Kinetics of Bose-Einstein Condensation in a Trap

C. W. Gardiner,[1] P. Zoller,[2] R. J. Ballagh,[3] and M. J. Davis[3]
[1]*Physics Department, Victoria University, Wellington, New Zealand*
[2]*Institut für Theoretische Physik, Universität Innsbruck, 6020 Innsbruck, Austria*
[3]*Physics Department, University of Otago, Dunedin, New Zealand*
(Received 2 May 1997)

The formation process of a Bose-Einstein condensate in a trap is described using a master equation based on quantum kinetic theory, which can be well approximated by a description using only the condensate mode in interaction with a thermalized bath of noncondensate atoms. A rate equation of the form $\dot{n} = 2W^+(n)[(1 - e^{\{\mu_n - \mu\}/kT})n + 1]$ is derived, in which the difference between the condensate chemical potential μ_n and the bath chemical potential μ gives the essential behavior. Solutions of this equation give a characteristic latency period for condensate formation and appear to be consistent with the observed behavior of both rubidium and sodium condensate formation. [S0031-9007(97)03982-3]

PACS numbers: 03.75.Fi, 05.30.Jp, 51.10.+y

The experiments on Bose-Einstein condensation of dilute atomic gases [1–3] have stimulated theoretical effort, which has, however, not produced any definitive result for the growth of the condensate from the vapor, although there have been significant theoretical contributions [4–8]. This Letter will present a *quantitative* and *experimentally testable* description of the growth process, based on quantum kinetic theory [9,10], which can be simplified to a single first-order differential equation for the number n of atoms in the condensate.

Our formulation contains the following principal features. We use the Hamiltonian

$$H = \int d^3\mathbf{x}\, \psi^\dagger(\mathbf{x})\left(-\frac{\hbar^2}{2m}\nabla^2\right)\psi(\mathbf{x}) + \frac{1}{2}\int d^3\mathbf{x} \int d^3\mathbf{x}' \psi^\dagger(\mathbf{x})\psi^\dagger(\mathbf{x}') \times u(\mathbf{x} - \mathbf{x}')\psi(\mathbf{x}')\psi(\mathbf{x}) + \int d^3\mathbf{x}\, V_T(\mathbf{x})\psi^\dagger(\mathbf{x})\psi(\mathbf{x}). \quad (1)$$

The potential function $u(\mathbf{x} - \mathbf{x}')$ is as usual not the true interatomic potential, but rather a short range potential—approximately of the form $u\delta(\mathbf{x} - \mathbf{x}')$—which reproduces the correct scattering length [11].

We divide the condensate into two regions called the *condensate band* R_C, and the *noncondensate band* R_{NC}, as in Fig. 1. We treat R_{NC} as being thermalized, representing the majority of the atoms as a heat bath which provides the source of atoms for condensate growth. The condensate band is the region of energy levels less than a value E_R, which includes not only the ground state, in which the condensate forms, but also those levels which would be significantly affected by the presence of a condensate. [12] In the noncondensate band, with energy levels greater than E_R, there is no significant such effect.

The behavior in R_C is treated fully quantum-mechanically, and a description in terms of trap levels modified by the presence of a condensate is used. At any time there is a given number N of atoms in R_C, and the energy levels in such a situation can be described using the number-conserving Bogoliubov method devised by one of us [13], so that the state of R_C is fully described by the *total number* of atoms N in R_C, and the quantum state of the quasiparticles within R_C. In this formulation we can write the condensate band field operator in the form

$$\psi_C(\mathbf{x}) = B\left[\xi_N(\mathbf{x}) + \sum_m \frac{b_m f_m(\mathbf{x}) + b_m^\dagger g_m(\mathbf{x})}{\sqrt{N}}\right]. \quad (2)$$

The quasiparticles, of energy ϵ_N^m, are described by annihilation operators b_m, while $B^\dagger$ is the creation operator which takes the R_C system, for any N, from the ground state with N atoms to the ground state with $N + 1$ atoms. The condensate wave function is $\xi_N(\mathbf{x})$, and this satisfies the Gross-Pitaevskii equation

$$-\frac{\hbar^2}{2m}\nabla^2\xi_N + V_T\xi_N + Nu|\xi_N|^2\xi_N = \mu_N\xi_N. \quad (3)$$

The amplitudes $f_m(\mathbf{x})$, $g_m(\mathbf{x})$ are for creation and destruction of quasiparticles of energy ϵ_N^m, and are fully defined in [10,13], but will not play any significant part in this Letter.

