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Bose-Einstein condensation in the alkali gases: Some fundamental concepts

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> *Whatever can be said, can be said clearly; and whereof one cannot speak,*
> *thereof one should keep silent.*
> *L. Wittgenstein*

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The author presents a tutorial review of some ideas that are basic to our current understanding of the phenomenon of Bose-Einstein condensation (BEC) in the dilute atomic alkali gases, with special emphasis on the case of two or more coexisting hyperfine species. Topics covered include the definition of and conditions for BEC in an interacting system, the replacement of the true interatomic potential by a zero-range pseudopotential, the time-independent and time-dependent Gross-Pitaevskii equations, superfluidity and rotational properties, the Josephson effect and related phenomena, and the Bogoliubov approximation.

CONTENTS

I. INTRODUCTION. SCOPE OF THE REVIEW

The phenomenon known as Bose-Einstein condensation (hereafter abbreviated BEC) was predicted by Ein-

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stein in 1924 on the basis of ideas of Bose concerning photons: In a system of particles obeying Bose statistics and whose total number is conserved, there should be a temperature below which a finite fraction of all the particles "condense" into the same one-particle state. Einstein's original prediction was for a noninteracting gas, a system felt by some of his contemporaries to be perhaps pathological, but shortly after the observation of superfluidity in liquid ^{4}He below the λ temperature (2.17 K), Fritz London suggested that despite the strong interatomic interactions BEC was indeed occurring in this system and was responsible for the superfluid properties; this suggestion has stood the test of time and is the basis for our modern understanding of the properties of the superfluid phase. In 1995 BEC was realized in a system that is about as different as possible from ^{4}He, namely, dilute atomic alkali gases trapped by magnetic fields, and over the last few years these systems have been the subject of an explosion of research, both experimental and theoretical, which in addition to drawing on established lore in the areas of atomic collisions, quantum optics, and condensed-matter physics has generated problems and ideas specific to these novel systems.

Perhaps the single aspect of BEC systems that makes them most fascinating is best illustrated by the cover of *Science* magazine of December 22, 1995, in which the Bose condensate is declared "molecule of the year" and pictured as a platoon of soldiers marching in lockstep: every atom in the condensate must behave in exactly the same way, and this has the consequence, *inter alia*, that effects which are so small as to be essentially invisible at the level of a single atom may be spectacularly amplified. (An example is the phenomenon of superfluidity, discussed in Sec. VI.) In addition, as we shall see by implication, this property tests, in rather subtle ways, our understanding of the meaning of the formalism of quantum mechanics, the nature of "randomness," and much else.

This paper does not attempt to be a comprehensive review of the field of BEC in the alkali gases, even as regards its theoretical aspects. Rather, it is intended to be tutorial in nature, and the reader I have had specifically in mind is a graduate student about to embark on research, either experimental or theoretical, in this area. I believe that a major difficulty such a student is likely to face is that there are many ideas which are taken for granted by workers in the field (or at least by a subset of them) but for which it is difficult to give an explicit and useful reference; this is particularly true of ideas that were originally developed, in some cases as long ago as the 1940s, in the context and language of liquid helium and have not always been rephrased in the terminology that has become standard in the BEC field. My goal therefore has been to set out as clearly as I know how a set of concepts which I believe are basic to our understanding of BEC in the alkali gases, and to discuss in at least a schematic way how they relate to existing or contemplated experiments.

Even given this limited goal, space and other considerations dictate a severe restriction of the subject matter. Generally speaking, I have spent a fair amount of time on the derivation of fundamental equations such as the Gross-Pitaevskii equation and the associated conceptual issues, but much less on their applications to specific experimental systems. This is not, of course, because I feel that such applications are any less important, but because it is this part of the program that tends to be discussed explicitly in the regular journal literature, while the logically prior steps are often taken for granted. Second, I have taken advantage of the fact that there already exist several good reviews of the field (e.g., Parkin and Walls, 1998; Pethick and Smith, 2000; and several of the articles in Inguscio *et al.*, 1999). In particular, the May 1999 issue of this journal contains an excellent review by Dalfovo *et al.* (1999) of much of the experimental work and relevant theory of the first three years of the subject, and I have therefore been able simply to refer the reader to that for many of the standard applications of the ideas I shall discuss. However, one aspect that is barely touched on by Dalfovo *et al.* and that has taken center stage over the last 18 months or so is the special class of phenomena associated with the hyperfine degree of freedom, so I spend a fair amount of time on this. For reasons explained in Sec. IX, I have not attempted to cover the important subject of nonlinear kinetics. Finally, purely for reasons of space, I have been unable to mention at all the highly nontrivial experimental techniques required to cool the alkali gases into the BEC regime [on this, see, for example, the Nobel lectures of Chu, Cohen-Tannoudji, and Phillips (1998) and Ketterle *et al.* (1999)] and have mentioned trapping and imaging techniques (in Sec. II) only to the extent that it is necessary to motivate the subsequent theoretical discussion. Some further material that I would have included here had space allowed may be found in Leggett (2000a).

The plan of the review is as follows. In Sec. II I give a brief introduction to the experimental systems, with emphasis on orders of magnitude and on the role of the hyperfine degree of freedom. Section III is devoted to the origin, definition, and occurrence of BEC and some related concepts such as the order parameter and superfluid velocity. In Sec. IV I discuss in some detail the effective interatomic interaction (a topic that tends to be passed over in most papers in a couple of lines), with some attention to the infamous "factor of 2," which is liable to confuse newcomers to the field, particularly in the multispecies case. Section V derives and discusses the time-independent and time-dependent Gross-Pitaevskii equations, including their generalizations to finite temperature and to multispecies systems. Section VI is devoted to the rotational properties of a Bose condensate and the associated notion of superfluidity; here, in contrast to much of the existing alkali-gas literature, I tend to play down "vortices" and concentrate on intrinsically multiply connected topologies, as I believe that this permits a much clearer conceptual picture. In Sec. VII, which is the longest in the paper, I discuss in some detail the "toy model" that results when the N bosons in question are restricted to a single two-dimensional Hilbert space; this permits a discussion of various phenomena (Josephson effect, phase diffusion, etc.) that have more complicated, and in my opinion often less well-understood, analogs in the case of an extended system. Section VIII introduces the Bogoliubov approximation, from a point of view that is not the majority one in the literature, and discusses its relation to the time-dependent Gross-Pitaevskii description. Section IX briefly lists and comments on some further topics which for various reasons are not covered in the main text.

The reader who compares this review with much of the existing literature on BEC, whether in ^{4}He or the alkali gases, will be struck by the fact that I virtually bend over backwards to avoid introducing the idea of "spontaneously broken gauge symmetry." (I do use it once, reluctantly, in Sec. VIII, but only for the purpose of making contact with the formalism that has become standard in the literature.) It would be disingenuous of me to attempt to conceal the fact that I believe the utility of this idea is outweighed by its dangers; see Sec. III.D.1

Finally, a note on referencing policy. In these days of automated databases, I do not believe it is particularly useful for a review of this type to attempt to provide a comprehensive list of papers in the literature that deal with the various topics described, still less to grade them according to relative significance. Generally speaking, when I am discussing basic conceptual issues I have tried to reference at least a selection of what I regard as the most important discussions (which are not necessarily the chronologically earliest ones); however, once it comes to applications of the basic equations I have often referenced only one or two recent papers from which I believe most of the rest of the relevant literature can be traced. Obviously the choice of these is highly subjective and indeed arbitrary, and I hope that the many authors whose papers I have failed to reference will not attribute this to malice!

II. THE SYSTEMS

A. General

The experimental systems I shall be addressing in this review are collections of individual neutral alkali-gas atoms,[1] with total number N ranging from a few hundred up to $\sim 10^{10}$, confined by magnetic and/or optical means to a relatively small region of space. Their (maximum) densities range from $\sim 10^{11}$ cm^{-3} to $\sim 5\times 10^{15}$ cm^{-3}, and their temperature, in the regime of interest to us, is typically in the range of a few tens of nK–~ 50 μK. It is needless to mention that such an atomic gas cannot in fact be the stable thermodynamic state of the N atoms, which would at these temperatures certainly correspond to a solid; however, the formation of the solid requires as a first step the recombination of two atoms to form a diatomic molecule, and while this process is certainly exothermic (with formation energies typically $\sim$0.4–1.2 eV) it is very slow in the absence of a third atom to carry off the surplus energy, angular momentum, etc. Thus in practice the dominant recombination processes are usually "three-body" ones; the rate per atom is typically $\sim 10^{-29}$–10^{-30} cm^6 sec^{-1}, giving a sample lifetime of the order of a few seconds to a few minutes.

An alkali atom in its ground state has a single valence electron in an *ns* state outside one or more closed shells (except for H); the electronic ground state is therefore a doublet. Except in the case of H, the only electronic excited state that is of much interest is the *np* state (since it is overwhelmingly to this state that radiation in the optical regime will couple the ground state); the wavelengths λ of the "fundamental" ($ns \rightarrow np$) transition lie in the range 5000–7000 Å and the excited-state lifetimes in the range 16–35 nsec (see, for example, Weiner *et al.*, 1999, Table II). [In the case of H ($n=1$) there is of course no $1p$ state and a single photon will preliminarily excite the atom to the $2p$ state; however, a pair of photons can excite the $1s \rightarrow 2s$ transition, and this has played an important role in recent experiments.]

If we treat the atom for the moment as a single indivisible entity (see Sec. III.A) and consider the exchange of two atoms of the same (chemical and isotopic) species, this involves exchanging $Z+A$ fermions, and thus the total wave function should be symmetric or antisymmetric under this exchange according as $Z+A$ is even or odd. Since Z is automatically odd for the alkali elements, this means that a system of identical odd-A isotopes will obey Bose-Einstein statistics (and hence has the possibility to display BEC), while an even-A system such as ^{6}Li or ^{40}K will obey Fermi-Dirac statistics. We shall be interested from now on in the former case, although the latter is also very interesting (see de Marco and Jin, 1999). The odd-A isotopes, other than ^{1}H, in which BEC has been demonstrated at the time of writing, are ^{87}Rb, ^{23}Na, ^{7}Li, and, very recently, ^{85}Rb; as it happens, each of the first three has nuclear spin 3/2, so when discussing the effects of nuclear spin in Sec. II.C I shall concentrate on this case. A table of the principal stable or long-lived alkali Bose isotopes may be found in Pethick and Smith (2000), Chap. 3.

B. Trapping potentials

For the purposes of this review it is not necessary to go into the details of the various ingenious schemes that have been developed over the last 15 years or so for the trapping of neutral atoms (or, what is equally important for the real-life experiments, for their cooling into the μK–nK regime where BEC can occur); for these topics, the reader is referred, for example, to Ketterle *et al.* (1999) or to the 1998 Nobel lectures. However, it is important to appreciate the general features of the resulting effective potentials in which the atoms move, and in

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[1] It is convenient for the present purpose to include H in the alkalis. However, some of the values quoted as "typical" below do not apply to it.

particular their dependence (or not) on the hyperfine-Zeeman degree of freedom to be discussed in Sec. II.C.

1. Laser traps

For an excellent account of the general subject of atom-laser interactions, the reader is referred to Cohen-Tannoudji (1992). The effect that has been principally exploited in the laser trapping of atoms in the BEC regime (as distinct from their cooling into this regime) is the so-called dipole effect, which relies on the (conservative) interaction of the laser field with the electric dipole moment it induces on the atom. For the purposes of an initial discussion, let us ignore the fine and hyperfine structure and define the detuning of the $ns \rightarrow np$ transition frequency in the standard way:

$$\Delta \equiv \hbar \omega_{las} - (E_{np} - E_{ns}) (\equiv \hbar \omega_{las} - 2\pi \hbar c/\lambda). \tag{2.1}$$

It is also convenient to define the saturation intensity I_o, that is, the laser-beam intensity, which, when exactly on resonance, will induce a population of order unity of the excited (p) state. To within a numerical factor of order unity which depends on polarization, etc., this is given by

$$I_o = \epsilon_0 c \Gamma^2 / d^2, \tag{2.2}$$

where d is an appropriately defined dipole matrix element for the transition in question and $\Gamma \equiv \hbar/\tau$; a typical value of I_o is of order $100\,\mathrm{W/m}^2$. Then a convenient expresssion for the change in energy of the atom in the laser field is, in the limit $\Gamma \ll \Delta$,

$$\Delta E_{laser}(\mathbf{r}) = \left(\frac{I(\mathbf{r})}{I_o} \right) \frac{\Gamma^2}{\Delta}. \tag{2.3}$$

Note that in this formula I/I_o can be larger than 1 [provided it is $\ll (\Delta/\Gamma)^2$]. A region of high laser intensity thus provides an attractive potential for $\Delta < 0$ ("red detuning") and a repulsive potential for $\Delta > 0$ ("blue detuning"). It should be borne in mind that by arranging to have two counterpropagating laser beams, the potential can be varied over a scale of as short as half the laser wavelength, i.e., ~3000 Å.

An important question is the degree to which, if at all, laser-generated potentials are sensitive to the hyperfine-Zeeman index discussed in Sec. II.C. To the extent that spin-orbit coupling in the excited state is neglected, it is clear that there can be no effect at all, since the orbital ground state (s state) is unique. Moreover, for a linearly polarized laser beam the two electron-spin states are clearly equivalent by time reversal, so any effect would have to be at most of the order of the ratio of hyperfine-Zeeman splitting to the detuning, which in most experiments is $\lesssim 10^{-4}$ (see below). The case of a circularly polarized laser beam is more complicated, and by tuning fairly close to the (fine-structure-split) resonance a considerable sensitivity to the hyperfine index can be obtained; see Corwin *et al.*, 1999.

An important consideration in laser trapping is that one usually wishes as far as possible to avoid spontaneous emission processes [note that a single optical photon, in the (admittedly unlikely) event that its energy were totally absorbed in the atomic gas, would be more than enough to heat it right out of the BEC phase]. As shown in detail by Cohen-Tannoudji (1992), for $\Gamma \ll \Delta$ the emission probability per atom is of order $[I(\mathbf{r})/I_o]\hbar^{-1}\Gamma^3/\Delta^2$. In view of the Δ^{-2} falloff by comparison with the Δ^{-1} behavior in Eq. (2.3), it is generally advantageous to tune the laser(s) very far off resonance. In fact, it is quite common to detune by ~10% of the original optical frequency,[2] so that the ratio Γ/Δ is $\sim 10^{-7} - 10^{-6}$; then, even in the red-detuned case with, say, 10^6 atoms in one's sample, the spontaneous emission rate is only a fraction of a $\sec^{-1}$ and is unlikely to affect the experiment. When blue-detuned radiation is used to provide a barrier, the spontaneous emission effect is obviously less important, since the atoms do not appreciably penetrate the barrier region. The crucial qualitative point is that it is possible in this way to provide laser-generated potentials that are of an order greater than the thermal energy (or other characteristic energy scales; see Sec. III) without appreciable heating effects. Note also that the time scales over which such potentials can be manipulated are extremely short (being in fact typically limited by the turning-on time of the laser). For a more extended discussion of laser (optical) confinement I refer the reader to Stenger *et al.* (1998b).

2. Magnetic traps

The magnetic analog of Earnshaw's theorem forbids the magnitude of the magnetic field $\mathbf{B}(\mathbf{r})$ to have a local maximum in free space. However, nothing forbids the occurrence of a local minimum, and various methods can be used to provide such a minimum, the most widely used being variants of the "time-orbiting potential" and Ioffe-Pritchard traps; for a detailed description of these the reader is referred to the papers of Petrich *et al.* (1995) and of Pritchard (1983), respectively. Virtually all "pure" (i.e., non-laser-assisted) magnetic traps used in BEC experiments to date have had axial symmetry and a finite offset field, i.e., with an appropriate choice of cylindrical polar coordinate system the *magnitude* of the field has the form

$$|\mathbf{B}(\mathbf{r})| = B_o + \frac{1}{2}\alpha\rho^2 + \frac{1}{2}\beta z^2. \tag{2.4}$$

One might wonder why I have not specified the *direction* of the field as a function of $\mathbf{r}$. The reason is that even when this direction varies appreciably from its value at the origin, the atoms move so slowly that it is an excellent approximation to regard their magnetic moments as following the direction of the local field adiabatically (see Sec. V.D). Thus, if we consider a given hyperfine-Zeeman species, its potential energy will be a function

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[2] However, the detuning is usually still small enough relative to the resonance frequency that the counter-rotating terms (see Cohen-Tannoudji, *op. cit.*) can be neglected in the analysis.

only of the local field magnitude (2.4); in fact in the simplest case it will be proportional to it with a constant of proportionality μ (see below).

3. Gravity

For atoms in the nK–μK temperature regime, the effect of the Earth's gravitational field is by no means negligible: for a ^{87}Rb atom at 100 nK the thermal energy corresponds to a vertical displacement in this field of only about 1.6 μ, less than the extent of the thermal cloud in a typical trap in the absence of gravity. The effect of gravity is, crudely speaking, to shift the minimum of the potential in the vertical direction; in the case of a pure laser trap, where the original potential is nearly independent of the hyperfine-Zeeman species, this effect is not of great importance, but in the case of magnetic trapping the species-independent gravitational effect competes against a species-dependent magnetic force, and the effect is in general to displace the minimum of the potentials for different species relative to one another, an effect sometimes called "sag." However, in certain cases it is possible to eliminate this effect by a judicious choice of field (see below).

