NEW PROBLEMS

Charles H. Holbrow, *Editor*
Colgate University, Hamilton, New York 13346

The ''New Problems'' department presents interesting, novel problems for use in undergraduate physics courses beyond the introductory level. We will publish worked problems that convey the excitement and interest of current developments in physics and that are useful for teaching courses such as Classical Mechanics, Electricity and Magnetism, Statistical Mechanics and Thermodynamics, Modern Physics, or Quantum Mechanics. We challenge physicists everywhere to create problems that show how their various branches of physics use the central, unifying ideas of physics to advance physical understanding. We want these problems to become an important source of ideas and information for students of physics. This project is supported by the Physics Division of the National Science Foundation. Submit materials to Charles H. Holbrow, *Editor*.

Bose–Einstein condensation

Isaac F. Silvera
Department of Physics, Harvard University, Cambridge, Massachusetts 02138

(Received 11 September 1996; accepted 6 February 1997)

I. SCOPE

After a brief description of what Bose–Einstein condensation (BEC) is and why it is expected to occur in an unconfined three-dimensional volume, five problems are posed. Two of them show how cold and dense a sample must be before BEC is possible; the solutions of the other three illustrate how the critical temperature and the temperature dependence of the condensate density depend on dimensionality and on external potentials. To work the problems a student should be acquainted with the Bose distribution function and the chemical potential. The problems are appropriate for a statistical physics course such as might be taught out of Kittel and Kroemer.[1]

II. INTRODUCTION

In 1995 while studying a very dilute gas of rubidium atoms confined in space by an inhomogeneous magnetic field, physicists observed Bose–Einstein condensation in a gas of atoms for the first time.[2] The phenomenon was originally predicted in 1925 by Albert Einstein shortly after Satyendra Bose brought to his attention a simple derivation of the Planck radiation law that treated photons as particles that obeyed the counting rules that are today called Bose–Einstein statistics. Einstein showed[3] that a collection of atoms that obeyed these counting rules (bosons) might at the proper temperature and density suddenly populate the collection's ground state in observably large numbers. This macroscopic occupation of the ground state is a phase transition and takes place at critical temperature T_c and/or number density n_c, and was given the name ''Bose–Einstein condensation'' (BEC). Although BEC has been a textbook example[4] in statistical mechanics for a long time, and although BEC is believed to be responsible for superfluidity in liquid helium, it has taken more than 70 years of increasingly intensive effort to unambiguously observe BEC. An important experimental goal will be to show that Bose condensed gases possess the property of superfluidity. Other observations have been made, and there are current experiments to study a Bose gas in a two-dimensional geometry.[5]

III. BACKGROUND

Particles with integral spin (0,1,2,...) are called bosons. For an assembly of identical bosons there is no limit to the number of particles which can occupy a single quantum state. Bose and Einstein derived the expression for the thermal occupation of a state with energy ϵ at temperature T

$$\overline{N_\epsilon}=\frac{1}{\left[\exp\left[\frac{(\epsilon-\mu)}{k_BT}\right]-1\right]},\tag{1}$$

where k_B is the Boltzmann constant and μ is the chemical potential.

Although interactions are extremely important in a real gas, the problems are made tractable and the essential physics is retained by assuming an ideal gas of noninteracting particles. We also assume that the states are non-degenerate. The chemical potential, which is a measure of the change of internal energy of the system when a particle is added, is a very important quantity in the theory of BEC. In equilibrium the chemical potential must be uniform although quantities such as pressure and density may vary across an inhomogeneous system. We shall see that for $T\leqslant T_c$, $\mu=0$ and particles added to the system go into the zero-energy state. The chemical potential is determined by requiring that the sum of particles occupying every state be equal to the total number of particles N. From Eq. (1) we see that $\mu \leqslant 0$ because the occupation number must be positive. For a gas in the low-density, high-temperature limit μ is large and negative and goes to zero as temperature is decreased or density is increased to the critical value where BEC occurs.