In this number-conserving Bogoliubov method, the *atoms* are conserved, while the quasiparticles are mixtures of *phonon* states, and these phonons relate to the process

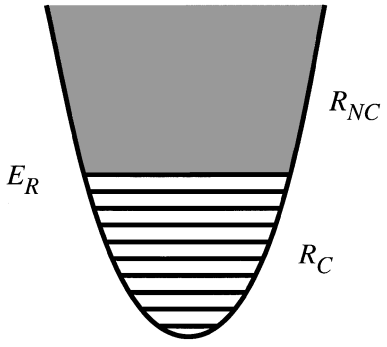

FIG. 1. The condensate and noncondensate bands.

of transferring an atom from an excited quantum state to the condensate level. Thus, the operators $b_m, b_m^\dagger$ do not change the total numbers of particles, while the operator B, which multiplies everything else in (2), reduces the total number of particles by 1.

The process we wish to describe is as follows: (i) Some of the collisions in R_{NC} will transfer an atom to R_C, so that $N \to N + 1$, and there is of course the reverse process where a collision of a noncondensate band atom with one within the condensate band transfers an atom from the condensate band into the noncondensate band, so that $N \to N - 1$. (ii) We consider a situation in which there is initially no condensate; however, the boundary between R_C and R_{NC} is fixed to be appropriate for the amount of condensate which is *finally* formed. (iii) By evaporative cooling, the chemical potential of the atoms in R_{NC} becomes non-negative; this is permissible provided the chemical potential does not exceed the lowest energy E_R of R_{NC}. (iv) With a weak interaction potential u, the Bogoliubov spectrum and wave functions are valid for *all* N, large and small, since for small N and u the results are not significantly different from perturbation theory.

Using quantum kinetic theory [10] it is possible to derive a simple master equation for the density operator ρ which describes the state of the condensate. The main processes are caused by an atom scattering into or out of R_C, and this can occur in six ways; that is, $N \to N \pm 1$ with no change in the number of quasiparticles, the creation of a quasiparticle, or the absorption of a quasiparticle.

The six transition probabilities can now all be written in terms of the functions $R^\pm$ as

$$W^+(N) = R^+(\xi_N, \mu_N/\hbar), \tag{4}$$

$$W^-(N) = R^-(\xi_{N-1}, \mu_{N-1}/\hbar), \tag{5}$$

$$W_m^{++}(N) = R^+\big(f_m, (\epsilon_N^m + \mu_N)/\hbar\big), \tag{6}$$

$$W_m^{--}(N) = R^-\big(f_m, (\epsilon_{N-1}^m + \mu_{N-1})/\hbar\big), \tag{7}$$

$$W_m^{+-}(N) = R^+\big(g_m, (-\epsilon_N^m + \mu_N)/\hbar\big), \tag{8}$$

$$W_m^{-+}(N) = R^-\big(g_m, (-\epsilon_{N-1}^m + \mu_{N-1})/\hbar\big). \tag{9}$$