C. The hyperfine and Zeeman interactions

For a general account of this subject, I refer the reader to Woodgate (1970), Chap. 9. Quite generally, a *hyperfine-Zeeman*[3] *sublevel* of an atom with given total electronic angular momentum J and nuclear spin I may be labeled by the projection m_F of total atomic spin $\mathbf{F} \equiv \mathbf{I}+\mathbf{J}$ on the axis of the field $\mathbf{B}$ (which is a good quantum number for any $|\mathbf{B}|$) and by the value of total $F[\mathbf{F}^2 \equiv F(F+1)]$ which characterizes it in the limit $|\mathbf{B}| \to 0$: F takes value from $|I-J|$ to $I+J$. In the present context, I shall specialize immediately to the electronic ground state of the alkalis ($J=S=1/2$) and approximate the electronic-spin g factor g_s by 2; moreover, since the only experiments to date involving more than one hyperfine species have been done on ^{87}Rb or ^{23}Na, I shall specialize to the I value characterizing both of these (and also ^{7}Li), namely, 3/2 (so $F=1$ or 2). Finally, for the moment I shall neglect the small nuclear Zeeman energy. Then the energies of the various hyperfine sublevels are given as a function of the magnetic-field magnitude B by the appropriate special case of the Breit-Rabi formula [see Woodgate, 1970, Eq. (9.80)]. It is convenient to choose the zero of energy to be the mean of the $B=0$ $F=1$ and $F=2$ energies and to define the zero-field splitting $E(F=2)-E(F=1)$ as $2A$. A has the sign of the nuclear g factor and is positive for all the $I=3/2$ alkali isotopes. We also introduce a characteristic hyperfine "crossover" field B_{hf} by $B_{hf} \equiv A/|\mu_B|$ $(\mu_B = e\hbar/2m_e)$. Then the energies of the various levels are given as follows:

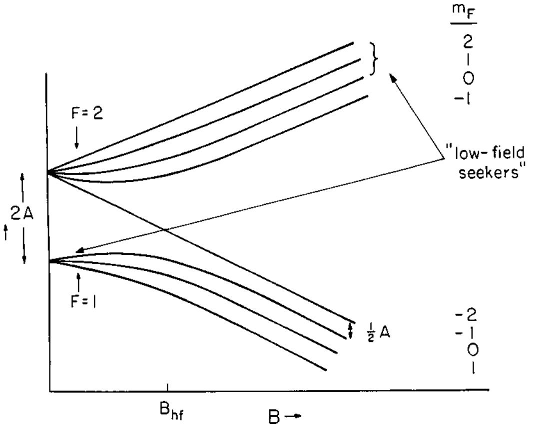

FIG. 1. The energies of the different hyperfine-Zeeman states as a function of magnetic field.

$$\begin{array}{ccl}
m_F & F & E(B) \\
2 & 2 & A(1+B/B_{hf}) \\
1 & \left\{\begin{matrix}2\\1\end{matrix}\right\} & \pm A[1+B/B_{hf}+(B/B_{hf})^2]^{1/2} \\
0 & \left\{\begin{matrix}2\\1\end{matrix}\right\} & \pm A[1+(B/B_{hf})^2]^{1/2} \\
-1 & \left\{\begin{matrix}2\\1\end{matrix}\right\} & \pm A[1-B/B_{hf}+(B/B_{hf})^2]^{1/2}) \\
-2 & 2 & A(1-B/B_{hf}),
\end{array} \tag{2.5}$$

where the plus sign corresponds to $F=2$ and the minus sign to $F=1$. A graph of these eigenvalues versus B is shown in Fig. 1; note in particular (1) the inversion of the order of the energies as a function of m_F in the lower multiplet relative to the upper one; (2) the nonmonotonic behavior of the two $m_F=-1$ states; and (3) the fact that (within this approximation) the initial slope of $E(B)$ is identical for the $F=2$, $m_F=1$ and $F=1$, $m_F=-1$ states.

Most BEC experiments have been done with fields that are much less than B_{hf} in the relevant region of space, and it is then usually legitimate, to a first approximation, to linearize Eqs. (2.5) in B:

$$E(B) \cong \pm \left\{ A + \frac{1}{2}|\mu_B| m_F B \right\}, \tag{2.6}$$

with the + (−) sign referring to the upper (lower) multiplet. We see that in a field configuration of the form (2.4), the states $F=2$, $m_F=-2,-1$ and $F=1$, $m_F=0$, -1 will be expelled from the trap (or in the case $F=2$, $m_F=-1$ displaced to the locus $B(\mathbf{r})=B_{hf}/\sqrt{2}$); these states are usually called "high-field seekers." On the other hand, the states $F=2$, $m_F=-2$, 1 or 0 and $F=1$, $m_F=-1$ (in the limit $B \ll B_{hf}$) are "low-field seekers" and will be attracted to the origin.

Now, if we start with a gas of pure $F=2$, $m_F=1$ or $F=2$, $m_F=0$ atoms, it turns out that even in the neglect of dipolar forces (which do not in general conserve the total m_F of the atoms involved), two-body collisions can

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[3] In the following I use "hyperfine" as a shorthand for "hyperfine-Zeeman"; thus two different hyperfine species may differ in the values of F and/or m_F.

produce lower-energy, high-field-seeking states, and for this reason most experiments to date on single hyperfine species in magnetic traps have been on one of the two "maximally stretched" states, namely, $F=2, m_F=2$ and $F=1, m_F=-1$. However, multispecies experiments have involved other states, in particular $F=2, m_F=1$. We see that given a field configuration of the form (2.4) with $B \ll B_{hf}$, the potential felt by an atom in a given hyperfine state is in our approximation expressed in the form

$$V(\rho,z)=\text{const}+\frac{1}{2}M\omega_r^2\rho^2+\frac{1}{2}M\omega_z^2z^2, \tag{2.7}$$

where the value of $\omega_r \equiv 2\pi\nu_r$ is identical for the $F=2$, $m_F=1$ and $F=1$, $m_F=-1$ states but a factor of $\sqrt{2}$ larger for the $F=2$, $m_F=2$ state (and similarly for $\omega_z \equiv 2\pi\nu_z$). Experimental papers reporting work on a single hyperfine species commonly specify the trap in terms of the relevant values of ν_r and ν_z. In practice, typical values of each lie in the region of a few Hz to a few kHz; there is no generic constraint on the ratio ν_r/ν_z, which may, depending on the trap, be $\gg 1$, ~ 1, or $\ll 1$.

Although Eq. (2.5) [and hence Eq. (2.6)] is usually an adequate approximation for $B \ll B_{hf}$, it is necessary on occasion to go beyond it. A case in point is the calculation of the relative equilibrium positions, in the presence of gravity, of the $F=2, m_F=1$ and $F=1, m_F=-1$ states. The position of the minimum in each case is determined by balancing the Earth's gravitational field against the gradient of the magnetic potential, and if we were to use Eq. (2.5) it would coincide for the two species. However, at this point it is necessary to take into account both the nuclear Zeeman term and the term of order B^2 in the expansion of formulas (2.5) (*the quadratic Zeeman effect*); it turns out that these two small effects exactly cancel when B has the special value (4/3) $\mu_n A/\mu_B^2$ ($\sim 1G$). A second respect in which the quadratic Zeeman effect plays a useful role is that by making the frequencies for (say) the $m_F=1 \rightarrow m_F=0$ and $m_F=0 \rightarrow m_F=-1$ transitions unequal it permits selective population, by an ordinary rf pulse acting on an originally purely $m_F=-1$ population, of the $m_F=0$ state without appreciable population of the $m_F=1$ state—something which is not possible so long as the (hyperfine) Zeeman energy is purely linear in m_F (on this, see Stenger *et al.*, 1998b, Sec. V).

D. Imaging

The raw data from which we infer the static and dynamic behavior of an ultracold trapped alkali gas, and in particular of a Bose-Einstein condensate, is almost without exception optical, involving the fundamental visible-region $ns \rightarrow np$ transition. I shall treat this subject quite briefly, simply to indicate broadly what kind of information can be obtained and with what order of accuracy. For further details I refer the reader to Ketterle *et al.* (1999).

The most important single point to appreciate is that the energy interval over which both the real and the imaginary parts of the dielectric constant of an atomic gas show substantial variation, namely, the linewidth Γ, is typically of order 0.5 mK (a few MHz) and hence small compared to the zero-field hyperfine ground-state splitting (100 mK–1 K). Thus there is no difficulty in measuring by optical means not only the total density of the gas but the density of atoms in the $F=2$ and $F=1$ multiplets separately. If one wishes to distinguish different sublevels within each multiplet, the energy resolution alone may or may not be sufficient, but one can exploit the sensitivity of a transition out of a particular sublevel to the polarization of the probe laser to make the distinction. In most, though not all, experiments the quantity that is directly measured is either the total atomic density or that of a particular species (usually integrated along the line of the probe laser beam) as a function of space and/or time.

The simplest optical imaging technique relies on straight absorption: the logarithm of the intensity transmitted through a column of gas is simply proportional to the integrated atomic density (or the density of the particular species selected). This method is inherently destructive (since real absorption processes are followed by spontaneous radiation and the accompanying heating), and in addition is difficult to apply at high densities (see Andrews *et al.*, 1996, p. 85, paragraph 2); thus in practice one often switches off the trap and allows the sample to expand (and thus rarefy) before switching on the probe laser beam.

A second, nondestructive measurement technique is dispersive (phase-contrast) imaging; this relies on the diffracting effect of the gas and does not involve (much) heating of the sample; it need not therefore be destructive, and it is believed that up to ~ 100 successive imagings may be obtained by this method (Andrews *et al.*, 1996). The spatial resolution obtainable is typically of the order of a few microns; as to the time resolution, it is apparently limited only by the switching-on time of the laser. As we shall see, this time is many orders of magnitude smaller than the typical time scales of the dynamics of the system, so optical measurements of density may reasonably be regarded as instantaneous.

E. Orders of magnitude

To aid our qualitative understanding, it is useful to compare typical orders of magnitude of various relevant energies for a set of ultracold atoms in a single system of units. In Table I, for definiteness we choose 10^6 ^{87}Rb atoms in a "typical" magnetic trap; numbers for the other heavier alkalis are generally comparable, but for H may be different by up to two or three orders of magnitude. In discussing the physical significance of some of these quantities I anticipate some of the results to be obtained in Secs. III–V.

It is worthwhile to note explicitly that the first three quantities in Table I, and the recoil energy, are characteristics of the isolated atom and do not depend on the

TABLE I. Energies for a set of 10^6 ultracold ^{87}Rb atoms in a typical magnetic trap.

	Temperature units	Frequency units
Energy of $ns \rightarrow np$ transition	$\sim 2\times 10^4$ K	4×10^{14} Hz
Zero-field hyperfine splitting	~ 0.3 K	~ 7 GHz
Energy width of transition ($\hbar\Gamma$)	~ 0.3 mK	~ 6 MHz
Characteristic two-body energy $\hbar^2/ma_s^2$	~ 0.3 mK	~ 6 MHz
Transition temperature $k_B T_c$	~ 500 nK	~ 10 kHz
Recoil energy $\hbar^2 k_{opt}^2/2M$	~ 200 nK	~ 5 kHz
Mean-field energy nU_o	~ 100 nK	~ 2 kHz
Zero-point energy in harmonic well	~ 5 nK	~ 100 Hz

conditions of confinement. The *two-body energy* $\hbar^2/ma_s^2$ can be tuned by adjusting the magnetic-field strength so as to vary the scattering length a_s (see Sec. IV.B) but is otherwise insensitive to the details of the trap geometry. By contrast, not only the zero-point energy $\hbar\omega_o$ but the transition temperature and the mean-field energy depend on the shape of the confining potential, as well as (in the latter two cases) on the total number of particles trapped; as we shall see in Sec. V.E, for a given species with a_s fixed, $k_B T_c$ is proportional to $N^{1/3}\omega_o$, while typical values of the mean-field energy in the condensed phase are proportional to $N^{2/5}\omega_o^{6/5}$. Thus variation in N, in particular, can result in substantial variations in these two quantities around the typical values quoted. Nevertheless, under realistic conditions with "typical" values of a_s ($\sim$50–100 Å; see Sec. IV.B) we almost always have the set of inequalities

$$\hbar^2/ma_s^2 \gg k_B T_c \gg nU_o \gg \hbar\omega_o, \tag{2.8}$$

although in the case of the second inequality the $\gg$ may represent a ratio that is only of order 5 (see Table I).

It is useful also to note some length scales characteristic of the BEC alkali-gas problem, and their relative orders of magnitude. Apart from the s-wave scattering length a_s, we define the (typical) mean interparticle spacing r_{int}, the "healing length" $\xi \equiv (2mnU_o\hbar^2)^{-1/2}$ (see Sec. V.A), the thermal de Broglie wavelength at T_c, λ_{DB}, and the oscillator length $a_{ho} \equiv (\hbar/m\omega_o)^{1/2}$, which is the zero-point spread of the ground-state wave function of a free particle in the trap in question. Under normal conditions, we then have the inequalities

$$a_s \ll r_{int} \sim \lambda_{\mathrm{DB}} \lesssim \xi \ll a_{ho}. \tag{2.9}$$

Typical values might be $a_s \sim 50$ Å, $r_{int} \sim 2000$ Å, $\xi \sim 4000$ Å, $a_{ho} \sim 1\,\mu$.

It is interesting to compare the above numbers with those characteristic of liquid helium.[4] In the case of helium at liquid densities, the concept of an s-wave scattering length is not really meaningful, but a somewhat similar role is played by the characteristic dimension of the hard-core part of the interatomic potential, which is around 2.5 Å. This should be compared with the interparticle spacing, which is about 3.5 Å; we see that the *dilute-gas condition* $a_s \ll r_{int}$ which is so characteristic of the BEC alkali gases is very far from satisfied for liquid helium. As a consequence, liquid helium is, in an intuitive sense, a much more strongly interacting system than the BEC gases, by many orders of magnitude, and this leads to a number of profound differences between the two systems. In particular, (1) in the alkali gases the behavior is extremely sensitive to the details of the trap, whereas in helium it is dominated by the interparticle interactions and very insensitive to the confining potential (which is in any case typically due to a fairly rigid "box" and thus flat over most of the region of interest); (2) in helium, interatomic collisions are so frequent that any process that is energetically allowed takes place virtually instantaneously, whereas in the alkali gases the kinetics of the process may be an important bottleneck (see Sec. VI.E); (3) on the theoretical front, quantitative calculations based on perturbation theory in the (effective) interatomic interaction are usually believed to be highly reliable for the alkali gases, whereas for helium they may fail miserably. There are other important differences between the two systems, in particular, that in the alkali gases both the external and, at least in principle, the interatomic potentials can be adjusted over a time scale very short compared to the time scales characterizing the dynamics of the system: this permits types of experiment, such as the celebrated interference experiment of Andrews *et al.* (1997; see Sec. VII.E), that, while as it were conceptually equally viable in superfluid ^{4}He, would in practice be totally impossible to realize. For a more detailed discussion of the analogies and differences between the superfluid phases[5] of ^{4}He and ^{3}He on the one hand, and the BEC phase of the alkali gases on the other, see Leggett (1999a).

III. THE DEFINITION, ORIGIN, AND OCCURRENCE OF BEC: THE ORDER PARAMETER

A. Definition of BEC

For pedagogic convenience let us start with the case in which the hyperfine degree of freedom can be ignored.

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[4] The numbers quoted are for ^{4}He at saturated vapor pressure; the numbers at pressures up to freezing, and for the light isotope ^{3}He, are similar in order of magnitude.

[5] The Fermi system ^{3}He is believed to become superfluid by forming Cooper pairs, which then effectively undergo BEC; the pairs are somewhat analogous to the alkali atoms in that they possess a hyperfine degree of freedom.

We thus consider a system of N identical spinless bosons characterized by spatial coordinates $\mathbf{r}_i$ $(i=1,2\cdots N)$, with arbitrary interparticle interactions and subject to some external potential, possibly time dependent, which for technical reasons we shall assume is such as to confine the particles in some finite region of space. We do not assume that the system is necessarily in thermal equilibrium, nor even in a steady state. The many-body wave functions $\Psi_N(\mathbf{r}_1\mathbf{r}_2\cdots\mathbf{r}_N:t)$ must be symmetric with respect to the interchange $\mathbf{r}_i\rightleftharpoons\mathbf{r}_j$ of any two particle coordinates.

For any given time t we can define the one-particle reduced density matrix $\rho(\mathbf{r},\mathbf{r}':t)$ in the standard way. We may as well go directly to the most general case, in which the description of the system is by a statistical mixture of mutually orthogonal many-body states $\Psi_N^{(s)}$ with probability p_s: the definition is

$$\begin{aligned}\rho(\mathbf{r},\mathbf{r}':t)&\equiv N\sum_s p_s\int d\mathbf{r}_2\cdots d\mathbf{r}_N\Psi_N^{*(s)}\\&\quad\times(\mathbf{r}\mathbf{r}_2\cdots\mathbf{r}_N:t)\Psi_N^{(s)}(\mathbf{r}'\mathbf{r}_2\cdots\mathbf{r}_N:t)\\&\equiv\langle\hat{\psi}^\dagger(\mathbf{r}t)\hat{\psi}(\mathbf{r}'t)\rangle,\end{aligned}\tag{3.1}$$

where in the last expression the quantity $\hat{\psi}(\mathbf{r})$ is the standard boson field operator, and the average indicated by the pointed brackets is in general statistical as well as quantum mechanical. Because of the Bose symmetry, the fact that in writing the second expression in Eq. (3.1) we have arbitrarily picked out the coordinate $\mathbf{r}_1$ as "special" need not worry us.

It follows from the definition (3.1) that the quantity $\rho(\mathbf{r},\mathbf{r}':t)$, when regarded as a matrix function of its indices $\mathbf{r}$ and $\mathbf{r}'$, is Hermitian, and can therefore be diagonalized with real eigenvalues. That is, it is always possible to find a complete orthonormal basis, in general time dependent, of single-particle eigenfunctions $\chi_i(\mathbf{r};t)$ such that we can write

$$\rho(\mathbf{r},\mathbf{r}':t)=\sum_i n_i(t)\chi_i^*(\mathbf{r}:t)\chi_i(\mathbf{r}':t).\tag{3.2}$$

It is important to note that in the general case (a) not only the eigenfunctions χ_i appearing in Eq. (3.2) but also the eigenvalues n_i may be functions of time; (b) the χ_i need not be eigenfunctions of any particular quantity [other than $\rho(\mathbf{r}\mathbf{r}':t)$ itself] and in particular are not necessarily eigenfunctions of the single-particle terms in the Hamiltonian; and (c) if we define operators a_i by

$$a_i(t)\equiv\int\hat{\psi}(\mathbf{r})\chi_i^*(\mathbf{r}:t)d\mathbf{r},\tag{3.3}$$

then while the $n_i(t)$ are the expectation values of the operators $a_i^\dagger(t)a_i(t)$, the many-body wave function is not in general an eigenfunction of the latter operator.

We are now in a position to formulate a definition of Bose-Einstein condensation (BEC). We shall say that at any given time t, the system shows BEC if one or more of the eigenvalues $n_i(t)$ is of the order of the total number of particles N; and further that it shows *simple BEC* if one and only one eigenvalue is of order N, all the rest being of order 1. Systems showing nonsimple BEC (i.e., having more than one eigenvalue of order N) are sometimes said to be fragmented. The phrase "of order $N(1)$" is somewhat vague in a situation where there is no simple thermodynamic limit, but in practice this does not usually lead to difficulty.

In the case of simple BEC, we shall arbitrarily use the value zero of the index i to refer to the unique state which has $n_i(t)\sim N$; we shall call the single-particle state $\chi_0(\mathbf{r}:t)$ the *condensate wave function* and the eigenvalue $N_0(t)$ (where we use the capital to emphasize the macroscopic value) the "(mean) number of particles in the condensate." A very important quantity associated with χ_0, the superfluid velocity $\mathbf{v}_s(\mathbf{r},t)$, will be introduced in Sec. III.D.

One point concerning the above definition is very important: In general, a statistical mixture of many-body states, each of which separately possesses (simple or general) BEC, need not itself possess BEC. (Consider, for example, a mixture of $p\sim N$ many-body states, each of which has a condensate in a different one of p mutually orthogonal states χ_0.) On the other hand, no mixture of many-body states that do not individually show BEC can itself show BEC.