In a gas of atoms obeying Maxwell–Boltzmann statistics there is a large continuum of energy or momentum states which are microscopically populated, i.e., the number of particles occupying any one state is a very small fraction of the total number of particles. Only at $T = 0$ is the ground state with $\epsilon = 0$ macroscopically populated by all of the particles. However, Einstein showed that for a gas of identical bosons, macroscopic occupation of the ground state, comparable to the total number of particles in the gas, can occur at a finite nonzero temperature. This phase change is BEC.

For a uniform space (no spatially varying potentials) the usual derivation of BEC is as follows. Equation (1) shows if $\mu = 0$ then $\overline{N_0}$, the occupation of the state with $\epsilon = 0$, diverges. $\overline{N_0}$ is called the condensate. When evaluating the chemical potential by summing all states, this term is separated out because of its possible divergent behavior,

$$N=\overline{N_0}+\sum_{\epsilon\neq 0}\frac{1}{\exp\left[\dfrac{(\epsilon-\mu)}{k_BT}\right]-1}. \tag{2}$$

This sum is bounded in three-dimensional space and can be evaluated by converting it to an integral, which you may do because the free particle states are very closely spaced, so that in the semi-classical approximation we can go over to a continuum model. Noting that the number of states equals the phase space volume divided by h^3, we have

$$\sum\rightarrow\int\frac{d\mathbf{p}_3\,d\mathbf{r}_3}{(2\pi\hbar)^3}=\frac{1}{(2\pi\hbar)^3}\int 4\pi p^2dp\,d\mathbf{r}_3. \tag{3}$$

Using $\epsilon = p^2/2M$, we have

$$\sum=\frac{4\pi\sqrt{2}}{(2\pi\hbar)^3}M^{3/2}\int\sqrt{\epsilon}d\epsilon\,d\mathbf{r}_3. \tag{4}$$

Since Σ is the number of states, you can recognize in Eq. (4) the number of states between ϵ and $\epsilon + d\epsilon$, i.e., $\rho(\epsilon)$ the density of states,

$$\rho(\epsilon)=\frac{4\pi\sqrt{2}M^{3/2}V\epsilon^{1/2}}{(2\pi\hbar)^3}, \tag{5}$$

where $V = \int d\mathbf{r}_3$ is the volume in a three-dimensional space, $\mathbf{r}_3$. Then Eq. (2) becomes

$$N=\overline{N_0}+\frac{4\pi\sqrt{2}}{(2\pi\hbar)^3}VM^{3/2}\int_0^\infty\frac{\epsilon^{1/2}d\epsilon}{\exp\left[\dfrac{(\epsilon-\mu)}{k_BT}\right]-1}\equiv\overline{N_0}+N^*. \tag{6}$$

For finite, negative μ all states are about equally, and microscopically, populated. But consider what happens to a system held at constant T and V when you add more particles. As N increases μ must adjust by increasing toward zero. Now for $\mu = 0$ the second term in Eq. (6) can be evaluated as

$$\frac{4\pi\sqrt{2}}{(2\pi\hbar)^3}VM^{3/2}(k_BT)^{3/2}\int_0^\infty\frac{x^{1/2}\,dx}{e^x-1}. \tag{7}$$

The integral has the value $2.612\sqrt{\pi}/2$. Clearly for any given V and T as μ approaches zero, the integral approaches its maximum value, and N^* in Eq. (6) cannot increase further. At this point T represents a critical value T_c at which the addition of more particles leads to new behavior. Writing the density $n = N/V$, we have

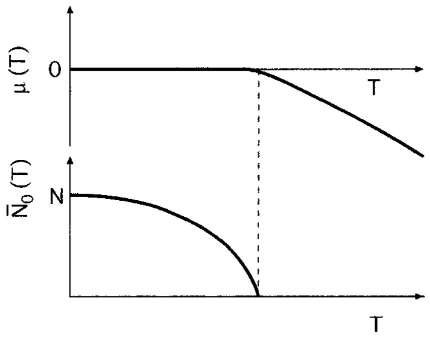

Fig. 1. The chemical potential μ and condensate population $\overline{N_0}$ of an ideal Bose gas as a function of temperature (adapted from Ref. 6).