The functions $R^\pm(y, \omega)$ are defined by

$$R^+(y,\omega) = \frac{u^2}{(2\pi)^5\hbar^2}\int d^3\mathbf{x}\int d\Gamma\,\Delta(\Gamma,\omega)F_1F_2(1+F_3)W_y(\mathbf{x},\mathbf{k}), \tag{10}$$

$$R^-(y,\omega) = \frac{u^2}{(2\pi)^5\hbar^2}\int d^3\mathbf{x}\int d\Gamma\,\Delta(\Gamma,\omega)(1+F_1)(1+F_2)F_3W_y(\mathbf{x},\mathbf{k}), \tag{11}$$

where we will use the notation

$$d\Gamma \equiv d^3\mathbf{K}_1 d^3\mathbf{K}_2 d^3\mathbf{K}_3 d^3\mathbf{k}, \tag{12}$$

$$\Delta(\Gamma,\omega) \equiv \delta[\Delta\omega_{123}(\mathbf{x}) - \omega]\delta(\mathbf{K}_1 + \mathbf{K}_2 - \mathbf{K}_3 - \mathbf{k}). \tag{13}$$

Here we use the notation

$$W_y(\mathbf{x},\mathbf{k}) = \frac{1}{(2\pi)^3}\int d^3\mathbf{v}\, y^*\Big(\mathbf{x} + \frac{\mathbf{v}}{2}\Big)y\Big(\mathbf{x} - \frac{\mathbf{v}}{2}\Big)e^{i\mathbf{k}\cdot\mathbf{v}} \tag{14}$$

to represent the Wigner function corresponding to the wave function $y(\mathbf{x})$. The function $F_i \equiv F(\mathbf{K}_i, \mathbf{x})$ is the noncondensate atom density per h^3 of phase space, and

$$\Delta\omega_{123}(\mathbf{x}) = \omega_{\mathbf{K}_1}(\mathbf{x}) + \omega_{\mathbf{K}_2}(\mathbf{x}) - \omega_{\mathbf{K}_3}(\mathbf{x}) \tag{15}$$

with

$$\hbar\omega_{\mathbf{K}}(\mathbf{x}) = \frac{\hbar^2\mathbf{K}^2}{2m} + V_T(\mathbf{x}). \tag{16}$$

We can write a stochastic master equation for the occupation probabilities $p(N,\mathbf{n})$, where $\mathbf{n} = \{n_m\}$, the set of all quasiparticle occupation numbers, in the form [14]

$$\begin{aligned}\dot{p}(N,\mathbf{n}) &= 2NW^+(N-1)p(N-1,\mathbf{n}) - 2(N+1)W^+(N)p(N,\mathbf{n}) + 2(N+1)W^-(N+1)p(N+1,\mathbf{n}) - 2NW^-(N)p(N,\mathbf{n})\\ &+ \sum_m [2n_m W_m^{++}(N-1)p(N-1,\mathbf{n}-\mathbf{e}_m) - 2(n_m+1)W_m^{++}(N)p(N,\mathbf{n})]\\ &+ \sum_m [2(n_m+1)W_m^{--}(N+1)p(N+1,\mathbf{n}+\mathbf{e}_m) - 2n_m W_m^{--}(N)p(N,\mathbf{n})]\\ &+ \sum_m [2(n_m+1)W_m^{+-}(N-1)p(N-1,\mathbf{n}+\mathbf{e}_m) - 2n_m W_m^{+-}(N)p(N,\mathbf{n})]\\ &+ \sum_m [2n_m W_m^{-+}(N+1)p(N+1,\mathbf{n}-\mathbf{e}_m) - 2(n_m+1)W_m^{-+}(N)p(N,\mathbf{n})].\end{aligned} \tag{17}$$

Here $\mathbf{e}_m = \{\ldots 0,0,1,0,0,\ldots\}$ has its only nonzero value at the position corresponding to the index m.

