_{\max}/k_B T}}{1 - e^{-\hbar\omega/k_B T}}. \quad (5)$$

However, this value is not critical; similar results are obtained for any $\Gamma(T)$ greater than about 10% of (5).

Growth.—A collision between a pair of atoms initially in the bath of atomic vapor results in *one* of the atoms having a final energy less than e_{\max} . This gives

$$\dot{n}_m|_{\text{growth}} = 2[(n_m + 1)W_m^+(n_0) - n_m W_m^-(n_0)], \quad (6)$$

where

$$W_m^+(n_0) = \frac{1}{2} \int_{e_{\max}}^{\infty} de_1 \int_{e_{\max}}^{\infty} de_2 \int_{e_{\max}}^{\infty} de_3 f(e_1)f(e_2) \times [1 + f(e_3)]\delta(e_1 + e_2 - e_3 - e_m), \quad (7)$$

$$W_m^-(n_0) = \frac{1}{2} \int_{e_{\max}}^{\infty} de_1 \int_{e_{\max}}^{\infty} de_2 \int_{e_{\max}}^{\infty} de_3 [1 + f(e_1)] \times [1 + f(e_2)]f(e_3)\delta(e_1 + e_2 - e_3 - e_m). \quad (8)$$

Because we assume the noncondensate band is in thermal equilibrium, with temperature T and chemical potential μ , we have

$$W_m^-(n_0) = \exp\left(\frac{(e_m - \mu)}{k_B T}\right) W_m^+(n_0). \quad (9)$$

The value of W_0^+ (henceforth W^+) differs significantly from that used previously [7] in that the integrals in (7) are performed only over energy levels higher than e_{\max} (previously over all levels), and the Bose-Einstein distribution function is used over all the range of integration (previously approximated by the Maxwell-Boltzmann distribution). With these changes we find that

$$W^+(n_0) = \frac{1}{2} \left(\frac{k_B T}{\hbar \omega}\right)^2 \left\{ [\log(1 - z)]^2 + z^2 \sum_{r=1}^{\infty} [z z(n_0)]^r [\Phi(z, 1, r + 1)]^2 \right\}, \quad (10)$$

where $z = \exp(\frac{\mu - e_{\max}}{k_B T})$ and $z(n_0) = \exp(\frac{\mu(n_0) - e_{\max}}{k_B T})$. The function Φ is the *Lerch transcendent* [12], defined by $\Phi(x, s, a) = \sum_{k=0}^{\infty} x^k / (a + k)^s$. These changes result in a significant correction, increasing W^+ by about a factor greater than 3 (dependent on T , μ , and the trap parameters) compared to that used previously in [7], and producing correspondingly faster growth.

By making a further approximation, that $W_m^+(n_0) \approx W^+(n_0)$, the calculations required are significantly simplified. We can do this because the $W_m^+(n_0)$ are an average over all the levels contained in the m th group, and hence are expected to be of the same order of magnitude as $W^+(n_0)$. As a validity check, it was found that the effect on the condensate growth rate was small when the $W_m^+(n_0)$ were altered by a factor in the range 0.5–2. We now have for the growth terms

$$\dot{n}_m|_{\text{growth}} = 2W^+(n_0) \{ [1 - e^{(e_m - \mu)/k_B T}] n_m + g_m \}, \quad (11)$$

$$\dot{n}_0|_{\text{growth}} = 2W^+(n_0) \{ [1 - e^{[\mu(n_0) - \mu]/k_B T}] n_0 + 1 \}. \quad (12)$$

The overall evolution of the system can now be found from the numerical solutions to the set of Eqs. (2). The parameters used are $\omega_x = \omega_y = 2\pi \times 82.3$ Hz and $\omega_z = 2\pi \times 18$ Hz, as in [8], and $a = 2.75$ nm, $e_{\max} \approx 2.2\mu(n_0(\text{eq}))$, where $n_0(\text{eq})$ is the final equilibrium value of n_0 , which is defined by $\mu(n_0(\text{eq})) = \mu$, the chemical potential of the vapor. The number of energy bands was set as large as possible, but it was required that there were at least four levels in the first group above the condensate, in order to represent the fact that the levels are discrete.

The improvements to this model over that used in [7] speed up the condensate growth by up to an order of magnitude, depending on the exact parameters, as anticipated in [7]. The major cause of this is the correction to W^+ arising from the use of the correct Bose-Einstein distribution. The inclusion of the scattering terms does not change the overall rate of growth substantially (which is dominated by the bosonic stimulated growth), but does

speed up the initial period of growth (dominated by spontaneous growth) and shortens the time before the stimulated term becomes significant. This gives a much sharper initial growth curve as compared to the smoother S-bend curves of [7]. In Fig. 3 we present an example of the results obtained for the growth of all the bands in R_C , in which a number of features may be seen.

(i) The effect of the initial conditions used can be seen from the front corner. In this example the initial populations for all but the top ten bands were set at zero, while the top ten bands had populations determined by the same Bose-Einstein distribution function as for R_{NC} . The figure shows that this initial condition is rapidly smoothed out by scattering processes. Different initial conditions merely generate a small change in the *initiation time* defined below.