$$k_BT_c=3.31\frac{\hbar^2}{M}n^{2/3}. \tag{8}$$

Now suppose you add more particles to the system. How can μ adjust further? The answer is found by expanding the expression for the condensate,

$$\overline{N_0}=\frac{1}{\exp\left(\dfrac{-\mu}{k_BT}\right)-1}\approx-\frac{k_BT}{\mu}.$$

In the thermodynamic limit ($N\rightarrow\infty$, $V\rightarrow\infty$ such that N/V remains constant), μ approaches zero as $1/N$. Thus, as $\mu\rightarrow 0$, $\overline{N_0}$ becomes macroscopically occupied in a very controlled way; as more particles are added below T_c, they all go into $\overline{N_0}$. The behavior of μ and $\overline{N_0}$ is shown in Fig. 1. Likewise, N and V can be held constant and T lowered below T_c, so that above-condensate particles N^* are transferred to the condensate. The gas is partitioned into two sets of particles, $\overline{N_0}$—the condensate—and the noncondensate particles, which are sometimes referred to as the ''above-condensate'' or ''normal'' particles. From Eq. (7) we have $N^* = N(T/T_c)^{3/2}$, which with Eq. (6) implies

$$\overline{N_0}=N\left[1-\left(\frac{T}{T_c}\right)^{3/2}\right]. \tag{9}$$

IV. PROBLEMS

A. De Broglie wavelength and BEC

In the semiclassical approximation at low density and high temperature, atoms are localized to wave packets with dimensions small compared to the average interatomic separation. The average de Broglie wavelength $\lambda = h/p$, which is a quantum measure of delocalization of a particle, must satisfy this criterion. Here, p is the momentum spread or momentum uncertainty of the wave packet. Indeed, in the other extreme for $T < T_c$, for particles in the zero momentum eigenstate the delocalization is infinite; i.e., the packet is spread over the entire volume V. BEC occurs when the interparticle separation is of the order of the delocalization. A useful quantity in the thermodynamics is the thermal de Broglie wavelength

$$\Lambda_{\mathrm{dB}}=\sqrt{\frac{2\pi\hbar^2}{Mk_BT}},$$

which is a measure of the thermodynamical uncertainty in the localization of a particle of mass M with the average thermal momentum.

(a) Determine the interparticle separation in terms of Λ_{dB} at the onset of BEC.

(b) Use the Heisenberg uncertainty principle and Maxwell–Boltzmann statistics to show that Λ_{dB} is, to within a factor of 2, just the uncertainty in the position of a particle $\Delta r=\sqrt{\langle r^2\rangle-\langle r\rangle^2}$.

B. Value of T_c for rubidium vapor

Recently, BEC has been reported to have been produced in a vapor of ^{87}Rb atoms at a number density of $n=2.5\times10^{12}\ \mathrm{cm}^{-3}$. Calculate T_c for such a gas in a uniform 3-D space and compare it with the temperature of 170 nK reported by the experimenters.[2]

C. BEC in an inhomogeneous magnetic field

Atoms with magnetic moments $\mathbf{m}$ in an external magnetic field $\mathbf{B}$ will have an interaction energy $U=-\mathbf{m}\cdot\mathbf{B}$.[7,8] Assume that the magnetic field varies quadratically and is of the form $B_0(z/a')^2+B_0(\rho/b')^2$, with $\rho^2=x^2+y^2$, so that

$$U=m_zB_0\left(\frac{z}{a'}\right)^2+m_\rho B_0\left(\frac{\rho}{b'}\right)^2\equiv\left(\frac{z}{a}\right)^2+\left(\frac{\rho}{b}\right)^2. \tag{10}$$

Find the critical temperature for BEC and the temperature dependence of the condensate. Simplify the problem by simplifying the potential to

$$U(z)=\left(\frac{z}{a}\right)^2. \tag{11}$$

Notice that in an inhomogeneous potential the density is inhomogeneous and peaked at the potential minimum. In an ideal gas the condensate forms only in the center of the cloud and is localized in space. In a quantum mechanical description, the ground harmonic oscillator state is macroscopically occupied and condensate atoms only occupy this state as the temperature is lowered.