Finally, let us generalize the above definitions to take account of the hyperfine degree of freedom. We now characterize the ith particle not just by its spatial coordinate $\mathbf{r}_i$ but by a discrete hyperfine index α_i, so that Ψ_N is a function of $\{\mathbf{r}_i,\alpha_i\}$, $(i=1,2\cdots N)$. The appropriate generalization of Eqs. (3.1) and (3.2) is then [omitting the intermediate expression in Eq. (3.1) whose generalization is obvious, and writing the field operator for hyperfine state α as $\hat{\psi}(\mathbf{r},\alpha)$ rather than the more conventional notation $\hat{\psi}_\alpha(\mathbf{r})$]

$$\begin{aligned}\rho(\mathbf{r}\alpha,\mathbf{r}'\alpha':t)&\equiv\langle\hat{\psi}^\dagger(\mathbf{r},\alpha)\hat{\psi}(\mathbf{r}',\alpha')\rangle\\&=\sum_i n_i(t)\chi_i^*(\mathbf{r},\alpha:t)\chi_i(\mathbf{r}',\alpha':t).\end{aligned}\tag{3.4}$$

The definition of (simple and general) BEC is then exactly as above, the only difference being that the condensate wave function $\chi_0(\mathbf{r},\alpha:t)$ now has a discrete (hyperfine) argument α as well as a continuous (position) one $\mathbf{r}$, i.e., it can be regarded as a spinor. We shall see below (Sec. V) that the BEC occurring in a situation where the hyperfine degree of freedom is important is often not of the simple variety.

B. Why BEC?

Whether or not BEC occurs in a given Bose system depends strongly on the sign of the "effective" interatomic interaction (a concept that will be defined precisely for the alkali gases in Sec. IV). The case of attractive interaction is rather subtle and is discussed briefly in Sec. IX; here we confine ourselves to the case of repulsive (or zero) interaction. For such a case the tendency of the system to undergo BEC, which is by no means confined to states of (or close to) thermal equilibrium, is a consequence of two mutually reinforcing effects, statistical and energetic. I discuss these in turn.

The statistical consideration is a standard textbook subject (though its generic significance is often somewhat obscured because it tends to be discussed in the specific context of a derivation of the equilibrium thermal distribution). Consider the problem of distributing N objects (atoms) among p different boxes (states). If the objects are distinguishable (the classical case), the number of different ways of distributing them so that the ith box contains n_i objects is the multinomial coefficient $N!/\Pi_{i=1}^{p} n_i!$. If on the other hand the objects in question are indistinguishable but there are no other constraints (the boson case), then clearly there is one and only one way of distributing them, for a given set of $\{n_i\}$. The difference becomes important when $N \gtrsim p$ (the *degeneracy condition*), and its effect, crudely speaking, is that in the bosonic case states in which many particles occupy the same state have a higher relative weight than in the classical (distinguishable) case.[6] This tendency of bosons to "cluster" is very generic; it is in no way restricted to thermal equilibrium, or to the noninteracting case.

If, however, we specialize for the moment to the case of noninteracting bosons in thermal equilibrium, and moreover are content to use the standard grand canonical ensemble,[7] the results take a very simple and standard form [see, for example, Huang (1987)]: at temperature T the formula for the mean number of particles n_i in the single-particle energy eigenstate i with energy ϵ_i has the standard Bose-Einstein form

$$n_i = \{\exp[\beta(\epsilon_i - \mu) - 1]\}^{-1} \quad \beta \equiv 1/k_B T, \tag{3.5}$$

where the chemical potential μ is fixed by the condition

$$\sum_i n_i(\mu, \beta) = N, \tag{3.6}$$

N being the average number of particles in the grand canonical ensemble.

The quantity $\mu(\beta{:}N) \equiv \mu(T,N)$ implicitly defined by Eq. (3.6) is very large and negative for $T \to \infty$; as T falls it increases monotonically. If at some temperature T_c condition (3.6) can be met with $\mu \to 0^-$, then below T_c the occupation of the lowest single-particle state (energy $\epsilon_0 = 0$ by convention) is of order N, while the other n_i's are still generally of order unity or less, i.e., BEC is realized. This condition is met, in free space, for dimension $D > 2$, and in a harmonic trap (isotropic or not)[8] for $D > 1$; see, for example, Dalfovo *et al.* (1999) or Pethick and Smith (2000). For each of these cases the transition temperature T_c can of course be calculated exactly as a function of N and the geometric parameters, but a simple rule of thumb, valid except very close to the borderline dimension, is that BEC occurs when the degeneracy condition $N \sim p$ is satisfied, with p taken to be the number of thermally accessible states, i.e., those with energies $\lesssim k_B T$. For example, in an anisitropic 3D trap with geometrical mean frequency $\overline{\omega_0} \equiv (\omega_r^2 \omega_z)^{1/3}$, where the mean density of single-particle states per unit energy $\mathcal{E}$ is $\mathcal{E}^2/(\hbar \overline{\omega_0})^3$, this argument gives for large N

$$k_B T_c = \text{const}\, \hbar \overline{\omega_0} \cdot N^{1/3}. \tag{3.7}$$

A quantitative calculation (see the cited references) confirms this result, with the constant fixed at 0.94.

For a noninteracting gas in any geometry in which BEC occurs, the condensate number $N_0(T)$ increases smoothly from zero at T_c to the total number N as T falls to zero. In particular, for the above anisotropic 3D trap we find

$$N_0(T) = N[1 - (T/T_c)^3]. \tag{3.8}$$

For a comparison of this (noninteracting-gas) formula with experiments in the alkali gases, see Hau *et al.* (1998).

In addition to the above effect of statistics, there is also an energetic effect: In a dilute Bose gas with weakly repulsive interactions, the interactions tend to reinforce the effect of statistics in forming BEC. To see this, we need to anticipate a result to be proved in Sec. IV, namely that, at least so long as we stay in the dilute limit, the Hartree-Fock energy of two identical spinless bosons in different orbital states is greater than that of two such bosons in the same state, by a factor between 1 and 2. This effect not only helps us understand why even in nonequilibrium situations *fragmentation* (i.e., an order-N occupation of two or more single-particle orbital states) is unusual in a spinless system; rather generally it says that, other things being equal, the more repulsive the interatomic interaction (i.e., the greater the s-wave scattering length; see Sec. III), the stronger the tendency to condense. (However, at some point this tendency will be balanced by the coherent scattering of pairs out of the condensate; see Sec. VIII.)

It is plausible that in the less common case of a negative scattering length (attractive interaction) condensation is likely to be inhibited, and we return to this point briefly in Sec. IX.

C. Rigorous results

In the realistic case of an interacting Bose system in more than one dimension, rigorous results concerning the existence and degree of BEC as a function of particle number, strength of interaction, etc. are rather few

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[6] This tendency may be seen already in the trivial case $N = p = 2$: for distinguishable particles, states involving double occupation are 50% of the whole, while for bosons they are 66%.

[7] Because of the critical role in the theory of BEC played by conservation of total particle number N, it is not entirely obvious *a priori* that the use of the grand canonical ensemble is justified. However, calculations using the microcanonical ensemble give similar results for large N (see, for example, Gajda and Rzazewski, 1997).

[8] The case $D = 1$ is rather delicate; see Dalfovo *et al.*, 1999.

and far between (see Lieb, 1999) and to the best of my knowledge are at present confined entirely to extended systems in the thermodynamic limit. Of course, many readers will no doubt take the view that in the context of the real-life alkali gases such results are of rather minor interest, since both experiment and theoretical prejudice suggest that perturbation theory starting from the noninteracting gas is likely to be a reliable description. Nevertheless I feel it is worthwhile to summarize without derivation the few rigorous results known to me for the extended case; most of them probably could be (but to my knowledge have not been) generalized to a realistic trap geometry.

(a) For a 3D system in free space, Gavoret and Nozières (1964) showed many years ago that if perturbation theory starting from the noninteracting Bose gas converges, then at $T=0$ the system displays BEC. However, their argument allows no inference about the condensed fraction $N_0(0)/N$, nor about the critical temperature T_c.

(b) If the real-life continuum is replaced by a "lattice gas" and the interatomic interaction modeled by a hard-core on-site repulsion, then for the case of half filling the existence of BEC at $T=0$ has been proved (Kennedy *et al.*, 1988).

(c) The best-known theorem concerning the (non)occurrence of BEC in extended D-dimensional space is due to Hohenberg (1967). Denoting by n_k the average number of particles per unit volume in the plane-wave state $\mathbf{k}(\neq 0)$, he demonstrates rigorously for any dimension the inequality

$$n_k \geqslant (n_0/n)(mk_BT/\hbar^2k^2)-1/2 \quad (n\equiv N/V). \tag{3.9}$$

It then follows (Hohenberg, 1967) that for $D\leqslant 2$, in the thermodynamic limit, BEC cannot occur at any finite temperature.

(d) While for $D=3$ Hohenberg's inequality places no upper limit on T_c, it does place a limit on the condensate fraction $N_0(T)/N$, which is nontrivial for $T \gtrsim T_c^{(0)}$, where $T_c^{(0)}$ is the transition temperature of the noninteracting gas. A simple form (not the tightest attainable) of this limit is

$$N_0(T)/N \leqslant \alpha(T_C^{(0)}/T), \quad \alpha=\left[\frac{3\zeta(3/2)}{4}\pi^{1/2}\right]^{2/3} \cong 2\cdot 3. \tag{3.10}$$

This limit is completely independent of the nature and even the sign of the interatomic potential.

(e) Finally, for a Bose gas with an interaction that is everywhere repulsive and has a space integral V_0, it is possible to place an upper limit on the condensate fraction which for small V_0 is stronger than Eq. (3.10) (Leggett, 2000b). For the special case $T=T_c^{(0)}$ this reads

$$N_0/N \leqslant \mathrm{const}(nV_0/k_BT_c^{(0)})^{1/3}, \tag{3.11}$$

where the current upper bound on the constant is about 2.5.

D. The order parameter and the superfluid velocity

1. Possible definitions of the order parameter

For the purposes of the present section, let us consider a spinless system[9] and assume that simple BEC is realized in the state $\chi_0(\mathbf{r}{:}t)$, with eigenvalue $N_0(t)$. Then the simplest and most direct definition of the order parameter $\Psi(\mathbf{r},t)$ [do not confuse with the many-body wave function $\Psi_N(\mathbf{r}_1\cdots\mathbf{r}_N{:}t)$] is

$$\Psi(\mathbf{r}t)\equiv\sqrt{N_0(t)}\,\chi_0(\mathbf{r}{:}t), \tag{3.12}$$

that is, apart from its normalization $\Psi(\mathbf{r}t)$ is simply the (Schrödinger) wave function of the single-particle state into which condensation occurs. Contrary to widespread popular belief, this definition [which is to all intents and purposes the one originally given by Penrose and Onsager (1956)] is perfectly adequate for all the purposes for which the concept of an order parameter has been (correctly) used in the literature. One point needs special emphasis: Since $\Psi(\mathbf{r}t)$ is in effect simply a Schrödinger wave function, it is clear that while its space and time derivatives (and in the case of a hyperfine degree of freedom the phase relations between its hyperfine components) are meaningful physical quantities, *the overall phase of the order parameter has no physical significance*.

Various alternative definitions of the order parameter are to be found in the literature. Some, such as the definition explicitly based on "off-diagonal long-range order" (Penrose and Onsager, 1956; Yang, 1962), are conceptually unexceptionable but obviously inapplicable in a trap geometry. However, there is one definition that is sufficiently common in the alkali-gas BEC literature that it calls for comment, namely, that based on the idea of so-called "spontaneously broken gauge symmetry." I refer the reader to Anderson (1966), Leggett and Sols (1991), and Leggett (1995a) for an extended discussion of this concept and its difficulties, and just summarize the basic idea here: One imagines that the superselection rule for the total particle number N is somehow violated, so that one can write the wave function of the system as a superposition of states corresponding to different N:

$$\Psi=\sum_N a_N\Psi_N. \tag{3.13}$$

This allows the single-particle destruction operator $\hat{\psi}(\mathbf{r}t)$ to have (possibly) a finite expectation value, and one then identifies the order parameter with the latter:

$$\Psi(\mathbf{r}t)\equiv\langle\psi(\mathbf{r}t)\rangle. \tag{3.14}$$

It should be emphasized that *there are no circumstances in which Eq. (3.13) is the physically correct de-*

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[9] The generalization to systems with internal degrees of freedom is made in Sec. V.D.

scription of the system,[10] or even of a part of it, and in the present author's opinion the definition (3.14), while possibly streamlining some calculations when judiciously used, is liable to generate pseudoproblems and is best avoided. However, the reader should be warned that this opinion is controversial and that there are even those who feel that Eq. (3.14) is not only a possible, but the only legitimate, definition of the order parameter.

2. The superfluid velocity

The simplest definition of the superfluid velocity $\mathbf{v}_s(\mathbf{r},t)$ is directly in terms of the phase gradient of the condensate wave function $\chi_0(\mathbf{r}t)$: writing $\chi_0(\mathbf{r}t) \equiv |\chi_0(\mathbf{r}t)| \exp[i\varphi(\mathbf{r}t)]$, we define

$$\mathbf{v}_s(\mathbf{r},t) \equiv \frac{\hbar}{m} \nabla \varphi(\mathbf{r}t). \tag{3.15}$$

Clearly, since N_0 is by definition not a function of position, we could equally well have defined $\mathbf{v}_s$ in terms of the phase of the order parameter $\Psi(\mathbf{r}t) \equiv \sqrt{N_0}\chi_0(\mathbf{r}t)$. We see directly from its definition that $\mathbf{v}_s$ satisfies two important constraints, namely, the condition of irrotationality

$$\operatorname{curl} \mathbf{v}_s(\mathbf{r},t) \equiv 0 \tag{3.16}$$

and the celebrated Onsager-Feynman quantization condition

$$\oint \mathbf{v}_s(\mathbf{r}t) \cdot d\mathbf{l} = nh/m \quad (n \text{ integral}). \tag{3.17}$$

Obviously, in a simply connected geometry with $\chi_0(\mathbf{r}t)$ finite everywhere Eq. (3.16) implies Eq. (3.17) with $n = 0$, but there are more general cases, e.g., involving vortices, in which n can be nonzero; see Sec. VI below.

The reason the quantity defined by Eq. (3.15) is important in the theory of superfluidity, and more generally of BEC, is that on the one hand it reflects the properties of a single quantum state [unlike the hydrodynamic velocity $\mathbf{v}(\mathbf{r}t) \equiv \mathbf{j}(\mathbf{r}t)/\rho(\mathbf{r}t)$, which is an average over many different states and thus fails in general to satisfy Eq. (3.16) or Eq. (3.17)], while on the other hand, unlike the analogous quantity in single-particle Schrödinger quantum mechanics, which while perfectly definable is subject to huge quantum fluctuations, $\mathbf{v}_s$ characterizes the behavior of a macroscopic number of particles (the condensate) and can thus in effect be regarded as a classical quantity. (For further discussion, see Leggett, 2000a.)

Finally, I want to reemphasize that the definitions of the order parameter and of the superfluid velocity given in this subsection rely essentially on the assumption of simple Bose condensation, i.e., that there is one and only one eigenvalue of the single-particle density matrix of order N. Generalizations to the case of multiple condensates, while possible, need to be carefully defined.

IV. THE EFFECTIVE INTERACTION IN A COLD DILUTE GAS

A. Statement of the problem: neglect of $l \neq 0$ partial waves

In this section I consider the effect of atom-atom interactions in a gas at the very low temperatures and densities characteristic of the alkalis under BEC conditions; for a much more detailed treatment of this topic, see Dalibard (1999) and Weiner *et al.* (1999). For pedagogical simplicity I assume, in Secs. I–III, that two colliding atoms can be "tagged" (as would be the case if they were of different chemical and/or isotopic species); this will allow us to postpone discussion of the effects of indistinguishability to Sec. IV.D. However, it will turn out that none of the results of Secs. IV.A–IV.C depend on this assumption. Furthermore, we neglect for the moment the hyperfine degree of freedom, assuming that for each atom its initial and final values in a collision are equal. The only relevant variable, for a given pair of atoms, is then their relative coordinate $\mathbf{r}$, and the outcome of a collision will be determined by the value of the (initial) relative kinetic energy $E \equiv \hbar^2 k^2 / 2m_r$ (here and subsequently m_r denotes the reduced mass and k the relative wave vector).

Consider the true interatomic potential $V_{at}(r)$ as a function of the separation r of the two centers of mass (c.m.). At short distances, of the order of molecular dimensions, this potential may not even be definable (since the standard Born-Oppenheimer separation of the c.m. and internal degrees of freedom may break down, see Weiner *et al.*, 1999), but at distances $\gtrsim 5$ Å (beyond which the Born-Oppenheimer approximation should certainly be good), $V_{at}(r)$ should be well defined and well approximated[11] in the limit $r \to \infty$ by the lowest-order van der Waals interaction $-C_6/r^6$; if we express energies and lengths in the standard atomic units (bohrs and hartrees, respectively), C_6 ranges from ~ 1400 for Li to ~ 6300 for Cs (see, for example, Marinescu *et al.*, 1994). This form of potential defines a characteristic *van der Waals length*, namely, $r_0 \equiv (2m_r C_6/\hbar^2)^{1/4}$, the physical significance of which is that it is the typical extent of the last bound state in the potential; this length is of the order of 50 Å, much larger than a typical molecular dimension, and the associated characteristic energy $E_c \sim \hbar^2/m_r r_0^2$ is of order 0.1–1 mK.[12]

An important simplification of our problem results from the fact that for all the alkalis (including H), the values of thermal energy $k_B T$ characterizing BEC conditions are small compared to the above energy. Since

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[10] An interesting attempt to justify Eqs. (3.14) and (3.13) via the concept of a "phase standard" has been made by Dunningham and Burnett (1998) and is discussed in Leggett (2000a).

[11] Strictly speaking, in the limit $r \to \infty$ the leading term in $V_{at}(r)$ is the electromagnetic interaction between the electron spins, which falls off only as r^{-3}. However, for all the alkalis, including H, the mean field due to this term may be verified to be small compared with the "standard" mean field calculated below.

[12] This is one respect in which H is very different: $C_6 \sim 6.5$, $r_o \sim 5$ Å, $E_c \sim 3$ K.

for $l \neq 0$ the probability of finding the two atoms at a distance r_0 from one another in a collision process falls off as $(kr_0)^{2l}$, where l is the relative orbital angular momentum, this means that for $l \neq 0$ the effective scattering amplitude, and hence the contribution to the effective interaction (see below) is smaller than that arising from s-wave scattering by a factor of order $(k_B T/E_c)^l$ and thus is normally negligible. It follows that in our subsequent discussion we may legitimately restrict ourselves to $l=0$ (s-wave) scattering.

B. The *s*-wave scattering length

The theory of low-energy s-wave scattering of two distinguishable particles interacting via a central potential $V(r)$ is a standard textbook subject; see, for example, Landau and Lifshitz (1959), Sec. 108. The principal result we need in the present context is the following. Provided $V(r)$ falls off, as $r \to \infty$, faster than r^{-3}, then in this limit and the limit $k \to 0$ (but for kr possibly >1), the s-wave scattering solution to the time-independent Schrödinger equation has, quite generically, the simple form

$$\psi(r) = \text{const}\, \frac{\sin[k(r-a_s)]}{r}, \tag{4.1}$$

where the quantity a_s is known as the (zero-energy) *s-wave scattering length* and, depending on the details of the potential, may have either sign. In the case of positive a_s one can say that by comparison with the noninteracting case the relative wave function is repelled from the origin, whereas with negative a_s the wave function is attracted; in the repulsive case a_s may be visualized as the radius of the hard-sphere potential, which would give rise to the same relative wave function. However, it should be emphasized that in the real problem $\psi(r)$ does not vanish for $r < a_s$.