We can interpret functions $R^\pm(y,\omega)$ as forward and backward collision rates for those collisions which result in a particle entering (+) or leaving (−) the condensate with an energy $\hbar\omega$. The collision must also take place in a position where the condensate Wigner function is nonzero. The terms in (17) representing transitions to the ground state of the condensate exhibit a stimulated increase in collision rate of approximately N, which can be a number up to 10^7, but the transition probabilities $W_m^{\pm\pm}$ defined in (6)–(9) are multiplied only by n_m, which does not become large. Thus as an

initial approximation we drop the quasiparticle terms, which are smaller by a factor of N, and are thus negligible for most of the condensation process. We note that the condensate wave function is in practice sharply peaked at $\mathbf{x} = 0$ by comparison with the phase space distribution function $F(\mathbf{K}, \mathbf{x})$, and thus replace $\mathbf{x}$ wherever it occurs by 0, except in $W_{\xi_N}(\mathbf{x}, \mathbf{k})$, whose integral gives the $\mathbf{k}$ space condensate probability density $|\tilde{\xi}_N(\mathbf{k})|^2$. We finally get the simple master equation which consists of only the first line of (17), and in which the transition matrix elements take the simplified form

$$W^+(N) = \frac{u^2}{(2\pi)^5\hbar^2}\int d\Gamma\Delta[\Gamma, \mu(N)/\hbar] \times F_1F_2(1 + F_3)|\tilde{\xi}_N(\mathbf{k})|^2, \quad (18)$$

$$W^-(N) = \frac{u^2}{(2\pi)^5\hbar^2}\int d\Gamma\Delta[\Gamma, \mu(N)/\hbar] \times (1 + F_1)(1 + F_2)F_3|\tilde{\xi}_N(\mathbf{k})|^2. \quad (19)$$

The evaluation of $W^{\pm}$ can be done in various degrees of approximation; we shall take here a thermal R_{NC} with

$$F(\mathbf{K}, \mathbf{x}) \approx [e^{(\hbar\omega\mathbf{k}+V_T(\mathbf{x})-\mu)/kT} - 1]^{-1} \quad (20)$$

from which one easily obtains [choosing $V_T(\mathbf{0}) = 0$]

$$W^+(N) = e^{(\mu-\mu_N)/kT}W^-(N), \quad (21)$$

which indicates that a steady state is reached at large N when the chemical potential of the condensate almost equals that of the noncondensate. (Inclusion of the smaller terms in the master equation also shows that the temperatures of R_C and R_{NC} are equal in equilibrium.) Evaluation of W^+ can be done by taking the energy range of R_C to be negligible compared to that of $F(\mathbf{K}, \mathbf{0})$, and by taking the range of $\mathbf{k}$ to be small compared to that of $\mathbf{K}$ in $F(\mathbf{K}, \mathbf{0})$. We also approximate the Bose function (20) by its Boltzmann equivalent for most of the range of integration since the integrals can then be evaluated analytically; however, this is a purely technical issue, which does not affect the essence of the results. (However, a fully quantum mechanical treatment could increase ω^+ by about an order of magnitude). Using $u = 4\pi a\hbar^2/m$, where a is the s-wave scattering length, we get

$$W^+(N) = \frac{4m(akT)^2}{\pi\hbar^3}e^{2\mu/kT}\left[\frac{\mu_N}{kT}K_1\left(\frac{\mu_N}{kT}\right)\right]. \quad (22)$$

Here $K_1(z)$ is a modified Bessel function. Notice also that the prefactor $4m(akT)^2/\pi\hbar^3$ is essentially the elastic collision rate $\rho\sigma v$, where the quantities are evaluated at the critical point for condensation. Under the assumption that the majority of the atoms are in the condensate, the major behavior of the master equation (17) is given by the rate equation for the mean number of atoms in the condensate (written as n),