(ii) The *initiation time* (here 60 ms) is defined by the critical line C-C. Up to this point the population of the condensate level is relatively small. The behavior up to the initiation time is similar to that found by Svistunov [10] and Kagan *et al.* [5]. In particular, the populations of the levels increase to approach a limiting dependence on the energy of $f(E) \propto E^{-1.61}$ on the critical line C-C, which is in good agreement with their prediction of $E^{-5/3}$ [13] for the case of a harmonic trap.

(iii) After the initiation time the condensate grows enormously. However, the occupations of the other trap levels actually decrease quite rapidly to their equilibrium values, and then remain nearly constant while the condensate continues to grow—by a factor of about 10 in this case. At the same time the energy spectrum of the trap levels in R_C changes according to (1). This accounts for the small variation in occupations of these levels which is still evident in Fig. 3.

Figure 4 compares with the experimental data of Ref. [8], for two different temperatures. The MIT group fitted their data to an uncorrected growth equation

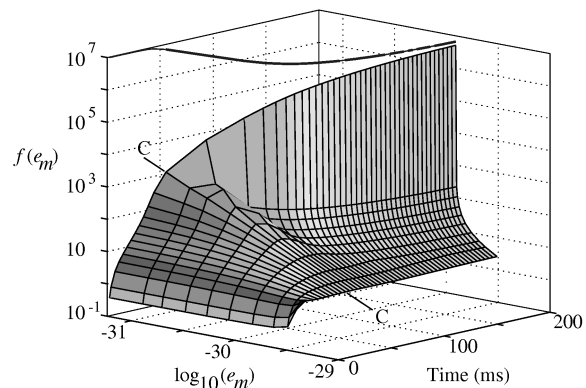


FIG. 3. $f(e_m)$ vs energy e_m as a function of time. Note that the lines almost parallel to the time axis are not lines of constant energy, but rather lines of $f(e_m)$ for constant level number whose energies change with condensate growth. The solid curve in the plane at the top of the axes represents the curve $\log_{10}[e_0] \equiv \log_{10}[\mu(n_0)]$ as a function of time.

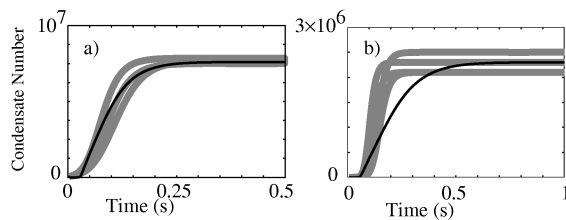


FIG. 4. Comparison of theoretical growth curves (black) with experimentally fitted curves (gray) from [8]. (a) Theory $T = 830$ nK, $n_0(\text{eq}) = 7.6 \times 10^6$; experiment $T = 810\text{--}890$ nK, $n_0(\text{eq}) = (7.5\text{--}7.85) \times 10^6$; (b) theory $T = 590$ nK, $n_0(\text{eq}) = 2.3 \times 10^6$; experiment $T = 580\text{--}610$ nK, $n_0(\text{eq}) = (2.1\text{--}2.5) \times 10^6$.

$\dot{n}_0 = \gamma n_0 \{1 - [n_0/n_0(\text{eq})]^{2/5}\}$, and reported only values of the parameter γ . To represent that the experimental curve is a fitted curve rather than the raw data, the curve has been plotted as a broad band. The MIT group used the initial population for their curves as free parameters in their fit. We have set the initial populations for the MIT curves so as to give the best agreement with the initiation time of our growth.

In the $T = 830$ nK case, Fig. 4a, the growth speed predicted agrees with that experimentally found. The $T = 590$ nK case in Fig. 4b shows a theoretical growth rate some 3 times slower than is measured. The discrepancy between theory and experiment at lower temperatures is hard to evaluate using the data in the form presented in [8], which do not allow for direct comparison between the actual projected spatial distributions as given by phase-contrast microscopy, and theoretical spatial distributions. These are not difficult to calculate from our many-level growth curves—the methodology will be published elsewhere. The MIT method fits to a zero chemical potential vapor plus a nonzero chemical potential condensate—a reasonable estimate in the absence of any theoretical description of the spatial distribution of the vapor. But a detailed description might give quite different results for temperature, and for condensate and vapor numbers.

In summary, we have given a description of condensate growth covering the full range of behaviors, both before and after initiation of the condensate. It is *quantitative* and agrees quite well with experiment. The behavior before initiation is essentially as given by the quantum Boltzmann equation, and agrees with computations based on this equation [5,10,14]. We are able to give a value for the initiation time which appears to be consistent with experiment. After the initiation of the condensate, the occupations of the noncondensate levels are clamped by their fast relaxation time to quasiequilibrium values, which change with the rise in trap levels induced by the

very much slower growth of the condensate to its final occupation.

We believe the future development of the theory for this problem will involve mainly refinements of our picture, such as including depletion of our fixed bath of vapor. But for quantitative comparison with experiment, it will be necessary to have more extensive data on spatial distributions at a range of temperatures.

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