The general behavior of the scattering length is related to the s-wave bound states occurring in the potential. If we imagine starting from the noninteracting state ($a_s \equiv 0$) and gradually increasing the strength of the potential (whose shape is taken to be typical of a real atomic one), then a_s will initially (or at any rate after a little) take increasingly negative values. As the point at which the potential is just enough to sustain a bound state is approached, a_s will approach $-\infty$, and when the state is just bound, will take a large positive value (which approaches $+\infty$ as the potential is reduced again to the critical value). In this region ($a_s \gg r_0$) the asymptotic form of the bound-state wave function is $r^{-1}\exp(-r/a_s)$ and its energy is $-\hbar^2/2m_r a_s^2$; the form of the zero-energy scattering state may be viewed as a consequence of the need to make it orthogonal to the bound state. This general behavior is expected near the points where further bound states appear in the well; it is worth bearing in mind that for the heavier alkalis there are a large number of such $l=0$ bound states ($\sim$120 for ^{87}Rb; see Mies *et al.*, 1996). The $^3\Sigma$ channel of H is an exception in this respect: a_s is positive even though there are no bound states.

The value of the s-wave scattering length, which in general is a function not only of the chemical and isotopic species involved but of the hyperfine indices of the two atoms (see Sec. IV.E) and even of the magnetic and/or laser field, is a basic datum for the alkali-gas problem. It may be obtained experimentally by the technique of photoassociative spectroscopy (see Tiesinga *et al.*, 1996) or from a knowledge of the atomic mean free path in the gas (see Sec. IV.C). Alternatively, for the lightest alkalis one can attempt to calculate it from first principles. A partial list of values found in the literature is given (in atomic units) in Table III of Weiner *et al.* (1999). Inspection of this table reveals two obvious features: Except for the case of H, a_s is generally much greater than a typical (vibrational-ground-state) molecular radius and is in fact typically of the order of the van der Waals length r_0, and positive values are appreciably more common than negative ones. Neither of these features is an accident; see Gribakin and Flambaum (1993), or for a concise version of the argument Pethick and Smith (2000), Sec. 5.3.[13]

Although the magnitude of a_s is thus often large on an atomic scale, it is very important for the theory of the BEC alkali gases that under normal BEC conditions it is still small compared to all the other characteristic lengths L_c (thermal de Broglie wavelength, interparticle spacing, and zero-point length of the trap). In particular, if we denote the density by n, the so-called *gas parameter* na_s^3, whose significance will become clear subsequently, is under normal BEC conditions at most of order 10^{-4} and often much smaller. Although in principle it is possible to make $|a_s|$ tend to infinity (so that $na_s^3 \gtrsim 1$) by appropriate tuning of the magnetic field (Feshbach resonance), in practice very large values of a_s tend to lead to rapid three-body recombination (see Stenger *et al.*, 1999). Very recent work, however, has indicated that such recombination may not be inevitable (Cornish *et al.*, 2000).

In view of some considerations that will emerge in the context of the Bogoliubov approximation (Sec. VIII), it is worthwhile to close this brief discussion with a note on the question of depletion. It is clear that even if the asymptotic value of the relative wave vector $\mathbf{k}$ is zero (as it will be if atoms are part of a spatially homogeneous Bose condensate), the short-range interatomic interaction will induce a finite probability p_q of a nonzero relative wave vector q. Taking for definiteness the case $a_s > 0$, $a_s \gg r_0$ (where r_0 is a measure of the effective range of the potential, e.g., the van der Waals length defined above), and normalizing in volume V, we find (most easily by requiring the zero-energy scattering state to be

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[13] It may be worthwhile to note that the zero-energy Schrödinger equation can be solved explicitly for any potential of the form $-\alpha/r^n$ (and in particular for the van der Waals potential, $n=6$) in terms of Bessel and Neumann functions; see Gribakin and Flambaum, 1993, Eq. (13).

orthogonal to the bound state; see, for example, Leggett, 1999b) that for $qr_0 \ll 1$ we have

$$p_q \cong \left(\frac{4\pi a_s / V}{q^2 + a_s^{-2}} \right)^2 . \tag{4.2}$$

If we assume that for $N \equiv nV$ atoms the contributions to the total depletion from the various pairs are additive, we find for the total depletion $\delta N \equiv \Sigma_{q \neq 0} \langle n_q \rangle$ the estimate

$$\delta N / N \sim n a_s^3 . \tag{4.3}$$

This single-pair contribution should be carefully distinguished from the Bogoliubov-level depletion to be discussed in Sec. VIII, which is a genuinely collective effect and, as we shall see, proportional to $(na_s^3)^{1/2}$. In fact, it is conventional to exclude[14] the contribution (4.3) from the depletion.

C. The effective interaction

I now turn to the effects of the atom-atom scattering on the properties of the many-body alkali-gas system. The fundamental result is that under appropriate conditions, and with appropriate qualifications, the true interaction potential $V_{at}(r)$ of two atoms of reduced mass m_r may be replaced by a delta function of strength $2\pi\hbar^2 a_s / m_r$, where a_s is the low-energy s-wave scattering length. The case of most frequent interest is that of two similar particles each of mass m (which may or may not be in the same hyperfine state);[15] thus the commonly quoted form of the effective interaction is

$$U(\mathbf{r}) = \frac{4\pi a_s \hbar^2}{m} \delta(\mathbf{r}). \tag{4.4}$$

It is actually rather more physically meaningful to express the result (4.4), plus the necessary qualifications, in the following alternative way: the mean interaction energy of the many-body system is given by the expression

$$\langle E_{int} \rangle = \frac{1}{2} \cdot \frac{4\pi a_s \hbar^2}{m} \sum_{ij} |\Psi(r_{ij} \overset{\sim}{\rightarrow} 0)|^2 , \tag{4.5}$$

where Ψ is the many-body wave function and the notation $r_{ij} \overset{\sim}{\rightarrow} 0$ means that the separation r_{ij} of the two atoms, while large compared to a_s, is small compared to any other characteristic length (thermal de Broglie wavelength, interparticle spacing, ...). (An equivalent statement is that $|\Psi|^2$ should be understood as averaged over a volume $\gg a_s^3$.) As we shall see, the very existence of this limit implies some conditions for the validity of Eq. (4.5). With this understanding, it is clear that Eq. (4.5) follows from Eq. (4.4) if (and only if) in evaluating $\langle E_{int} \rangle$ we work to first order only in a_s.

Let us briefly list the conditions necessary for the validity of Eq. (4.5) in the time-independent case. First, $l \neq 0$ scattering must be negligible. Second, the very existence of the limit indicated by the notation $\overset{\sim}{\rightarrow}$ implies the condition $k_c a_s \ll 1$, where k_c is the characteristic wave-vector scale of the many-body wave function Ψ and is of the order of the inverse of the smallest of the L_c listed in the last subsection (cf., however, below). As we have seen, these conditions are relatively well fulfilled for the alkali Bose gases under BEC conditions. The question of the validity of Eq. (4.5) in a time-dependent situation is a little more subtle, and I return to it in Sec. VI.

Equation (4.5) [or Eq. (4.4)] is possibly the single most important result in the whole of the physics of the dilute ultracold alkali gases (note that it in no way requires Bose statistics). While one can find many derivations of it in the literature [e.g., Huang (1987), Secs. 13.1–3 and 5, or Stoof *et al.* (1996)], few of them are sufficiently general to cover the spatially and, often, temporally inhomogeneous situations typical of the BEC alkali gases; I therefore now sketch an argument that, while not particularly rigorous, is at least rather general, and indicates the justification for the above conditions of validity.

Let us consider a system of N particles and arbitrarily pick out two of them, say 1 and 2, denoting their relative and center-of-mass coordinates, respectively, by $\mathbf{r}$ and $\mathbf{R}$. The most general (pure) states of the many-body system will then be described by a wave function $\Psi(\mathbf{r}{:}\mathbf{R},\{\xi\},t)$ where $\{\xi\}$ schematically denotes the coordinates of the remaining $N-2$ particles. In the following, it is the dependence on $\mathbf{r}$ that is crucial, and the parametric dependence of Ψ on $\mathbf{R}$, ξ, and t will not be written out explicitly.

The essential question we wish to answer is: How does the interaction $V_{at}(r)$ between the pair 1 and 2 affect the (mean) total energy of the many-body system? Actually, this question is ambiguous. One interpretation would be: How do the energies of the exact many-body eigenstates change when the interaction $V_{at}(r)$ is "switched on?" This question is difficult to answer in general, and in any case is not of very obvious physical relevance, especially in the context of time-dependent problems. A more physical question would seem to be: Consider two different states of the system for which [for all $(\mathbf{R},\{\xi\},t)$] the form of $\Psi(\mathbf{r})$ for r greater than or equal to some cutoff $r_c \gg a_s, r_o$ is identical; subject to this condition they are constructed to minimize, in the first case, the kinetic energy of relative motion, and in the second, the sum of the latter and the potential energy $V_{at}(r)$. What is the difference in their (mean) total energies? Denote the first solution by $\psi_0(r)$ and the second by $\psi(r)$; in the following it is an essential assumption that the relevant forms of $\psi_0(r)$ can be taken constant for $r \geq r_c$ (which is crudely speaking equivalent to the condition $k_c a_s \ll 1$; see above). We denote the constant value simply by ψ_0.

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[14] If we attempt an estimate of the kinetic energy on the basis of Eq. (4.2), we find it is linearly divergent, so that at this point we must go back to the true short-range ($r \lesssim r_0$) behavior of $\psi(r)$. We return to this point in Sec. VIII.C.

[15] However, to avoid having to consider the effects of indistinguishability at this stage we continue to assume they can be "tagged."

Define the cutoff radius r_c such that $a_s \ll r_c \ll k_c^{-1}$ (where k_c is, as above, a characteristic wave vector for the states described by Ψ) and consider a trial wave function of the form

$$\psi(r) = \psi_0, \quad r \geqslant r_c$$

$$\psi(r) = \frac{(1 - a_s/r)}{(1 - a_s/r_c)} \psi_0, \quad r_o \ll r \leqslant r_c$$

$$\psi(r) = \text{complicated}, \quad r \lesssim r_o. \tag{4.6}$$

This wave function is not, strictly speaking, normalized [if $\psi_0(r)$ is] but it may be checked that the effect of correcting for this is to change the energy by a term of order $(k_c^2 r_c^2)\hbar^2 a_s \psi_0^2/m$, which is smaller than the result (4.5) by a factor $k_c^2 r_c^2 \ll 1$; thus we may consistently neglect this effect. The form (4.6) of $\psi(r)$ is also not a solution of the two-particle zero-energy time-independent Schrödinger equation $(-\hbar^2/m)\nabla^2\psi(r) = -V_{at}(r)\psi(r)$, because of the slope discontinuity at $r = r_c$, but it can be made so by introducing a fictitious shell-like potential $V_{ps}(r)$ of the form

$$V_{ps}(r) = -(\hbar^2 a_s/m r_c^2)\,\delta(r - r_c). \tag{4.7}$$

If we now evaluate the expectation value of $V_{ps}(r)$ in the state (4.6), we find, independently of the value of r_c,

$$\langle V_{ps} \rangle = -(4\pi\hbar^2 a_s/m)|\psi_0|^2. \tag{4.8}$$

Since with V_{ps} present state (4.6) is an eigenfunction of Schrödinger's equations with eigenvalue zero, and hence has $\langle H_{ps} \rangle \equiv \langle H \rangle + \langle V_{ps} \rangle = 0$, the expectation value $\langle H \rangle = \langle H_r \rangle - \langle V_{ps} \rangle$ of the actual energy of the state (4.6) is $-\langle V_{ps} \rangle$. Thus, summing over the contributions of all pairs i,j, we reproduce Eq. (4.5). Note that this result is independent of the value chosen for r_c provided it lies in the given window, and moreover should be applicable equally to a time-dependent situation under appropriate conditions (see Sec. IV.F). Incidentally, it is interesting that while in the above argument the condition $r_c \gg r_o$ is essential, the condition $r_c \gg a_s$ is not, and thus it may be possible to reformulate the argument so as to apply it to the dense conditions obtaining close to a Feshbach resonance ($n r_o^3 \ll 1$ but $n a_s^3 \gg 1$); I shall not attempt to discuss this question here.

Assuming that Eq. (4.5) is indeed justified under the conditions we consider, it is sometimes helpful to write it in second-quantized form:

$$\langle E_{int} \rangle = \frac{1}{2} \cdot \frac{4\pi\hbar^2 a_s}{m} \left\langle \int \psi^\dagger(\mathbf{r})\psi^\dagger(\mathbf{r})\psi(\mathbf{r})\psi(\mathbf{r})\,d\mathbf{r} \right\rangle, \tag{4.9}$$

where, however, in evaluating two-particle operators like $\psi(\mathbf{r})\psi(\mathbf{r})$, we should bear in mind that they are the appropriate $\overset{\sim}{\rightarrow}$ limit as $\mathbf{r}_1 \to \mathbf{r}_2$ of $\psi(\mathbf{r}_1)\psi(\mathbf{r}_2)$. A third form, valid to relative order N^{-1}, which is sometimes helpful to our intuition, is

$$\langle E_{int} \rangle = \frac{1}{2} \cdot \frac{4\pi\hbar^2 a_s}{m} \left\langle \int \rho^2(r)\,dr \right\rangle. \tag{4.10}$$

D. Effects of indistinguishability

In the preceding sections, it has been assumed that the two atoms whose interactions we are considering are in some way tagged, i.e., are distinguishable. It will turn out (see Sec. IV.E) that this is in effect so, even for atoms that are chemically and isotopically identical, if their initial hyperfine indices are different. However, let us consider a collision in which the incoming atoms are identical in all respects including their hyperfine indices, and thus indistinguishable (and obey Bose statistics). What difference does this make?

Actually, as regards the results of Secs. IV.A–IV.C, the answer is: none at all. The reason is that we have confined the discussion to s-wave states, and for those the wave function is automatically symmetric with respect to interchange of the atomic center-of-mass coordinates ($\mathbf{r} \to -\mathbf{r}$). In particular, the validity of Eq. (4.5) [or Eqs. (4.4), (4.9), or (4.10)] is completely independent of the distinguishability or otherwise of the atoms involved.

Nevertheless, there are two important relations that *are* affected by the statistics. The first is the relation between a_s and the total elastic-scattering cross section σ as conventionally defined, that is, the ratio of the number of particles scattered per unit time to the flux incident from infinity. For distinguishable particles σ can be calculated in the standard way from the partial-wave expansion of the incoming wave (see, for example, Landau and Lifshitz, 1959, Sec. 105), and in particular in the limit $k r_0 \ll 1$ of relevance to us is given by $4\pi a_s^2$. However, for indistinguishable bosons the odd partial waves in the expansion are forbidden, so that for given incident intensity the probability of the particles' being in a relative s state is multiplied by 2. Consequently, for indistinguishable bosons one has

$$\sigma = 8\pi a_s^2, \tag{4.11}$$

twice the value for distinguishable particles.

Indistinguishability has a second effect, which will be crucial for arguments about the metastability of superflow and related things (Sec. VI): As noted, the validity of Eq. (4.5) is independent of the statistics. However, the relation between the quantity $|\Psi(0)|^2$ occurring on the right-hand side, which is the probability of finding two particles at the origin of their relative coordinate, and the single-particle wave functions does depend on the statistics. As in the last subsection, we focus on a particular pair of atoms and do not write out explicitly the dependence on ξ and t, which enter only parametrically; moreover, we assume for simplicity that (the $r_{12} \to \infty$ limit of) the two-particle wave function *prima facie* factorizes (the Hartree-Fock approximation), i.e., that ignoring indistinguishability we would have

$$\Psi(\mathbf{r}_1, \mathbf{r}_2) \cong \varphi(\mathbf{r}_1)\chi(\mathbf{r}_2), \tag{4.12}$$

where φ and χ are each normalized over the volume of the system.

Suppose first that the states φ and χ are identical. Then we get from Eq. (4.5) a contribution from this pair to the total interaction energy of the form

$$\langle E_{int}\rangle_{12}=\frac{4\pi\hbar^2 a_s}{m}\int|\chi(\mathbf{r})|^4\,d\mathbf{r}. \tag{4.13}$$

Now suppose that $\varphi(\mathbf{r})$ and $\chi(\mathbf{r})$ represent different, mutually orthogonal states. Then we must symmetrize $\Psi(\mathbf{r_1},\mathbf{r_2})$ with respect to the interchange of (1) and (2), i.e., replace Eq. (4.13) by the normalized expression

$$\Psi(\mathbf{r_1},\mathbf{r_2})=\mathbf{2}^{-\mathbf{1/2}}[\varphi(\mathbf{r_1})\chi(\mathbf{r_2})+\chi(\mathbf{r_1})\varphi(\mathbf{r_2})]. \tag{4.14}$$

The result is that the probability density at the relative origin is multiplied[16] by a factor of 2:

$$|\Psi(r_{12}\overset{\sim}{\to}0)|^2=2|\varphi(\mathbf{r})|^{\mathbf{2}}|\chi(\mathbf{r})|^{\mathbf{2}}\quad(\mathbf{r}=\mathbf{r_1}=\mathbf{r_2}), \tag{4.15}$$

and as a result the contribution to the interaction energy is now

$$\langle E_{int}\rangle_{12}=\frac{8\pi\hbar^2 a_s}{m}\int|\varphi(\mathbf{r})|^{\mathbf{2}}|\chi(\mathbf{r})|^{\mathbf{2}}\,d\mathbf{r}. \tag{4.16}$$

Crudely speaking, Eq. (4.16), when compared with Eq. (4.13), says that two bosons in different (but mutually overlapping) states, e.g., two different momentum eigenstates, interact twice as strongly as when they are in the same state (or as they would if distinguishable).

It is clear that this result can be generalized to an arbitrary many-body state. Expanding the field operators $\psi(\mathbf{r})$, $\psi^\dagger(\mathbf{r})$ in Eq. (4.9) in an orthogonal one-particle basis $\chi_i(\mathbf{r})$, we rewrite that equation as

$$E_{int}=\frac{4\pi\hbar^2 a_s}{m}\cdot\frac{1}{2}\cdot\sum_{ijkl}\langle a_i^\dagger a_j^\dagger a_k a_l\rangle \times\int\chi_i^*(\mathbf{r})\chi_j^*(\mathbf{r})\chi_k(\mathbf{r})\chi_\ell(\mathbf{r})d\mathbf{r}, \tag{4.17}$$

and a standard Hartree-Fock decoupling of the expectation value then gives

$$E_{int}=\frac{4\pi\hbar^2 a_s}{m}\cdot\frac{1}{2}\cdot\sum_{ij}n_i n_j(2-\delta_{ij}) \times\int|\chi_i(\mathbf{r})|^{\mathbf{2}}\cdot|\chi_{\mathbf{j}}(\mathbf{r})|^{\mathbf{2}}\,d\mathbf{r}. \tag{4.18}$$

The salient consequence of Eq. (4.18) is that *a repulsive interaction* ($a_s>0$) *favors multiple occupation of a single one-particle state*—an effect that is in addition to the statistical one of Sec. III and is sometimes called an "attraction in momentum space" (Huang, 1987; Nozières, 1995).