Hint: Note that the kinetic energy of a particle now depends on position so that the integral of the energy over $d\mathbf{r}_3$ [see Eq. (4)] must be executed.

D. Does BEC occur in a uniform 2-D space?

Show that BEC will not occur in a 2-D gas in a uniform space, i.e., one in which there is no external potential. BEC or the separation of the particles into a condensate and above-condensate part takes place only if the sum (or integral) in Eq. (2) does not diverge when $\mu\rightarrow0$. If it does diverge faster than $\overline{N}_0$, the occupation of $\overline{N}_0$ does not become favored and macroscopic.[9] It is convenient to show the divergence of Eq. (2) by rewriting the sum in terms of $z=e^{\beta\mu}$, where $\beta=1/k_BT$.

E. Show that BEC occurs for a 2-D gas in a quadratic potential

An applied external potential can change the results of the previous problem.[10,11] To see that this is so, redo the previous problem using, for simplicity, a one-dimensional potential in the x direction,

$$U=-u_0\left(1-\frac{x^2}{a^2}\right), \tag{12}$$

where u_0 is the depth of the potential well and a is a measure of its extent in the x direction. The results are easily extended to a 2-D potential.

V. SOLUTIONS

A. De Broglie wavelength and BEC

(a) It is straightforward from Eq. (8) to show that the interparticle spacing is

$$n^{-1/3}=\frac{\Lambda_{\mathrm{dB}}}{1.38}.$$

(b) From the uncertainty principle find Δr,

$$\Delta r\sim\frac{\hbar}{\Delta p}=\frac{\hbar}{\sqrt{\langle p^2\rangle-\langle p\rangle^2}}.$$

From Maxwell–Boltzmann statistics you know that

$$\langle p^2\rangle=3Mk_BT,\quad \langle p\rangle^2=\frac{8Mk_BT}{\pi},$$

from which it follows that

$$\Delta r=0.59\Lambda_{\mathrm{dB}}\approx\Lambda_{\mathrm{dB}}.$$

B. Value of T_c for rubidium vapor

This answer is obtained by substituting the appropriate numbers into Eq. (8),

$$T_c=\frac{3.31\times(1.05\times10^{-34})^2\times(2.5\times10^{18})^{2/3}}{1.38\times10^{-23}\times87\times1.67\times10^{-27}}$$
$$=34\times10^{-9}\ \mathrm{K}=34\ \mathrm{nK}.$$

Recent measurements show better agreement with theory.[12] To calculate the critical temperature for the actual experimental conditions one should use an expression for an inhomogeneous field like that given in Problem 4.3. However, in an inhomogeneous field BEC still takes place at the peak density region where $n_c\approx\Lambda_{\mathrm{dB}}^{-3}$, the condition given by Eq. (8).

C. BEC in an inhomogeneous magnetic field

The kinetic energy of a particle in the potential is $\epsilon=p^2/2M+U(r)$ so that the density of states function, Eq. (5), becomes

$$\rho(\epsilon)=\frac{4\pi\sqrt{2}M^{3/2}}{(2\pi\hbar)^3}\int_{V^*}\sqrt{\epsilon-U(z)}\,d\mathbf{r}_3,$$

where V^* is the accessible volume.