$$\dot{n} = 2W^+(n)[(1 - e^{\{\mu_n-\mu\}/kT})n + 1]. \quad (23)$$

Since (21) has been used, this represents a situation in which a condensate (which may be initially unoccupied) is in contact with a bath of noncondensed atoms. If (23) is used alone, it describes a situation in which the thermal bath is not depleted as the condensate evolves. A very simple form for the differential equation can be given in this case by using (22), together with a harmonic trap potential $V_T(\mathbf{x}) = m(\omega_x^2x^2 + \omega_y^2y^2 + \omega_z^2z^2)/2$, and the Thomas-Fermi approximation $\mu_N = (15Nu\omega_x\omega_y\omega_zm^{3/2}/16\pi\sqrt{2})^{2/5}$ [with, however, a linear interpolation as $N \to 0$ to give the correct noninteracting value of $\mu(0) = \hbar(\omega_x + \omega_y + \omega_z)/2$] yields a differential equation which can be easily integrated numerically. We present solutions for the parameters of the original rubidium [1] and sodium [2] experiments in Fig. 2. In both cases there is a latency time during which the condensate is initiated by the spontaneous term [the last term inside the curly brackets in (23)], after which the stimulated term [the term proportional to N inside the curly brackets in (23)] takes over, causing a rapid growth until saturation sets in when the condensate chemical potential μ_n approaches the chemical potential μ of the bath.

The time scales for the growth of the condensate are of the same order of magnitude as experimentally observed, although no measurements have been published. In comparing with experiment, one should bear in mind that this treatment (i) neglects fluctuation effects and (ii) neglects the quasiparticle effects. Inclusion of these should not change the growth curve in the region where N is substantially larger than 1, but could possibly speed up the process by which the first 100 or so atoms enter the condensate.

The solutions in Fig. 2 assume that μ and T, the chemical potential and temperature of the bath of noncondensed atoms, are constant. They nevertheless exhibit the fundamental nature of the process of condensation. For a treatment more appropriate to comparison with experiment, one must couple the condensate growth equation (23) to appropriate time development equations for the process of evaporative cooling, such as those of [15–17]. There are three principal time scales in the problem; the time scale of equilibration of the noncondensate "bath," which is very fast, the time scale of condensate growth, as given by solutions of (23), and the time scale of the evaporative cooling process, which is in practice considerably slower than both of the others. Under these conditions one would

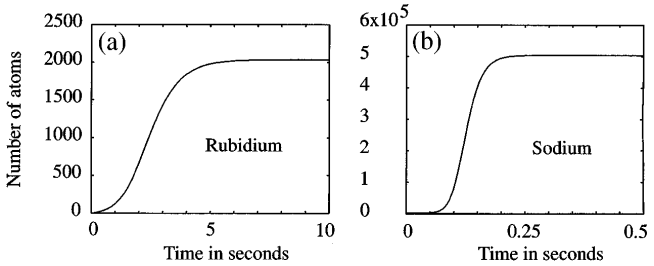

FIG. 2. Condensate growth for (a) rubidium and (b) sodium. Scattering lengths are 5.71 and 2.75 nm, respectively.

expect that a model in which the noncondensate bath distribution function is considered to be always thermalized for particles below the "cut" energy, which we shall call ηkT, and is zero above this cut energy would be valid. Provided the cooling process is slow enough, we can use (21) with the resulting time-dependent $\tilde{T}$ and $\tilde{\mu}$ (values appropriate to the truncated distribution), after modifying the evaporative cooling equations to take account of the transfer of particles and energy between condensate and noncondensate.

One should also note that the Boltzmann function with a cutoff at the energy ηkT, typically with $\eta = 5-7$, is a distribution which is significantly out of thermal equilibrium; for $\eta = 5$ or 7 we find, respectively, 12.5% and 2.9% of the full Boltzmann distribution is above ηkT. However, collisions which are of the correct kinematic configuration to permit one of the atoms to enter the condensate are a selection of the full Boltzmann distribution in which the density of states factor, proportional to E^2 for the harmonic oscillator, becomes approximately independent of E; for them only 0.67% and 0.091% have energy greater than ηkT. Thus the truncated distribution behaves like a genuine thermal distribution for the collisions which can populate the condensate.

Using this more complete model of condensate formation, we have simulated a number of different evaporative cooling paths that are consistent with the published descriptions of Bose condensate formation (e.g., [1,2]). Although differing in detail, the results are broadly in agreement with those shown in Fig. 2. One of the features of the experimental process is that the cooling process is halted, and the system allowed to thermalize for a short period before the condensate is observed. Our simulations show that the nonequilibrium noncondensate distribution evolves to a true Boltzmann distribution in a few mean collision times, and it is easy to show that the new temperature is always less than $\tilde{T}$, while the new chemical potential may be larger or smaller than $\tilde{\mu}$. Typically, in the regime appropriate to the experiments, μ increases during this relaxation, and may change from a value below to a value above μ_C . This crucial step in the formation of the condensate, of μ evolving to exceed μ_C, may thus have occurred only during the relaxation process.