E. Effect of the hyperfine degree of freedom

I shall assume here for simplicity that while the hyperfine index may be different for the two atoms involved in the collision of interest, the pair of outgoing levels is the same as the pair of incoming ones ("elastic" collision). This excludes the exothermic collision processes that are often responsible for depopulation in magnetic traps; it also excludes a rather delicate effect that may occur when different pairs of levels are very nearly degenerate (see Sec. IX).

If the two atoms in question are in the same orbital state, the situation is straightforward; they must then be in a symmetric state as regards their hyperfine (internal) degrees of freedom, and this state then just factors out of the calculation. The interaction energy is just given by the expression (4.14) with a_s replaced by the generalized scattering length $a_{\alpha\beta}^{(s)}$ defined below.

Consider a pair of otherwise identical Bose atoms characterized by hyperfine labels α, β ($\alpha\neq\beta$) and occupying mutually orthogonal orbital states φ, χ. The simplest description of their collisions is obtained in terms of the odd and even wave functions,

$$\Psi_+\equiv\eta_+\zeta_+,\quad\Psi_-\equiv\eta_-\zeta_-, \tag{4.19}$$

where $\eta_\pm$, $\zeta_\pm$ are, respectively, normalized spin and orbital wave functions of the form

$$\eta_\pm\equiv2^{-1/2}(\alpha_1\beta_2\pm\alpha_2\beta_1),\quad\zeta_\pm\equiv2^{-1/2}(\varphi_1\chi_2\pm\chi_1\varphi_2), \tag{4.20}$$

where $\varphi_1\equiv\varphi(\mathbf{r}_1)$, etc. Because the antisymmetric orbital function ζ_- has zero probability density at the relative origin, it undergoes no scattering and contributes nothing to the interaction. We now define a generalized s-wave scattering amplitude $a_{\alpha\beta}^{(s)}$ just as in Sec. IV.B, in terms of the asymptotic behavior of the s-wave part of ζ_+; note that this definition refers only to the phase of ζ_+ as $r_{12}\to\infty$ and is completely independent of its magnitude. We then see by the arguments of Sec. IV.D that the energy shift associated with the (normalized) state $\eta_+\zeta_+$ is $8\pi\hbar^2 a_{\alpha\beta}^{(s)}/m$ (i.e., including the factor of 2). Consider now what this means for a collision in which, in the incoming state, the atom with hyperfine index α is in orbital state $i(\equiv\varphi)$ and that with hyperfine index β is in orbital state $j(\equiv\chi)$, and label it for brevity $|\alpha_i,\beta_j\rangle$; note that this state is physically distinguishable from $|\alpha_j,\beta_i\rangle$. If now we write the (correctly symmetrized and normalized) wave function of the state $|\alpha_i\beta_j\rangle$ in terms of the Ψ_+ and Ψ_- defined in Eq. (4.19), and take into account that Ψ_- drops out, we find that the effective interaction Hamiltonian is a 2×2 matrix in the space spanned by $|\alpha_i,\beta_j\rangle$ and $|\alpha_j,\beta_i\rangle$ of the form

$$\hat{H}=\begin{pmatrix}1&1\\1&1\end{pmatrix}\times\frac{4\pi\hbar^2 a_{\alpha\beta}^{(s)}}{m}\delta(r_{12}). \tag{4.21}$$

Following Oktel and Levitov (1999), it is convenient to call the process $|\alpha_i,\beta_j\rangle\to|\alpha_i,\beta_j\rangle$ a *forward collision* and the process $|\alpha_i,\beta_j\rangle\to|\alpha_j,\beta_i\rangle$ a *momentum-exchange collision*; we see from Eq. (4.21) that the matrix elements for those two processes are identical in sign and magnitude.

A similar analysis in terms of Ψ_+ and Ψ_- demonstrates that the total cross section $\sigma_{\alpha\beta}$ for (incoherent) mutual scattering of two different hyperfine species is

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[16] By an obvious extension of the argument, the probability of finding three particles at the same point is six times larger when they are all in different states than when they are all in the same one-particle state. As pointed out by Kagan *et al.* (1985), this leads to a significant reduction of three-body recombination processes in the BEC state, a prediction verified experimentally by Burt *et al.* (1997).

$4\pi(a_{\alpha\beta}^{(s)})^2$ (no factor of 2)—a result that could have been obtained intuitively by the argument that the hyperfine index is as good a "label" of a particular atom as a chemical or isotopic one.

Finally, a note on the relation of the scattering lengths $a_{\alpha\beta}^{(s)}$ for different pairs of hyperfine indices α, β: In some cases an exact relation can be obtained by using rigorous invariance principles such as rotational invariance (see Sec. V.D). It is usually not possible to go beyond this. In particular, the tempting idea of trying to obtain relations between (e.g.) the three different amplitudes involving atoms in $F=2$, $m_F=1$ and $F=1$, $m_F=-1$ states by taking purely electronic singlet and triplet amplitudes and weighting them with the probability of finding, in the initial (asymptotic) states, the two electrons to be in a relative singlet or triplet usually does not work very well (see Tiesinga *et al.*, 1996); the near equality of these three amplitudes for ^{87}Rb (see Julienne *et al.*, 1997) is believed to be a coincidence resulting from the near vanishing of the electronic triplet amplitude for two ^{87}Rb atoms.

F. Time-dependent situations: the MIT hydrogen experiments

How fast do the physical conditions have to change in time before the replacement of the true interatomic potential $V_{at}(r)$ by the scattering-length approximation (4.4) becomes invalid or dubious? It is, at least, extremely plausible that the answer should be the slower of the rates $\hbar/m_r r_o^2$ and $\hbar/m_r a_s^2$ (where r_0 was defined in Sec. IV.A); this is the maximum time the system needs to adjust the relative wave function out to distances of the order of the r_c defined in Sec. IV.C. Now, it follows from the results to be obtained in Sec. V [see Eq. (5.13)] that if the time dependence is due to a change in the trap potential, then even if this is itself very fast the typical inverse time taken by the mean-field wave function to respond is at most of the order of $nU_0/\hbar \equiv 4\pi n\hbar a_s/m$; under BEC conditions ($na_s^3 \ll 1$) this is small compared to the above rates, and thus it is self-consistent to assume that Eq. (4.4) is valid at all times.

A different situation may, however, occur when it is $V_{at}(r)$ itself that is changed in time, for example by sweeping the system through a Feshbach resonance. In that case it is possible in principle for the rate of change to be large compared to $\hbar/ma_s^2$, and in particular in the immediate vicinity of the resonance this will always be true. Under these conditions the use of Eq. (4.4) may be dubious.

An interesting real-life case in which not only the above considerations but those of Secs. IV and V become relevant is the experiment of Fried *et al.* (1998), who reported the first observation of BEC in atomic hydrogen. The authors tuned a laser to approximately half the $1s$-$2s$ transition frequency and directed it on trapped atomic hydrogen, arranging to have the beam retroreflected so that it passed through the sample twice in opposite directions; the probability of excitation of the $2s$ state as a function of laser frequency was inferred by monitoring the prompt fluorescence produced when the $2s$ state (which is highly metastable) was mixed with the rapidly decaying $2p$ state by application of an electric field. Although in general the interpretation of the data would be complicated by the Doppler effect, the authors were able to identify the "Doppler-free" part of the spectrum, which is due to absorption of two photons traveling in opposite directions and hence not subject to this complication. Thus one can regard the raw data as being the probability $P(\Delta\nu)$ of absorption at a given value of the laser frequency, which differs by $\Delta\nu$ from the free-space value; $\Delta\nu$ is interpreted as the effect of the interatomic interactions (the *cold collision frequency shift*) as follows.

The crucial point is that the interatomic potential $V_{at}(r)$ is different for two atoms both in the $1s$ ground state and for a pair in which one atom is in the $2s$ excited state (the probability of both being in the $2s$ state is negligible). Since the rate of increase of the $2s$ amplitude, which is given by the two-photon Rabi frequency[17] Ω, is almost certainly very tiny compared to $\hbar/ma_s^2$, or even $\hbar/mr_0^2$, the above considerations justify us in replacing $V_{at}(r)$ in both cases by the appropriate s-wave scattering length a_{1s-1s} or a_{1s-2s} (Oktel and Levitov, 1999). So, at a point $\mathbf{r}$ where the atomic density is $n(\mathbf{r})$, the expression for the interaction correction to the $1s$-$2s$ energy difference (i.e., for the quantity $2h\Delta\nu$) should be of the form $\eta\cdot 4\pi\hbar^2(a_{1s}-a_{2s})n(r)/m$. But is η equal to 1, 2, or neither? The simplest argument is that the action of the laser cannot suddenly change the value of $|\Psi(r_{12}\simeq 0)|^2$; thus for a state with 100% BEC the quantity η should be 1, and in the normal state (where to order N^{-1} all atoms should be in different orbital states) η should be 2. For a state with a fraction f of the atoms in the condensate, a naive extension of this argument would give the result $\eta=2-f$. However, as pointed out by Oktel and Levitov (1999), a given atom may commute between the condensate and the normal component on a time scale $\ll\Omega^{-1}$, and under those conditions it may be necessary to take careful account of the momentum-exchange terms (Sec. IV.E); they conclude that in this case there are two different resonance frequencies for any given f. The situation is further complicated by the fact that, as noted by Fried *et al.* (1999, p. 3813, col. 2, paragraph 3), an analysis of their data according to the above considerations, i.e., assuming that a pure condensate occurs and results in a value 1 of η, yields a total condensate that is implausibly large from the point of view of the cryogenics; in fact, the authors analyze their data under the assumption that $\eta=2$ everywhere. (The change in the absorption spectrum on the onset of BEC then comes entirely from the change in the density distribution.) At the time of writing, this whole complex of questions remains controversial.

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[17] See, for example, Mandel and Wolf (1995), p. 752.

V. THE GROSS-PITAEVSKII APPROXIMATION

The simplest possible approximation for the wave function of a many-body system is a (correctly symmetrized) product of single-particle states, i.e., the Hartree-Fock ansatz. In the case of a BEC system at $T=0$, this approximation is usually known as the Gross-Pitaevskii or mean-field approximation. It results in a very simple equation or set of equations, which are very convenient for numerical calculations and, in the case of the BEC alkali gases, appear to give a rather good quantitative description of the behavior in a large variety of experiments. In the following I first treat, using this ansatz, a gas of a single hyperfine species ("spinless" gas) in equilibrium at zero temperature, and then generalize the treatment to finite temperature (Sec. V.B), to the time-dependent case (Sec. V.C), and finally to the case of more than one hyperfine species (Sec. V.D). Section V.E briefly reviews some applications. Unless explicitly stated otherwise, I shall assume the effective interaction(s) to be all repulsive (all $a_{\alpha\beta}^{(s)}>0$); for the case of a single species with attractive interaction, see Dalfovo *et al.* (1999), Sec. II.C.

A. The Gross-Pitaevskii ground state of a spinless system

In this subsection I consider a gas of N atoms all of the same hyperfine species (and will drop the associated label), in equilibrium in some trapping potential $V_{ext}(r)$ at zero temperature. The Hartree-Fock ansatz for the ground state is simply[18]

$$\Psi_N(\mathbf{r}_1\cdots\mathbf{r}_N)=\prod_{i=1}^{N}\chi_0(\mathbf{r}_i), \tag{5.1}$$

where $\chi_0(r)$ is some normalized single-particle wave function, to be determined. With this ansatz and the considerations of Sec. III, the expectation value of the energy takes the form

$$\langle H\rangle_N=N\int d\mathbf{r}\left\{\frac{\hbar^2}{2m}|\boldsymbol{\nabla}\chi_0(\mathbf{r})|^2+V_{ext}(\mathbf{r})|\chi_0(\mathbf{r})|^2\right\}$$
$$+\frac{1}{2}N(N-1)U_0\int d\mathbf{r}|\chi_0(\mathbf{r})|^4, \tag{5.2}$$

where the effective interaction constant U_0 is given, according to Sec. III, by

$$U_0\equiv 4\pi\hbar^2 a_s/m. \tag{5.3}$$

Since typically in BEC experiments N is at least 10^5, in the following I shall neglect the difference between $N-1$ and N. Minimization of the right-hand side of Eq. (5.2) subject to the constraint of normalization of χ_0, followed by division by N, then yields the Hartree equation for condensed bosons,

$$-\frac{\hbar^2}{2m}\nabla^2\chi_0(\mathbf{r})+V_{ext}(\mathbf{r})\chi_0(\mathbf{r})+NU_0|\chi_0(\mathbf{r})|^2\chi_0(\mathbf{r})$$
$$=\mu\chi_0(\mathbf{r}), \tag{5.4}$$

where μ enters as N^{-1} times the Lagrange multiplier associated with the normalization of χ_0. Because of the nonlinearity of Eq. (5.4), μ is not in general the energy per particle $\langle H\rangle_N/N$; rather, by multiplying Eq. (5.4) by $\chi_0^*(\mathbf{r})$, integrating over $\mathbf{r}$, and using the fact that $\langle H\rangle_N$ is stationary against small variations of $\chi_0(\mathbf{r})$, we see that μ is equal to $\delta\langle H\rangle_N/\delta N$, i.e., the chemical potential (whence the notation). Note that the form of the solution $\chi_0(\mathbf{r})$ of Eq. (5.4) is itself implicitly a function of N.

In the literature it is conventional to rewrite the nonlinear Schrödinger equation (5.4) in terms of the order parameter $\Psi(\mathbf{r})$ defined by Eq. (3.12) (with $N_0=N$ at zero temperature); it then reads

$$-\frac{\hbar^2}{2m}\nabla^2\Psi(\mathbf{r})+V_{ext}(\mathbf{r})\Psi(\mathbf{r})+U_0|\Psi(\mathbf{r})|^2\Psi(\mathbf{r})$$
$$=\mu\Psi(\mathbf{r}), \tag{5.5}$$

with $\Psi(\mathbf{r})$ normalized so that the space integral of its squared modulus is N. Equation (5.5) is the celebrated Gross-Pitaevskii equation;[19] note that in the present (time-independent) case this is strictly equivalent to the one-particle equation (5.4).[20]

Associated with Eq. (5.4) or Eq. (5.5) is the important concept of a *healing length*. Consider a situation in which in a given region of space the particle density $\rho(\mathbf{r})=|\Psi(\mathbf{r})|^2$ is nearly constant at a value n. Then the (local) healing length ξ is defined by

$$\xi\equiv\left(\frac{2mnU_0}{\hbar^2}\right)^{-1/2}=(8\pi n a_s)^{-1/2}. \tag{5.6}$$

To see the physical significance of ξ, consider for a moment the case (of course unrealistic for the alkali gases) of a gas of $N\equiv nV$ atoms confined to a cubic box of volume $V\equiv L^3$; $V_{ext}\equiv 0$ within the box, but the wave function $\chi_0(\mathbf{r})$ [hence $\Psi(\mathbf{r})$] must of course vanish on the walls. For a noninteracting gas, $\Psi(\mathbf{r})$ would be a product of sine waves with wavelength $2L$. However, it is intuitively clear that, in the presence of repulsive interactions, it is energetically favorable to make $\rho(\mathbf{r})$ nearly constant in the bulk of the box, and in the fact explicit solution of the Gross-Pitaevskii equation (5.4) shows this to be the case. As we approach a wall ($z\to 0$) $\Psi(z)$ falls off to zero as $\tanh z/(\sqrt{2}\xi)$ (in fact, for a half-infinite space this is the exact form of the solution). Thus ξ is indeed the length over which the perturbing effect of the wall is "healed." Note that under normal BEC conditions ($na_s^3\ll 1$) ξ is large compared to a_s (but generally small compared to typical trap dimensions; see

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[18] Strictly speaking this is an oversimplification: even at this level, the many-body wave function must build in the short-range ($r_{ij}\lesssim a_s$) correlations discussed in Sec. IV.B. In the following I implicitly assume that this has been done.

[19] Strictly speaking, the $T=0$ time-independent Gross-Pitaevskii equation.

[20] Similar remarks apply to Eq. (5.9) below.

Sec. II.E); we shall see in Sec. VIII that ξ is also in a sense the length over which the gas heals from internal collisions.

B. The spinless gas: finite-temperature equilibrium

The extension of the Gross-Pitaevskii (Hartree-Fock, mean-field) ansatz to excited states of the many-body system, and thus to finite temperatures, is at first sight straightforward: We assume that the approximate energy eigenstates of the many-body system are characterized by specifying a complete orthonormal set of single-particle wave functions $\chi_i(\mathbf{r})$ and occupying each of them with n_i bosons, in such a way that $\Sigma_i n_i = N$. The form of the $\chi_i(\mathbf{r})$ must be obtained self-consistently by generalizing the argument used in Sec. V.A for the ground state: see below. For the case of thermal equilibrium at temperature $T \equiv (\beta k_B)^{-1}$, we take the expectation value of n_i for $i \neq 0$ to be given by the usual Bose distribution:

$$\langle n_i(T) \rangle = \{\exp[\beta(\epsilon_i - \mu) - 1]\}^{-1} \tag{5.7}$$

and substitute this expression in the interaction term in the energy. The number N_0 of particles in the condensate (if any), that is, in the special single-particle state $\chi_0(\mathbf{r})$, is obtained from the prescription

$$N_0(T) = N - \sum_{i \neq 0} \langle n_i(T) \rangle. \tag{5.8}$$

In the following I shall neglect terms of relative order n_i/N, $i \neq 0$.

Bearing in mind the expression (4.18) for the interaction energy, and noting that terms with $i = j \neq 0$ are of order N^{-1} relative to those with $i \neq j \neq 0$, we see that for any particular energy eigenstate the function χ_0 and χ_j $(j \neq 0)$ are given, respectively, by the solutions of the equations

$$\begin{aligned}\Bigg\{ &-\frac{\hbar^2}{2m}\nabla^2 + V_{ext}(\mathbf{r}) \\ &+ \frac{4\pi\hbar^2 a_s}{m}\left(N_0|\chi(\mathbf{r})|^2 + 2\sum_{i \neq 0} n_i |\chi_i(\mathbf{r})|^2 \right) \Bigg\} \chi_0(\mathbf{r}) \\ &= \mu \chi_0(\mathbf{r}),\end{aligned} \tag{5.9}$$

$$\begin{aligned}\Bigg\{ &-\frac{\hbar^2}{2m}\nabla^2 + V_{ext}(\mathbf{r}) \\ &+ \frac{4\pi\hbar^2 a_s}{m}\left(2N_0|\chi(\mathbf{r})|^2 + 2\sum_{i \neq 0} n_i |\chi_i(\mathbf{r})|^2 \right) \Bigg\} \chi_j(\mathbf{r}) \\ &= \epsilon_j \chi_j(\mathbf{r}) \quad (j \neq 0),\end{aligned} \tag{5.10}$$

where the chemical potential μ is defined as $\delta\langle E \rangle / \delta N$ at constant $\{n_i\}$, or what comes to the same thing, constant entropy. In thermal equilibrium Eqs. (5.9) and (5.10) must be solved self-consistently by replacing the quantities n_i and N_0 by their thermal expectation values (5.7) and (5.8), respectively.