A particle with a given energy can have an excursion in the potential to an extreme where $p=0$ or $\epsilon=U(z)$, yielding the limits on the integral $z=\pm z_m=\pm a\sqrt{\epsilon}$, so that

$$\rho(\epsilon)=\frac{4\pi\sqrt{2}M^{3/2}}{(2\pi\hbar)^3}S\int_{-z_m}^{z_m}\left(\epsilon-\frac{z^2}{a^2}\right)^{1/2}dz$$

$$=\frac{4\pi\sqrt{2}M^{3/2}}{(2\pi\hbar)^3}S\frac{\pi}{2}a\epsilon,$$

where $S=\int dx\ dy$.

Now Eq. (7) becomes

$$N\approx\frac{4\pi\sqrt{2}M^{3/2}}{(2\pi\hbar)^3}S\frac{\pi}{2}a(k_BT)^2\int_0^\infty\frac{x\ dx}{e^x-1}.$$

The definite integral has the value $\pi^2/6$ so that

$$T_c=\left[\frac{N}{S}\frac{(2\pi\hbar)^3}{\sqrt{2}\pi^4k_B^2aM^{3/2}}\right]^{1/2}=2.32\frac{\hbar^{3/2}}{ak_BM^{3/4}}\sigma^{1/2},$$

where $\sigma = N/S$ is the areal density in the unconfined plane. Following the procedure leading to Eq. (9) we find

$$\overline{N_0}=N\left[1-\left(\frac{T}{T_c}\right)^2\right].$$

If we solve for the potential of Eq. (10), we find

$$T_c=1.33\frac{\hbar}{k_BM^{1/2}}\left(\frac{N}{ab^2}\right)^{1/3}.$$

D. BEC in a uniform 2-D space

Rewritten in terms of $z = e^{\beta\mu}$, Eq. (2) becomes

$$N=\sum_\epsilon\frac{ze^{-\beta\epsilon}}{1-ze^{-\beta e}}=\sum_\epsilon ze^{-\beta\epsilon}\sum_{l=0}^{\infty}(ze^{-\beta\epsilon})^l,$$

since $1/(1-x)=\Sigma_0^\infty x^l$. Next, collect terms as follows:

$$N=\sum_\epsilon\sum_{l=0}^{\infty}(ze^{-\beta\epsilon})^{l+1}=\sum_\epsilon\sum_{l=1}^{\infty}(ze^{-\beta\epsilon})^l$$

$$=\sum_l z^l\sum_\epsilon e^{-l\beta\epsilon}.$$

Up to this point the result is independent of dimension. Now in 2-D

$$\sum_\epsilon\rightarrow\frac{1}{h^2}\int 2\pi p\ dp\int d\mathbf{r}_2,$$

so

$$N=\left(\sum z^l\right)\frac{S}{h^2}2\pi\int_0^\infty p\ dp\ \exp\left(\frac{-l\beta p^2}{2M}\right).$$

The momentum integral is easily evaluated to give

$$\frac{Mk_BT}{l}$$

or

$$N=\sum_{l=1}^{\infty}\frac{z^l}{l}\frac{S}{\Lambda_{\mathrm{dB}}^2}.$$

The sum can be recognized

$$\sum\frac{z^l}{l}=-\ln(1-z),$$

so

$$N=-\frac{S}{\Lambda_{\mathrm{dB}}^2}\ln\left(1-\exp\left(\frac{\mu}{k_BT}\right)\right).$$

N diverges when $\mu\rightarrow 0$. Therefore, BEC does not take place in 2-D.

Note that when you went over from the sum to the integral, you could have separated out the condensate fraction. In 3-D the integral representing the above-condensate particles is bounded, so that for $T\leqslant T_c$ particles ''flow'' into the condensate, and the total number of particles remains bounded. In 2-D if you partition the particles into zero-momentum and normal parts, you find that both parts diverge at T_c and there is no phase transition.