The condensate growth equation (23) is like the kind of equation one finds for laser. Thus there is the spontaneous emission term (the $+1$ inside the curly brackets), and a gain term. The gain here is determined entirely by the difference between the condensate chemical potential μ_n, which is quantum mechanically determined, and that of the noncondensate bath μ, which is determined by statistical mechanics. The fact that the quasiparticles play no significant role in the process is analogous to the behavior of a multimode laser, in which nearly all photons go into the mode with the highest gain, even if it is only marginally the highest gain.

One can also conclude that adaptations of the condensate growth equation for different configurations of the noncondensate bath will prove a useful tool in the eventual design of an atom laser, or "Boser."

This work was supported by the Marsden Fund under contract number PVT-603, and by Österreichische Fonds zur Förderung der wissenschaftlichen Forschung.

[1] M. Anderson, J. R. Ensher, M. R. Matthews, C. E. Wieman, and E. A. Cornell, Science **269**, 198 (1995).
[2] K. B. Davis, M-O. Mewes, M. R. Andrews, N. J. van Druten, D. S. Durfee, D. M. Kurn, and W. Ketterle, Phys. Rev. Lett. **75**, 3969 (1995).
[3] C. C. Bradley, C. A. Sackett, J. J. Tollet, and R. Hulet, Phys. Rev. Lett. **75**, 1687 (1995).
[4] Yu. M. Kagan, B. V. Svistunov, and G. V. Shlyapnikov, Sov. Phys JETP **75**, 387 (1992).
[5] *Bose-Einstein Condensation*, edited by A. Griffin, D. W. Snoke, and S. Stringari (Cambridge University Press, Cambridge, 1995).
[6] H. T. C. Stoof, Phys. Rev. Lett. **66**, 3148 (1991); Phys. Rev. A **49**, 3824 (1994).
[7] D. V. Semikoz and I. I. Tkachev, Phys. Rev. Lett. **74**, 3093 (1995).
[8] J. Anglin, "Cold, dilute, trapped bosons as an open quantum system", Los Alamos Server Report, No. quant-ph/9611008.
[9] C. W. Gardiner and P. Zoller, Phys. Rev. A **55**, 2902 (1997).
[10] C. W. Gardiner and P. Zoller (to be published).
[11] A. A. Abrikosov, L. P. Gorkov, and I. E. Dzyaloshinski, *Methods of Quantum Field Theory in Statistical Physics* (Dover, New York, 1963).
[12] Numerical investigations show that for the usual trap potentials the choice $E_C \approx 3\mu_N$ means that the higher levels are equal to those of the noncondensed system to at least an accuracy of 5%. Typically, μ_N is about an order of magnitude less than kT. Under these conditions a thermal distribution of energies corresponds to over 95% of the atoms being thermalized and within R_{NC}. Even after condensation, the majority of the atoms are still in R_{NC}.
[13] C. W. Gardiner, Phys. Rev. A **56**, 1414 (1997).
[14] A full master equation which treats off-diagonal elements can be similarly derived and will be presented elsewhere [10].
[15] M. Holland, J. Williams, K. Oakley, and J. Cooper, Quantum Semiclass. Opt. **8**, 571 (1996); M. Holland, J. Williams, and J. Cooper, Phys. Rev. A **55**, 3670 (1997).
[16] O. J. Luiten, M. W. Reynolds, and J. T. M. Walraven, Phys. Rev. A **53**, 381 (1996).
[17] M. J. Davis, *Evaporative Cooling and Bose-Einstein Condensation*, B.Sc. Hons. Thesis, Otago University (1996).