We note that while the effective potential felt by the "normal" (or "thermal") $(i \neq 0)$ particles is a function only of the total density $\rho(\mathbf{r})$ given by

$$\rho(\mathbf{r}) = N_0|\chi_0(\mathbf{r})|^2 + \sum_{i \neq 0} n_i |\chi_i(\mathbf{r})|^2 \equiv n_c(\mathbf{r}) + n_T(\mathbf{r}), \tag{5.11}$$

the potential felt by the condensate is sensitive to n_c and n_T separately. This creates a small technical problem, since it is not guaranteed that the solutions of Eq. (5.9) are necessarily orthogonal to that of Eq. (5.10). This point is discussed in detail by Huse and Siggia (1982), who conclude that in realistic circumstances its correction is unlikely to change much the conclusions drawn from Eqs. (5.9) and (5.10); however, a more satisfactory resolution is to note that, while the finite-temperature Gross-Pitaevskii theory is indeed not strictly internally consistent in this respect, the next (Bogoliubov) level of approximation (see Sec. VIII) will remove the inconsistency while still in many cases leaving Eqs. (5.9) and (5.10) as quantitatively good approximations.

C. The spinless gas: time-dependent Gross-Pitaevskii theory

In attempting to generalize the considerations of Secs. I and II to the time-dependent case, we encounter a nontrivial complication: The order parameter $\Psi(\mathbf{r},t)$ is conventionally defined, as in Eq. (3.12), as $\sqrt{N_0(t)} \cdot \chi_0(\mathbf{r}t)$, where $N_0(t)$ is the single macroscopic eigenvalue of the single-particle density matrix $\rho(\mathbf{r}\mathbf{r}':t)$ and $\chi_0(\mathbf{r}t)$ is the associated normalized single-particle eigenfunction. Now, we can write down the obvious time-dependent generalizations of Eqs. (5.4) and (5.5), respectively (neglecting for the moment terms in n_i, $i \neq 0$),

$$\begin{aligned} i\hbar \frac{\partial \chi_0(\mathbf{r}t)}{\partial t} &= -\frac{\hbar^2}{2m}\nabla^2 \chi_0(\mathbf{r}t) + V_{ext}(\mathbf{r}t)\chi_0(\mathbf{r}t) \\ &\quad + N_0(t) U_0 |\chi_0(\mathbf{r}t)|^2 \chi_0(\mathbf{r}t) \end{aligned} \tag{5.12}$$

and

$$\begin{aligned} i\hbar \frac{\partial \Psi(\mathbf{r}t)}{\partial t} &= -\frac{\hbar^2}{2m}\nabla^2 \Psi(\mathbf{r}t) + V_{ext}(\mathbf{r}t)\Psi(\mathbf{r}t) \\ &\quad + U_0 |\Psi(\mathbf{r}t)|^2 \Psi(\mathbf{r}t). \end{aligned} \tag{5.13}$$

In the literature, one can find the term "time-dependent Gross-Pitaevskii equation" used to refer either to Eq. (5.12) or to Eq. (5.13). However, it is clear that, unlike their time-independent analogs, Eqs. (5.12) and (5.13) are *not equivalent* unless the condensate number $N_0(t)$ is conserved in time; since this condition itself follows from Eq. (5.13), it is clear that Eq. (5.13) implies Eq. (5.12) but not vice versa. A very systematic analysis of the time-dependent problem, in terms of an expansion in a parameter that is essentially the typical value of the quantity $(na_s^3)^{1/4}$, has been given by Castin and Dum (1998); see also Gardiner (1997). In this subsection I adopt a less rigorous but hopefully rather intuitive approach to the question of the validity of Eqs. (5.12) and (5.13).

We work at $T=0$ and start from the many-body Hamiltonian consisting of the usual kinetic and external potential-energy terms plus the interaction term $\frac{1}{2}U_0\Sigma_{ij}\delta(\mathbf{r}_i-\mathbf{r}_j)$, and insert it in the many-body Schrödinger equation. We then make for the solution of the latter the Hartree-type ansatz which is the obvious generalization of Eq. (5.1):

$$\Psi_N(\mathbf{r}_1\mathbf{r}_2\cdots\mathbf{r}_N:t)=\prod_{i=1}^{N}\chi_o(\mathbf{r}_i:t). \tag{5.14}$$

Note that in making this ansatz we already explicitly assume that $N_0(t)=N=\text{const}$. Substituting this ansatz into the time-dependent many-body Schrödinger equation, we obtain

$$\begin{aligned} i\hbar\sum_{i=1}^{N}\frac{\partial\chi_0(\mathbf{r}_i,t)}{\partial t}\cdot\Lambda_i(\{\mathbf{r}_j\}:t) &= \sum_i\left[\left\{-\frac{\hbar^2}{2m}\nabla_i^2+V_{ext}(\mathbf{r}_i)+\frac{1}{2}U_0\right.\right.\\ &\quad\left.\left.\times\sum_{j\neq i}^{N}\delta(\mathbf{r}_i-\mathbf{r_j})\right\}\cdot\chi_0(\mathbf{r}_i:t)\Lambda_i(\{\mathbf{r}_j\}:t)\right], \end{aligned} \tag{5.15}$$

where $\Lambda_i(\mathbf{r}_j:t)$ is simply a shorthand for the ($\mathbf{r}_i$-independent) quantity $\Pi_{j\neq i}^{N}\chi_0(\mathbf{r}_j:t)$. In view of the product nature of the ansatz (5.14), it is consistent to take the density of particles other than i at $\mathbf{r}_i$, $\Sigma_{j\neq i}^{N}\delta(\mathbf{r}_i-\mathbf{r}_j)$, to be given by its expectation value over Eq. (5.14), namely, the total density $\rho(\mathbf{r}t)\equiv\Sigma_{i=1}^{N}|\chi_0(\mathbf{r}_i:t)|^2$ (where as usual we ignore the difference between $N-1$ and N). Then it is clear that Eq. (5.15) is satisfied if Eq. (5.12) is; moreover, since we have already assumed that $N_0(t)=N=\text{const}$, Eq. (5.13) also follows. The argument can clearly be generalized (with some labor) to the case of finite temperature (i.e., $\langle n_i\rangle\neq 0$ for $i\neq 0$), and the result is, as we might intuitively expect, simply to replace μ in Eq. (5.9) and ϵ_i in Eq. (5.10) by the quantities $i\hbar\partial\chi_0(\mathbf{r}t)/\partial t$ and $i\hbar\partial\chi_i(\mathbf{r}t)/\partial t$, respectively.[21]

The above simple argument shows that once we have made the ansatz (5.14) for the many-body wave function, then the unique consistent choice of $\chi_0(\mathbf{r}t)$ is the function determined by Eq. (5.12). However, it does not of course assure us that the ansatz (5.14) is consistent, and indeed in the presence of finite interactions it is not—even if we start at $t=0$ with a simple product wave function of the type (5.14), the last term in Eq. (5.15) will in general mix in more complicated (correlated) many-body states. Thus we should expect Eq. (5.13) to be valid only to lowest order in $\epsilon\equiv(na_s^3)^{1/4}$, and indeed the rigorous calculation of Castin and Dum (1998) shows this to be so. What is less expected, but also emerges from their calculation, is that if we define the condensate wave function $\chi_0(\mathbf{r}t)$ in the more general way described in Sec. III (i.e., as the wave function of the unique "macroscopically occupied" single-particle state), then it still satisfies Eq. (5.12) at the order in ϵ where Eq. (5.13) fails. It should be noted that the quantity ϵ may itself depend on time.

It is often useful to define a "reference" solution to Eq. (5.13)—call it $\Psi_0(\mathbf{r}t)$—and then study the behavior of small deviations $\delta\Psi(\mathbf{r}t)$ from Ψ_0. Because of the presence of the nonlinear term, we get a pair of coupled equations for $\delta\Psi(\mathbf{r}t)$ and its complex conjugate $\delta\Psi^*(\mathbf{r}t)$:

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}\delta\Psi(\mathbf{r}t) &= -\frac{\hbar^2}{2m}\nabla^2\delta\Psi+V_{ext}(\mathbf{r}t)\delta\Psi(\mathbf{r}t)\\ &\quad+U_0|\Psi_0(\mathbf{r}t)|^2\delta\Psi(\mathbf{r}t)\\ &\quad+U_0[\Psi_0(\mathbf{r}t)]^2\delta\Psi^*(\mathbf{r}t). \end{aligned} \tag{5.16}$$

The equation for $\delta\Psi^*$ is the complex conjugate of Eq. (5.16). A case of special interest is when $\Psi_o(rt)$ represents the Gross-Pitaevskii ground state: in that case, to get agreement between Eqs. (5.13) and (5.5) we write

$$\Psi_o(\mathbf{r}t)=\Psi(\mathbf{r})\exp-i\mu t/\hbar, \tag{5.17}$$

where $\Psi(\mathbf{r})$ satisfies the time-independent Gross-Pitaevskii equation (5.5). It is then convenient to write $\delta\Psi(\mathbf{r}t)$ in the form

$$\begin{aligned} \delta\Psi(\mathbf{r}t) &= \exp-i\mu t/\hbar[u(\mathbf{r})\exp-i\omega t\\ &\quad+v^*(\mathbf{r})\exp+i\omega t], \end{aligned} \tag{5.18}$$

and some straightforward algebra then shows that the functions $u(\mathbf{r})$, $v(\mathbf{r})$ satisfy the *Bogoliubov–de Gennes equations*

$$\hbar\omega u(\mathbf{r})=\{\hat{H}_o-\mu+2U_o|\Psi(r)|^2\}u(\mathbf{r})+U_o\Psi^2(\mathbf{r})v(\mathbf{r}) \tag{5.19}$$

$$\begin{aligned} -\hbar\omega u(\mathbf{r}) &= \{\hat{H}_o-\mu+2U_o|\Psi(r)|^2\}v(\mathbf{r})\\ &\quad+U_o\Psi^{*2}(\mathbf{r})u(\mathbf{r}), \end{aligned} \tag{5.20}$$

where $\hat{H}_o$ is a shorthand for $[-(\hbar^2/2m)\nabla^2+V_{ext}(r)]$. We shall rederive Eqs. (5.19) and (5.20) from a different point of view in Sec. VIII. In the special case of a weakly interacting gas in free space $[V_{ext}\equiv 0,\Psi(\mathbf{r})=\sqrt{n_o}\cong\sqrt{n}]$ it is clear that $u(\mathbf{r})$ and $v(\mathbf{r})$ have the form of plane waves: $u(\mathbf{r})=A\exp(i\mathbf{k}\cdot\mathbf{r}),v(\mathbf{r})=B\exp(i\mathbf{k}\cdot\mathbf{r})$, and moreover from Eq. (5.5) μ is simply equal to $U_o n$. Explicit solution of Eqs. (5.19) and (5.20) then yields the dispersion relation

$$\hbar\omega(k)=[\epsilon_k(\epsilon_k+2nU_0)]^{1/2}\quad(\epsilon_k\equiv\hbar^2k^2/2m). \tag{5.21}$$

Introducing the hydrodynamic speed of sound c_s by

$$c_s^2=\frac{n}{m}\frac{\partial^2E}{\partial n^2}=\frac{nU_0}{m}, \tag{5.22}$$

we can rewrite Eq. (5.21) in the form

$$\omega(k)=(c_s^2k^2+\hbar^2k^4/4m^2)^{1/2}. \tag{5.23}$$

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[21] The quantity $\langle n_i\rangle$ is then constant in time and determined by its $t=0$ value.

This is the famous Bogoliubov spectrum for a dilute Bose gas; it reduces to $\epsilon_k/\hbar$ for $k \gg \hbar/mc_s$ [i.e., $k\xi \gg 1$, since ξ can be written from Eqs. (5.6) and (5.22), as $\sqrt{2}\hbar/mc_s$] but in the opposite limit has the sound-wave form $c_s k$. We return to Eq. (5.21) in Sec. VIII, just noting here that regardless of the value of $\mathbf{k}$ the fluctuation of the atomic density $\rho(\mathbf{r}t) = |\Psi(\mathbf{r}t)|^2$ around its equilibrium value n is given by the standard sound-wave form

$$\delta\rho(\mathbf{r}t) = \text{const}\cos[\mathbf{k}\cdot\mathbf{r} - \omega(k)t]. \tag{5.24}$$

D. Effects of the hyperfine degree of freedom

Introduction of an internal (hyperfine) degree of freedom leads immediately to at least three complications in the picture developed above. First, the axes in the hyperfine space with respect to which the external potential is diagonal may vary in (real) space and, possibly, in time. Second, the s-wave scattering amplitude will in general have a matrix structure in the hyperfine space. Third, "simple" BEC is no longer the only natural possibility (see Nozières, 1995).

In dealing with these complications we have a choice of basis in the hyperfine space: Either we regard the axes as fixed independently of the spatial coordinates $\mathbf{r}$ and time t, or we allow them to depend on $\mathbf{r}$ and, possibly, t, for example in such a way that the local external potential is everywhere diagonal (adiabatic basis).

Let us first briefly use the latter choice to discuss the very simplest case, in which the spinor $\Psi(\mathbf{r},\alpha)$ describing the condensate is of the form $\Psi(\mathbf{r})|\alpha_o\rangle$ where $|\alpha_o\rangle$ is a fixed spinor in the adiabatic basis (e.g., that corresponding to $F=1, m_F=1$);[22] it can be shown (Ho and Shenoy, 1996) that this is a good approximation for the ground state when the axes of the latter basis are sufficiently slowly varying. Then it turns out that if we wish to define a superfluid velocity $\mathbf{v}_s$ in the natural way, so that the local particle current is $\mathbf{v}_s|\Psi(\mathbf{r})|^2$, the appropriate definition is no longer Eq. (3.15) but rather

$$\mathbf{v}_s(\mathbf{r}t) = \frac{\hbar}{m}\mathbf{D}\varphi(\mathbf{r}t), \quad \varphi(\mathbf{r}t) \equiv \arg\Psi(\mathbf{r}t), \tag{5.25}$$

where $\mathbf{D}$ is the covariant derivative introduced by the "bending" in space of the hyperfine axes (see Weinberg, 1972, Chap. 4). As a result, $\mathbf{v}_s$ no longer satisfies the irrotationality condition (3.16), and even in a simply connected geometry the equilibrium state may sustain a finite orbital angular momentum (Ho and Shenoy, 1996; cf. Loss *et al.*, 1990).

For most purposes, however, and in particular where the effects of interactions are important, a choice of hyperfine axes that is independent of spatial coordinate (and time) is much more convenient, and I shall use it from now on. For the moment let us assume simple BEC, so that we can define, as in Sec. III.D, a unique order parameter $\Psi(\mathbf{r},\alpha)$ which is a spinor in the space of the hyperfine axes. The kinetic-energy operator then has the standard form $-(\hbar^2/2m)\nabla^2$, and the local external potential is a matrix $V_{\alpha\beta}(\mathbf{r})$ with respect to the hyperfine axes. It remains to consider the interaction energy.

By an obvious generalization of the considerations of Sec. IV, it is intuitively plausible that the general expression for the atomic interaction energy is

$$E_{int} = \frac{1}{2}\sum_{\alpha\beta,\gamma\delta} U_{\alpha\beta\gamma\delta}\langle\psi_\alpha^\dagger(\mathbf{r})\psi_\beta^\dagger(\mathbf{r})\psi_\gamma(\mathbf{r})\psi_\delta(\mathbf{r})\rangle, \tag{5.26}$$

where $\psi_\alpha^\dagger(\mathbf{r})$ is the creation operator for an atom at point $\mathbf{r}$ and with spin (hyperfine) index α, and $U_{\alpha\beta\gamma\delta}$ is related to the s-wave scattering length matrix $a_{\alpha\beta\gamma\delta}$ by

$$U_{\alpha\beta\gamma\delta} = \frac{4\pi\hbar^2}{m}a_{\alpha\beta\gamma\delta}. \tag{5.27}$$

Note that because of the Bose statistics $U_{\alpha\beta\gamma\delta}$ may be taken to be symmetric under the exchanges $\alpha \leftrightarrow \beta$ and $\gamma \leftrightarrow \delta$. In any given physical situation the possible forms of the matrix $a_{\alpha\beta\gamma\delta}$ may be constrained by symmetry considerations. Consider, for example, the case of a system moving in a small magnetic field $\mathbf{B}(\mathbf{r}) = \hat{\mathbf{n}}(\mathbf{r})|\mathbf{B}(\mathbf{r})|$, $|\mathbf{B}(\mathbf{r})| \ll B_{hf}$, and suppose that all atoms are known to be in the lower $(F=1)$ hyperfine manifold, as in the experiments of Stenger *et al.* (1998a). Under these conditions the local interaction energy can be a function only of the only two quantities one can form that are linear in $\psi_\alpha^\dagger\psi_\beta^\dagger\psi_\gamma\psi_\delta$ and invariant under spin rotation, namely, the squares of the total density $\rho(\mathbf{r})$ and of the spin density $\mathbf{S}(\mathbf{r})$. Expressing these quantities as linear combinations of $\psi_\mu^\dagger(\mathbf{r})\psi_\nu(\mathbf{r})$ and using Eq. (5.27), we find (see Ho, 1998)

$$a_{\alpha\beta\gamma\delta} = \frac{1}{2}[a_1\delta_{\alpha\gamma}\delta_{\beta\delta} + a_2\mathbf{S}_{\alpha\gamma}\cdot\mathbf{S}_{\beta\delta} + (\alpha \leftrightarrow \beta)], \tag{5.28}$$

where $\mathbf{S}$ is the (vector) spin operator for the $F=1$ state. The quantities a_1 and a_2 can be related to the scattering amplitudes of two atoms in the $K=2$ and $K=0$ states, where K is the magnitude of the (conserved) total atomic spin $\mathbf{K} \equiv \mathbf{F}_1 + \mathbf{F}_2$. By considering, for example, the $K=0$ state $(\mathbf{S}_{\alpha\gamma}\cdot\mathbf{S}_{\beta\delta} = -2)$ and the $K=2, m_K=2$ state $(\mathbf{S}_{\alpha\gamma}\cdot\mathbf{S}_{\beta\delta} = 1)$ we find

$$a_1 = \frac{1}{3}(a_{K=0} + 2a_{K-2}), \quad a_2 = \frac{1}{3}(a_{K=2} - a_{K=0}). \tag{5.29}$$

To obtain a Gross-Pitaevskii formalism in a general choice of axes, we assume as above simple BEC, i.e., make the ansatz

$$\Psi_N = \prod_{i=1}^{N}\chi_o(\mathbf{r}_i, \alpha_i : t), \tag{5.30}$$

consider a particular point $\mathbf{r}$ (and time t), and use our freedom to choose the axes arbitrarily to choose them, temporarily, so that only a single component (call it α_o) of the spinor $\chi_o(\mathbf{r},\alpha)$, or equivalently of the order parameter $\Psi(\mathbf{r},\alpha)$, is nonvanishing: $\Psi(\mathbf{r},\alpha_o) \equiv \delta_{\alpha\alpha_o}\Psi(\mathbf{r})$.