E. BEC in 2-D in a quadratic potential

Substituting Eq. (12) into Eq. (2) gives the following integral to be evaluated:

$$N\approx\int d\mathbf{p}_2\int\frac{dx\ dy}{\left[\exp\left[\frac{(\epsilon-\mu)}{k_BT}\right]-1\right]}.$$

Rather than evaluate the integral directly, make a transformation to the dummy variable p_z,

$$x=\frac{p_za}{\sqrt{2Mu_0}}$$

so that

$$\epsilon=\frac{p_x^2+p_y^2}{2M}+U=\frac{p_x^2+p_y^2}{2M}-u_0+\frac{u_0x^2}{a^2}$$

becomes

$$\epsilon=\frac{p_x^2+p_y^2+p_z^2}{2M}-u_0,$$

and the integral becomes

$$N=\frac{ab}{\sqrt{2Mu_0}}\int\frac{d\mathbf{p}_3}{\left[\exp\left[\frac{\left(\frac{p_x^2+p_y^2+p_z^2}{2M}-u_0-\mu\right)}{k_BT}\right]-1\right]}$$

$$=\frac{ab}{\sqrt{2Mu_0}}\int\frac{d\mathbf{p}_3}{\left[\exp\left[\frac{\left(\frac{p_x^2+p_y^2+p_z^2}{2M}-\bar{\mu}\right)}{k_BT}\right]-1\right]},$$

where b is a measure of the size of the system along y, and we have defined $\bar{\mu}=u_0+\mu$. The integral is now identical to the integral for BEC in 3-D that was carried out to give Eq. (8). BEC takes place when $\bar{\mu}=0$ or $\mu=-u_0$. The result is that with a confining potential BEC will take place in 2-D.

[1] C. Kittel and H. Kroemer, *Thermal Physics* (Freeman, San Francisco, 1980), 2nd ed.

[2] M. H. Anderson, J. R. Ensher, M. R. Matthews, C. E. Wieman, and E. A. Cornell, ''Observation of Bose–Einstein condensation in a dilute atomic vapor,'' Science **269**, 198–201 (1995).

[3] A. Einstein, Quantentheorie des einatomigen idealen Gases, Sitzsungber-

ichte, Preussische Akademie der Wissenschaften, Berlin, 261–267 (1924) and 3–14 (1925).

[4] K. Huang, *Statistical Mechanics* (Wiley, New York, 1987).

[5] I. F. Silvera, ''The quest for Bose–Einstein condensation in atomic hydrogen,'' J. Low Temp. Phys. **101**, 49–58 (1995).

[6] P. Nozières, ''Some comments on Bose–Einstein condensation,'' in *Bose–Einstein Condensation*, edited by A. Griffin, D. W. Snoke, and A. Stringari (Cambridge U. P., Cambridge, 1995), pp. 15–30.

[7] V. V. Goldman, I. F. Silvera, and A. J. Leggett, ''Atomic hydrogen in an inhomogeneous magnetic field: Density profile and Bose–Einstein condensation,'' Phys. Rev. B **24**, 2870–2873 (1981).

[8] V. Bagnato, D. E. Pritchard, and D. Kleppner, ''Bose–Einstein condensation in an external potential,'' Phys. Rev. A **35**, 4354–4358 (1986).

[9] P. C. Hohenberg, ''Existence of long-range order in one and two dimensions,'' Phys. Rev. **158**, 383–386 (1967).

[10] S. I. Shevchenko, ''Theory of two-dimensional superfluidity in a nonuniform external field,'' Sov. Phys. JETP **73**, 1009–1019 (1991).

[11] V. Bagnato and D. Kleppner, ''Bose–Einstein condensation in low-dimensional traps,'' Phys. Rev. A **44**, 7439–7441 (1991).

[12] K. B. Davis, M.-O. Mewes, M. R. Andrews, N. J. van Druten, D. S. Durfee, D. M. Kurn, and W. Ketterle, ''Bose–Einstein condensation in a gas of sodium atoms,'' Phys. Rev. Lett. **75**, 3969–3973 (1995); J. R. Ensher, D. S. Jin, M. R. Matthews, C. E. Wieman, and E. A. Cornell, ''Bose–Einstein condensation in a dilute gas: Measurement of energy and ground-state occupation,'' *ibid.* **77**, 4984–4987 (1996).