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[22] In words, the condensate atoms are in the lower hyperfine manifold and their spins are everywhere oriented along the direction of the local magnetic field.

Then the formulas of Sec. IV go through verbatim, and we find for the local interaction energy density $E_{int}(\mathbf{r})$ within the Gross-Pitaevskii approximation the simple expression

$$E_{int}(\mathbf{r})=\frac{1}{2}\cdot\frac{4\pi\hbar^2}{m}\overline{a_s}|\Psi(\mathbf{r})|^4, \tag{5.31}$$

where $\overline{a_s}$ denotes the component of $a_{\alpha\beta\gamma\delta}$ corresponding to $\alpha=\beta=\gamma=\delta=\alpha_o$. Transforming back to a general frame and integrating over $\mathbf{r}$, we obtain for the total interaction energy the expression[23]

$$E_{int}=\frac{1}{2}\sum_{\alpha\beta\gamma\delta}U_{\alpha\beta\gamma\delta}\int\Psi^*_\alpha(\mathbf{r})\Psi^*_\beta(\mathbf{r})\Psi_\gamma(\mathbf{r})\Psi_\delta(\mathbf{r})d\mathbf{r}, \tag{5.32}$$

$$U_{\alpha\beta\gamma\delta}\equiv\frac{4\pi\hbar^2}{m}a_{\alpha\beta\gamma\delta} \tag{5.33}$$

[where $\Psi_\alpha(\mathbf{r})$ and hence E_{int} may also be a function of time]. The right-hand side of Eq. (5.32) is the general expression, within the $T=0$ Gross-Pitaevskii approximation, for the interaction energy of a Bose system exhibiting simple BEC, and it is routinely used in the literature for the analysis of such a system.

We now proceed by straightforward analogy with the arguments of Secs. V.A–V.C above. Given the ansatz (5.30), the time-independent $T=0$ Gross-Pitaevskii equation is obtained by minimizing the total energy and takes the form of a set of equations for the j spinor components $\Psi_\alpha(\mathbf{r})$,

$$-\frac{\hbar^2}{2m}\nabla^2\Psi_\alpha(r)+\sum_\beta V_{\alpha\beta}(r)\Psi_\beta(r)+\sum_{\beta\gamma\delta}U_{\alpha\beta\gamma\delta}\Psi^*_\beta(\mathbf{r})\Psi_\gamma(\mathbf{r})\Psi_\delta(\mathbf{r})=\mu\Psi_\alpha(\mathbf{r})\quad(\alpha=1\cdots j). \tag{5.34}$$

Similarly, the zero-temperature time-dependent Gross-Pitaevskii equation takes the form

$$i\hbar\frac{\partial\Psi_\alpha}{\partial t}(\mathbf{r}t)=\frac{\hbar^2}{2m}\nabla^2\Psi_\alpha(\mathbf{r}t)+\sum_\beta V_{\alpha\beta}(\mathbf{r}t)\Psi_\beta(\mathbf{r}t)+\sum_{\beta\gamma\delta}U_{\alpha\beta\gamma\delta}\Psi^*_\beta(\mathbf{r}t)\Psi_\gamma(\mathbf{r}t)\Psi_\delta(\mathbf{r}t)\quad(\alpha=1\cdots j). \tag{5.35}$$

Just as in the case of a simple one-particle Schrödinger equation, the time-independent solution $\Psi_\alpha(\mathbf{r})$ of Eq. (5.34) may be regarded as related to a special case of the solution $\Psi_\alpha(\mathbf{r}t)$ of Eq. (5.35) by

$$\Psi_\alpha(\mathbf{r}t)=\exp(-i\mu t/\hbar)\Psi_\alpha(r). \tag{5.36}$$

It is worth noting explicitly that in Eqs. (5.34) and (5.36) the chemical potential μ is common to all components $\Psi_\alpha(\mathbf{r})$; see below.

The generalization of even the static Gross-Pitaevskii theory (let alone the time-dependent one) to nonzero temperature in the multicomponent case appears not to be entirely trivial, and to the best of my knowledge has not been much discussed in the literature for the most general case. The basic difficulty is that while we can certainly define normal-component eigenfunctions $\chi_{i\lambda}(\mathbf{r},\alpha)$, we have in general no *a priori* guarantee that their spinor structure will be simply related to that of the condensate [in particular, the relevant spinors need not be locally parallel or orthogonal to the condensate spinor $\Psi(\mathbf{r},\alpha)$].[24] I shall therefore discuss here only the simplest case, namely, that in which not only does the external potential $V_{\alpha\beta}(\mathbf{r})$ have $\mathbf{r}$-independent eigenvalues but the condensate has an $\mathbf{r}$-independent spinor structure, i.e., $\Psi(\mathbf{r},\alpha)=\Psi(\mathbf{r})\xi_o(\alpha)$; it is convenient to choose the basis so that $\xi_o(\alpha)=\delta_{\alpha\alpha_o}$. Then, in this basis, the normal eigenfunctions within the Hartree-Fock approximation will also be fixed spinors: $\chi_{i\lambda}(\mathbf{r},\alpha)=\varphi_{i\lambda}(\mathbf{r})\xi_\lambda(\alpha)$, where one of the ξ_λ's is $\xi_o(\alpha)$ and the rest are orthogonal to the latter. One can then go through the standard Hartree-Fock decoupling of the interaction energies in Sec. IV, with the upshot that the interaction between normal particles in states λ and λ' has the factor of 2 only for $\lambda=\lambda'$, and the interaction of the condensate with a normal particle of hyperfine index λ has it only for $\lambda=0$.

I now turn to the question of simple versus multiple (general) BEC. A very important consideration here is that the generic factor of 2, which for a spinless system with repulsive interactions opposes simultaneous occupation of two different (but spatially overlapping) orbital states, is absent in the case of simultaneous occupation of two mutually orthogonal hyperfine states, and thus such occupation (fragmentation) is not at all uncommon. For pedagogical convenience let us consider the very simplest situation, that of a spatially uniform system with only two relevant hyperfine states characterized by $\mathbf{r}$-independent spinors $|\alpha\rangle,|\beta\rangle$. (We choose the basis to diagonalize the external potential energy.) Then, normalizing in unit volume and setting the particle density equal to n, we see that the ground-state Gross-Pitaevskii order parameter has the form

$$\Psi_\alpha(\mathbf{r})=n^{1/2}C_\alpha,\qquad \Psi_\beta(\mathbf{r})=n^{1/2}C_\beta\quad(|C_\alpha|^2+|C_\beta|^2=1), \tag{5.37}$$

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[23] Needless to say, if we accept the concept of spontaneously broken U(1) symmetry (see Sec. III.D), the above derivation may be short-circuited by the replacements, in Eq. (5.26), $\langle\psi^\dagger_\alpha(\mathbf{r})\psi^\dagger_\beta(\mathbf{r})\psi_\gamma(\mathbf{r})\psi_\delta(\mathbf{r})\rangle\to\langle\psi^\dagger_\alpha(\mathbf{r})\rangle\langle\psi^\dagger_\beta(\mathbf{r})\rangle\langle\psi_\gamma(\mathbf{r})\rangle\langle\psi_\delta(\mathbf{r})\rangle$, $\langle\psi_\alpha(\mathbf{r})\rangle\to\Psi_\alpha(\mathbf{r})$, etc. I prefer to avoid this "automatic" derivation both for the reasons given in Sec. III.D and because it makes the generalization to general (nonsimple) BEC less transparent.

[24] The origin of this difficulty is essentially the point noted at the end of Sec. V.B above, namely, that within the Hartree-Fock (Gross-Pitaevskii) approximation the condensate and the normal quasiparticles experience different effective Hamiltonians.

i.e., the many-body ground state has the form [including (part of) the time dependence]

$$\Psi_N = \Pi_i\{(C_\alpha|\alpha_i\rangle + C_\beta|\beta_i\rangle)\exp - i\mu t/\hbar\}. \tag{5.38}$$

Substituting Eq. (5.37) in the time-independent Gross-Pitaevskii equation (5.34), we find that the coefficients C_κ ($\kappa=\alpha,\beta$) satisfy the equation

$$E_\kappa C_\kappa + \sum_{\lambda,\mu,\nu=\alpha,\beta} nU_{\kappa\lambda\mu\nu}C_\lambda^* C_\mu C_\nu = \mu C_\kappa \quad (\kappa=\alpha,\beta), \tag{5.39}$$

where E_κ is the eigenvalue of the single-particle Hamiltonian (kinetic plus external potential energy) corresponding to hyperfine state $|\kappa\rangle$. In general Eq. (5.39) will have more than one solution (see below), and for the ground state we must choose that corresponding to the lowest value of the total energy.

Let us now consider the case in which the interaction term commutes with the single-particle part of the Hamiltonian, so that the numbers of particles in states α and β are separately constant. Expressed in terms of the matrix elements $U_{\kappa\lambda\mu\nu}$, this means that the only allowed terms correspond to the choices $\kappa=\mu$, $\lambda=\nu$ or $\kappa=\nu$, $\lambda=\mu$. Introducing the notation

$$U_{\alpha\alpha\alpha\alpha} \equiv U_{\alpha\alpha}(\equiv 4\pi\hbar^2 a_s^{(\alpha\alpha)}/m), \tag{5.40}$$

$$U_{\beta\beta\beta\beta} \equiv U_{\beta\beta}(\equiv 4\pi\hbar^2 a_s^{(\beta\beta)}/m), \tag{5.41}$$

$$U_{\alpha\beta\alpha\beta}(\equiv U_{\alpha\beta\beta\alpha}, \text{etc.}) \equiv \frac{1}{2}U_{\alpha\beta}\left(\equiv \frac{1}{2}4\pi\hbar^2 a_s^{(\alpha\beta)}/m\right), \tag{5.42}$$

we find that Eq. (5.39) reduces to

$$\left(E_\alpha + \sum_{\lambda=\alpha,\beta} nU_{\alpha\lambda}|C_\lambda|^2\right)C_\alpha = \mu C_\alpha \tag{5.43}$$

and a similar equation with $\alpha\to\beta$ for C_β. It is straightforward to verify that the (lowest) solution of Eq. (5.42) minimizes the total energy per particle,

$$E(C_\alpha, C_\beta) = \sum_{\kappa=\alpha,\beta} E_\kappa|C_\kappa|^2 + \frac{1}{2}\sum_{\kappa,\lambda=\alpha,\beta}(nU_{\kappa\lambda})|C_\kappa|^2|C_\lambda|^2, \tag{5.44}$$

with respect to arbitrary variations of C_α and C_β subject to the normalization constraint $|C_\alpha|^2+|C_\beta|^2=1$ [i.e., in effect, with respect to arbitrary variation of $\langle n_\alpha\rangle - \langle n_\beta\rangle$].

However—and here is the crunch—if processes that change $\langle n_\alpha\rangle - \langle n_\beta\rangle$ are really absent as we have assumed, then the physically interesting states of the many-body system, even at $T=0$, are by no means restricted to states of the form (5.38). Let us in fact consider states of the more general form

$$\Psi_N = \Pi_i\{C_\alpha|\alpha_i\rangle\exp - i\mu_\alpha t/\hbar + C_\beta|\beta_i\rangle\exp - i\mu_\beta t/\hbar\} \tag{5.45}$$

where we do *not* assume that $\mu_\alpha=\mu_\beta$. This corresponds to an order parameter of the form

$$\Psi_\alpha(r,t) = n^{1/2}C_\alpha\exp - i\mu_\alpha t/\hbar,$$
$$\Psi_\beta = n^{1/2}C_\beta\exp - i\mu_\beta t/\hbar. \tag{5.46}$$

Substituting this into the time-dependent Gross-Pitaevskii equation (5.35) and using the form of $U_{\alpha\beta\gamma\delta}$ given by Eqs. (5.40)–(5.42), we find that Eq. (5.46) is a solution of Eq. (5.35) provided the μ_κ satisfy

$$\mu_\kappa = E_\kappa + \sum_{\lambda=\alpha,\beta} nU_{\kappa\lambda}|C_\lambda|^2, \quad \kappa=\alpha,\beta, \tag{5.47}$$

which is equivalent to the statement that (for example) μ_α is the partial derivative of the total energy with respect to n_α at constant n_β. It is not difficult to see that these results generalize to the more physical case in which the $\chi_{o\alpha}(\mathbf{r}), \chi_{o\beta}(\mathbf{r})$ are nonuniform and in general different (though see below). In this case we write the order parameter in the more general form

$$\Psi_\alpha(\mathbf{r}t) = \Psi_\alpha(\mathbf{r})\exp - i\mu_\alpha t/\hbar,$$
$$\Psi_\beta(\mathbf{r}t) = \Psi_\beta(\mathbf{r})\exp - i\mu_\beta t/\hbar, \tag{5.48}$$

and the generalized form of Eq. (5.47) [obtained by a substitution of (5.48) into (5.39)] is

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V_\kappa(\mathbf{r})\right)\Psi_\kappa(\mathbf{r}) + \sum_{\lambda=\alpha,\beta} U_{\kappa\lambda}|\Psi_\lambda(\mathbf{r})|^2\Psi_\kappa(\mathbf{r}) = \mu_\kappa\Psi_\kappa(\mathbf{r}) \quad (\kappa=\alpha,\beta) \tag{5.49}$$

—a form that is often used in the literature for cases in which the species numbers n_α, n_β are separately conserved.

It is actually possible to generalize the description (5.45) even to cases in which the interaction term does not commute with the single-particle Hamiltonian, since in that case also Eq. (5.47) [or in the spatially inhomogeneous case (5.49)] has more than one solution, and these can be superposed to generate a solution analogous to Eq. (5.45). However, this generalization does not appear to be of much practical interest in the context of current experiments, and in view of the notational complications I do not pursue the question here.

Returning to the simple case corresponding to Eq. (5.45), we reemphasize that this equation describes simple BEC (in a time-dependent state). However, provided that we are at no time interested in measuring operators that change the hyperfine state, it is clear that in the thermodynamic limit ($N\to\infty$) all experimental properties of the state (5.45) are identical to those of the state

$$\Psi_N' \equiv \mathcal{S}\prod_{i=1}^{n_\alpha}|\alpha_i\rangle\prod_{j=n_\alpha+1}^{N}|\beta_j\rangle, \tag{5.50}$$

where $\mathcal{S}$ denotes the symmetrization operator and n_α is (the nearest integer to) $|C_\alpha|^2 N$. It is clear that the single-particle density matrix corresponding to the state (5.50) has two eigenvalues, n_α and n_β, which are each of order N and thus that Ψ_N' displays multiple BEC (a *fragmented condensate*). We shall see in Sec. VII.C that Ψ_N'

can be represented (up to an overall phase) as a superposition of states of the generic form (5.45), i.e., of the form

$$\prod_{i=1}^{N}\{|C_\alpha|\cdot|\alpha_i\rangle+|C_\beta|\exp i\varphi|\beta_i\rangle\},\tag{5.51}$$

with random relative phase φ. Since in the absence of processes that change the hyperfine states no physical quantities can depend on φ, the properties of the state (5.50) are identical (in the thermodynamic limit) to those of Eq. (5.45).

A more general discussion of BEC in a two-state system is given in Sec. VII.

It is clear that the above discussion recovers most of the results of that given in Sec. IV.E (which was precisely for the case of conservation of the hyperfine index). However, even in the $T=0$ case (and *a fortiori* at finite temperatures) one might worry about the effects of the momentum-exchange term discussed there. At $T=0$, in the homogeneous case or more generally where the two condensate wave functions $\chi_{o\alpha}(\mathbf{r}),\chi_{o\beta}(\mathbf{r})$ are identical, this term vanishes, but in general it does not: its physical effect is, crudely, to scatter an atom initially in state $\chi_{o\alpha}(\mathbf{r})$ into the component of $\chi_{o\beta}(\mathbf{r})$, which is orthogonal to $\chi_{o\alpha}(\mathbf{r})$ and vice versa. By making the Gross-Pitaevskii (Hartree) approximation one of course ignores such processes, and I believe that, at least at zero temperature, if one is going to take them into account one should simultaneously take into account the terms taken at the next (Bogoliubov) level of approximation (see Sec. VIII); indeed, they may be regarded as simply a special case of the latter; see Sec. VIII.F. At finite temperature the effects of momentum-exchange collisions with the normal component may be more significant (Oktel and Levitov, 1999, see Sec. 4.6).

E. Applications

The applications of both the time-independent and the time-dependent Gross-Pitaevskii equation to a single-species alkali gas in a harmonic trap are excellently reviewed by Dalfovo *et al.* (1999), so I just recapitulate here the barest essentials, confining myself for simplicity to the isotropic case. A critical dimensionless parameter that controls the qualitative behavior is the quantity

$$\lambda\equiv(15Na_s/a_{ho})^{1/5},\tag{5.52}$$

where $a_{ho}\equiv(\hbar/m\omega_o)^{1/2}$ is the *oscillator length*. In most experiments to date λ lies in the range 5–10, and in the following I shall treat it as large compared to unity. In this limit we can neglect, in the $T=0$ Gross-Pitaevskii equation, the kinetic-energy term except very close to the edge of the condensate (the Thomas-Fermi approximation), and the form of the ground-state density distribution is then an inverted parabola:

$$\rho_o(r)=\rho_o(0)(1-r^2/r_o^2).\tag{5.53}$$

The chemical potential, the central density $\rho_o(0)$, and the condensate radius r_o are given in terms of λ by the formulas

$$\mu=\frac{1}{2}\hbar\omega_o\cdot\lambda^2,\tag{5.54}$$

$$r_o=\lambda a_{ho},\tag{5.55}$$

$$\rho(0)=\lambda^{-3}Na_{ho}^{-3}.\tag{5.56}$$

At finite temperatures the results for the condensate are the same except that N is replaced by N_o and the definition of λ is similarly modified. In practice the condition $\lambda\gg1$ is met until temperatures quite close to T_c, since it turns out that the free-gas formula $N_o=N[1-(T/T_c)^3]$ is not a bad approximation for the real trapped gases. What of the thermal (uncondensed, normal) component? Following Dalfovo *et al.* (1999), let us define a dimensionless parameter $\eta\equiv\mu(0)/k_BT_c\sim(N^{1/6}a_s/a_{ho})^{2/5}$. Then η lies in the range 0.3–0.4 for most existing experiments.[25] At T_c, the density n of the gas and hence the mean-field energy per atom nU_o are of the order of $\eta^{3/2}\sim0.1$ of their values at $T=0$; however, the competition of the mean field is not, as at $T=0$, with the zero-point energy $(\hbar\omega_o/2)$ but with the thermal energy k_BT_c, which is a factor ~100 larger [see Eq. (3.7)]. Thus, in the normal phase $(T>T_c)$ and in fact even below T_c, the mutual interactions of the atoms of the normal component are negligible. In fact, since at $T_c\lambda_{\rm DB}$ is of order $n^{-1/3}$, the dilute-gas condition $n\ll1$ automatically guarantees that $nU_0\ll kT$ for $T\geq T_c$. However, below T_c the interaction between the normal component and the condensate can have a non-negligible effect on the condensate fraction, reducing the latter according to the estimate of Dalfovo *et al.* by as much as 20% for $T/T_c=0.6$.

The application of the time-dependent Gross-Pitaevskii equation (5.13) to a single-species gas in a trap has been studied by many authors, both to calculate the collective excitation spectrum and to explore the nonlinear behavior; I particularly draw attention to the elegant scaling solution first constructed by Kagan and co-workers (1996) and by Castin and Dum (1997) for a harmonic trap with arbitrary time variation of the trapping frequency ω_o, which is exact in the Thomas-Fermi limit $\lambda\gg1$ (and exact in two dimensions for all λ). See Dalfovo *et al.* (1999), Sec. IV.D, and for an exhaustive discussion of the collective excitations, including effects associated with the normal component, Griffin (2000).

Turning to the multispecies case, a number of authors (e.g., Ho and Shenoy, 1996; Esry and Greene, 1999) have used Eq. (5.49) to study the equilibrium of two different hyperfine species in a trap. A rather generic result of such calculations is that even if the external potential is identical for the two species, phase separation will occur if, as in the case of the $F=2$, $m_F=+1$ (“$|2\rangle$”) and $F=1$, $m_F=-1$ (“$|1\rangle$”) states of

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[25] Note that the maximum value of na_s^3 is $\eta^6/(15)^{3/5}$.

^{87}Rb, the scattering lengths are all positive and satisfy the inequality $a_{12}^2 > a_{11}a_{22}$ (or, what is approximately the same condition for close values of the a_{ij}, $a_{12} > (1/2) \times (a_{11} + a_{22})$. In such a case, in a typical harmonic trap, one species (in this case $|1\rangle$) will form a ring or shell around the other, while the total density behaves (for close a_{ij}) almost identically to that of a single species. Such behavior has been verified in the experiments of Hall, Matthews, Ensher, *et al.* (1998); see their Fig. 1.

An even richer situation was realized in the experiments of Stenger *et al.* (1998a), in which all three substates of the $F=1$ ground multiplet were simultaneously confined in an optical trap and their distribution studied as a function of parameters such as the (spatially varying) magnetic field. In subsequent experiments the same group investigated metastable configurations of systems containing two of the three species (Miesner *et al.*, 1999) and their relaxation by quantum tunneling of the condensate (Stamper-Kurn *et al.*, 1999). It appears that a reasonably good quantitative account of all these experiments is given by calculations based on the time-independent Gross-Pitaevskii equation (5.49). An interesting difference from the case of ^{87}Rb (with $F=2$ and $F=1$ components) is that the "accidental" near degeneracy of the various scattering lengths observed in the latter case appears to be absent: the difference in the $K=2$ and $K=0$ scattering lengths in the $F=1$ ground multiplet (see Sec. V.D) is of order 10% relative to their mean (see Burke *et al.*, 1998), with $a_2 > a_0$. As a result, phase separation apparently occurs between the 0 and ± 1 components, while the latter two are mutually miscible (Stenger *et al.*, 1998a).

The time-dependent equation (5.35) has similarly been applied by a number of groups (e.g., Ho, 1998; Ohmi *et al.*, 1998; Ohberg and Stenholm, 1999; cf. Colson and Fetter, 1978) both to calculate collective excitations and to study the process of achievement of equilibrium when the relative concentration of the species is suddenly changed. In the latter context I particularly call attention to the analysis by Sinatra *et al.* (1999) of the experiment of Hall *et al.* [Hall, Matthews, Ensher, *et al.* (1998) and Hall, Matthews, Wieman, and Cornell (1998)], on which see also Sec. VII.D. A salient conclusion is that because of the very small difference in the a_{ij}'s for ^{87}Rb, equilibration will take a time (~60 msec) long compared to that associated with the average mean-field energy (~2 msec), as indeed observed. Another interesting conclusion is that the approach to equilibrium is nonmonotonic (as observed) and that the phenomenologically observed damping is a result of strongly chaotic behavior (see Sec. IX.E).

VI. ROTATIONAL PROPERTIES: SUPERFLUIDITY

A. Phenomenology of superfluidity in liquid ^{4}He

Fritz London's original suggestion in 1938 that liquid ^{4}He in its He-II phase below the λ temperature exhibits BEC was prompted primarily by the observation in that phase of the property of superfluidity. In the original measurements of Kapitza and of Allen and Misener, what was observed was the ability of the liquid to flow without apparent friction through channels so narrow that any ordinary liquid (including the He-I phase of ^{4}He above the λ temperature) would be almost totally clamped by viscous effects.

As so often occurs in physics, the original experiment is not the most conceptually clear-cut demonstration of the phenomenon. In fact, from a modern point of view, superfluidity is not a single phenomenon but a complex of phenomena, and the picture becomes clearer if one considers not a channel between two bulk reservoirs, as in the experiments of Kapitza and Allen and Misener, but rather an annular geometry.[26] Let us then consider a hollow cylinder of height h, inner radius $R-d/2$ and outer radius $R+d/2$, where $d \ll R$; for the moment we assume that deviations from exact cylindrical symmetry are small (but nonzero). Then, if the cylinder is filled with ^{4}He, we can observe two conceptually distinct (though related) phenomena. The first is sometimes called the Hess-Fairbank effect: the system appears to come out of equilibrium with its rotating container. To amplify this definition, we all know that if we take our annulus filled with water and set it on an old-fashioned gramophone turntable which we then set into rotation, the water will come (after a delay of maybe ≈ 1 min) into rotation with the annulus and will thereafter rotate with it as long as the turntable continues to rotate. When we stop the rotation, the water also gradually comes to rest. Imagine now that we do the same experiment with He, starting above the λ point and rotating *very slowly* (for a 1-cm-radius annulus, the angular velocity would have to be $\lesssim 10^{-4}$ rad/sec to see the specific behavior to be described; in practice smaller radii are used and the criterion is not quite so stringent). The He behaves in exactly the same way as the water, coming into rotation with the container. Now suppose that, while still rotating with this low angular velocity, we cool the system through the λ temperature. The He then appears to gradually come out of equilibrium with the container, i.e., to cease (*prima facie*) to rotate even though the container is still rotating! In fact, as T falls to zero, the He appears at first sight to come to rest in the laboratory frame (or, to be more precise, rather in the frame of the fixed stars). It is clear that this behavior cannot simply reflect very long relaxation times, since the liquid has come out of equilibrium with the container: *the "nonrotating" state must be the true thermodynamic state*. This Hess-Fairbank effect is the exact analog of the Meissner effect in a superconductor. It is conventional to define the *superfluid density* $\rho_s(T)$ [or superfluid fraction $\rho_s(T)/\rho$, where ρ is the total density] in terms of the experimentally observed value of the temperature-

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[26] All the ensuing considerations have close analogs in the theory of superconductivity, which indeed is nothing but superfluidity occurring in a charged system; see, for example, Vinen (1969) or Leggett (1995b).

dependent moment of inertia $I(T) \equiv L/\omega$ relative to its classical value $I_{cl} \equiv NmR^2$: $\rho_s(T)/\rho \equiv 1 - I(T)/I_{cl}$.

The second phenomenon is the following: Again put the He, above T_λ, in the annulus and set the latter into rotation, but this time much faster. This time, as we cool through T_λ, we see very little change: to all intents and purposes the liquid continues to rotate with the container. Now stop the container. The He continues to rotate, apparently indefinitely. One can show rigorously that for the container stationary the rotating state cannot be the thermodynamic equilibrium one, so what we are seeing here is an example of an extremely long-lived metastable state. I shall refer to this phenomenon as *metastability of superflow*. At first sight neither the Hess-Fairbank effect nor the metastability of superflow is obviously equivalent to the phenomenon originally observed in 1938; I discuss the relation to this and yet other possible definitions of superfluidity elsewhere (Leggett, 2000a).

A simple phenomenological understanding of both the Hess-Fairbank effect and the stability of supercurrents may be obtained if we assume (a) that in analogy to the electrons in an atom, the atoms of the condensate (which, we recall, must all behave as one) can have only integral values $\ell\hbar$ of their angular momentum, corresponding in the annular geometry to an angular velocity of rotation $\ell\hbar/mR^2 \equiv \ell\omega_c$, and (b) that (in distinction to the electrons in an atom) the passage of an atom (or rather of the condensate atoms as a whole) from one value of ℓ to another is impeded by a high free-energy barrier. Then it is intuitively plausible that on cooling through T_λ with $\omega \ll \omega_c$ the condensate will prefer to come to rest. On the other hand, if the angular velocity of the container is $\gg \omega_c$, say $n\omega_c$ where n is in general not integral, then on cooling through T_c the condensate will simply "choose" the value of ℓ that most closely matches its angular velocity to that of the container; in particular, if the latter is $\gg \omega_c/2$, the condensate will simply choose the integer ℓ closest to n, and the difference between ℓ and n will be barely observable, so that the liquid appears to continue to rotate with the container. However, when the rotation stops the free-energy barriers will prevent relaxation to $\ell = 0$.

B. Rotating frames of reference

In order to formulate a quantitative account of superfluidity, whether in liquid ^{4}He or in the BEC alkali gases, we need to know how to do statistical mechanics where the potential that confines the system (be it a physical container or a set of magnetic and/or laser fields) is rotating. This problem is discussed in textbooks of statistical mechanics (e.g., Landau and Lifshitz, 1969, Sec. 26), and I consider it in the specific alkali-gas context elsewhere (Leggett, 2000a); here I merely quote the standard result.

Consider a system that, when the "container" is stationary in the laboratory frame,[27] is described by the generic Hamiltonian

$$\hat{H}_{lab} = \sum_i \{(p_i^2/2m) + V_{ext}(\mathbf{r}_i)\} + \frac{1}{2}\sum_{ij} U(|\mathbf{r}_i - \mathbf{r}_j|). \tag{6.1}$$

We wish to know how to apply statistical mechanics when the container is rotated at angular velocity ω around an axis which by convention we shall choose as passing through the origin and along direction $\hat{\mathbf{z}}$:

$$V_{ext}(\mathbf{r}_i) \to V_{ext}(\mathbf{r}_i : t) \equiv V[\mathbf{r}_i'(t)], \tag{6.2}$$

where $\mathbf{r}_i'(t) \equiv (x_i \cos\omega t + y_i \sin\omega t, -x_i \sin\omega t + y_i \cos\omega t, z_i)$. In the following it is not required that $V_{ext}(\mathbf{r})$ have exact[28] or even approximate symmetry under rotation around the axis $\boldsymbol{\omega}$, but it is essential that the interparticle interaction have this property [for which the centrality of U specified in Eq. (6.1) is sufficient though not strictly speaking necessary]; see below.

The standard result is now the following: Consider a time $\tau = 2\pi n/\omega$ (n integral) such that the instantaneous configuration of the potential is its original stationary one. Then the thermodynamic equilibrium state of the system is determined by minimizing the expectation value of the quantity $\hat{H}_{eff} - TS$, where

$$\hat{H}_{eff} \equiv \hat{H}_{lab} - \omega \cdot \hat{\mathbf{L}}, \tag{6.3}$$

where $\hat{L}$ is the operator of total angular momentum. At other times the density matrix of the system is modified in such a way as to make it, and thus all physical properties of the system, time independent when viewed from the rotating frame. (Note that this does not imply that the system is necessarily stationary in that frame.)

The derivation of Eq. (6.3) will fail if the interatomic potential has a part that is not invariant under rotation around the axis of $\boldsymbol{\omega}$, as is in general the case when dipolar interactions are taken into account (assuming the magnetic field is not rotated, as in the experiment of Madison *et al.*, 2000). In such a case there is strictly speaking no frame of reference in which the Hamiltonian is time independent, and thus no thermodynamic equilibrium state: in fact, the situation is similar to that realized in Couette flow, and the best we can do is to find a steady state. Fortunately, in realistic geometries such as that of Madison *et al.* (2000) such effects appear likely to be a small perturbation.

In the remainder of this section I shall be discussing the spinless case unless explicitly otherwise stated; for (other) possible effects of the hyperfine degree of freedom, see the last paragraph of Sec. VI.D.

C. Equilibrium of a BEC system in a rotating container

Let us first apply formula (6.3) to a free Bose gas above the transition temperature in a nearly cylindri-

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[27] Strictly speaking, that of the fixed stars; I shall ignore the difference.

[28] In fact, the limit of exact cylindrical symmetry needs to be approached with some care; see Leggett (2000a).

cally symmetric annular container. With the above replacement, the Bose-Einstein distribution is simply

$$n_n = [\exp\beta(\epsilon_n - \hbar\omega\ell_n - \mu) - 1]^{-1} \tag{6.4}$$

and the angular momentum is

$$L = \sum_n n_n \hbar\ell_n = \sum_n \ell_n [\exp\beta(\epsilon_n - \hbar\omega\ell_n - \mu) - 1]^{-1}. \tag{6.5}$$

Now for a cylindrically symmetric geometry in the limit $d \ll R$ n can be taken as some pair of quantum numbers j,k describing the transverse motion (their detailed nature is irrelevant) plus the angular momentum quantum number ℓ: associated with the latter is an "angular" kinetic energy $\ell^2\hbar^2/{}^2mR^2$. Associating with (j,k) the energy $\tilde{\epsilon}_{jk}$, we thus have

$$L = \sum_{jk} \sum_{\ell} \hbar\ell \left\{ \exp\beta\left[\tilde{\epsilon}_{jk} + \left(\frac{\ell^2\hbar^2}{2mR^2} - \hbar\omega\ell - \mu \right) \right] - 1 \right\}^{-1}. \tag{6.6}$$

The crucial point is that for any realistic geometry and temperature the quantity $\beta\hbar^2/mR^2 \equiv \hbar^2/(mR^2 k_B T)$ will be extremely small (for example, even for Na in a 100μ annulus at 1 μK it is still only $\approx 10^{-6}$), so the sum over ℓ can be replaced by an integral and the origin shifted: $\ell' = \ell - mR^2\omega\hbar$. It is then clear from symmetry that the result is simply

$$L = NmR^2\omega \equiv I_{cl}\omega, \tag{6.7}$$

where $I_{cl} \equiv NmR^2$ is the classical moment of inertia.[29] Thus the gas rotates exactly in pace with the container, and $\rho_s(T) = 0$ from its definition.

What happens below T_λ? Consider for simplicity the case $T=0$. Now *all* the atoms must be condensed into the state with lowest "effective" energy, i.e., into the single-particle state that minimizes the quantity

$$E_{ang}(\ell) = \frac{\ell^2\hbar^2}{2mR^2} - \hbar\omega\ell, \quad \ell \text{ integral.} \tag{6.8}$$

It is clear that the value of ℓ that minimizes $E_{ang}(\ell)$ is the nearest integer to ω/ω_c, where $\omega_c \equiv \hbar/mR^2$. Thus for $0 < \omega < \omega_c/2$ the condensate stays in the original ground state $(\ell = 0)$, and thus the system has zero angular momentum; for $\omega_c/2 < \omega < 3\omega_c/2$ the condensate occupies the state $\ell = 1$ and the total angular momentum is $N\hbar$, and so on. At finite temperatures the angular momentum is the sum of that of the condensate, which behaves similarly to that described but with $N \rightarrow N_o(T)$, and that of the normal component, which behaves exactly as in the normal phase, i.e., rotates with the container and contributes an angular momentum $[N_n(T)/N] I_{cl}\omega$. $[N_n(T) \equiv N - N_o(T).]$ Thus in this simple model, $\rho_s(T)/\rho = N_o(T)/N$.

We see, then, that in a cylindrically symmetric container, even for a noninteracting Bose gas, the onset of BEC leads to the Hess-Fairbank effect. Moreover, this feature persists in more general geometries and in the presence of interactions. To see this, let us specialize for simplicity to the case $T=0$ and assume that the time-independent Gross-Pitaevskii theory will give at least a qualitative guide to the behavior. Thus we write the many-body wave function in the Gross-Pitaevskii (Hartree) form and minimize the effective Hamiltonian (6.3). Since the angular momentum operator of the ith particle can be written as simply $-i\hbar\partial/\partial\theta_i$ where θ_i is the polar angle relative to the rotation axis, the resulting Gross-Pitaevskii equation has the form

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + i\hbar\omega\frac{\partial}{\partial\theta} \right)\Psi(\mathbf{r}) + V_{ext}(\mathbf{r}) + \frac{4\pi\hbar^2}{M} a_s |\Psi(\mathbf{r})|^2 \Psi(\mathbf{r}) = \mu\Psi(\mathbf{r}), \tag{6.9}$$

and this must be solved subject to the "single-valuedness" boundary condition

$$\Psi(\theta + 2\pi) = \Psi(\theta). \tag{6.10}$$

The expectation value of the angular momentum is given (at $T=0$ within the Gross-Pitaevskii approximation) by the expression

$$\langle \hat{\mathbf{L}} \rangle \equiv \hat{\mathbf{z}} \sum_i \left(\Psi_N, -i\hbar\frac{\partial}{\partial\theta_i}\Psi_N \right) = \hat{\mathbf{z}} \int \Psi^*(\mathbf{r}) \left(-i\hbar\frac{\partial}{\partial\theta} \right) \Psi(\mathbf{r}) d\mathbf{r}. \tag{6.11}$$

In general there will be more than one solution of Eq. (6.9) that satisfies the boundary condition (6.10), and we must then choose the one that minimizes the expectation value of $\langle H_{eff} \rangle$. The above formulation applies independently of the container geometry[30] and the sign (and *a fortiori* the strength) of the interaction term.

For a first qualitative discussion it is convenient to separate the cases of toroidal and simply connected geometries. In the toroidal case let us provisionally assume that $\Psi(\mathbf{r})$ is finite and the derivatives of its phase $\varphi(\mathbf{r})$ exist everywhere in the torus; then we can write Eqs. (6.10) and (6.11), respectively, in the form[31]

$$\oint \frac{\partial\varphi(\mathbf{r})}{\partial\theta} d\theta = 2n\pi, \quad n = 0, \pm 1, \pm 2 \ldots, \tag{6.12}$$

$$\langle \mathbf{L} \rangle = \hat{\mathbf{z}}\hbar \int |\Psi(\mathbf{r})|^2 \frac{\partial\varphi}{\partial\theta} d\mathbf{r}, \tag{6.13}$$

where in Eq. (6.12) the integral is taken along any path that goes around the torus once, staying always within it.

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[29] There are slight complications, which I shall ignore, concerning the small shift in μ and the fact that (for d/R finite) a meniscus tends to form.

[30] However, in the following I shall implicitly assume that the axis of rotation lies within the container cross section, at least at some values of z (otherwise the problem becomes rather trivial and uninteresting).

[31] In the He literature it is conventional to express the ensuing argument in terms of the superfluid velocity $\mathbf{v}_s(\mathbf{r})$ defined by Eq. (3.15); the equation corresponding to Eq. (6.12) is the Onsager-Feynman quantization condition (3.17).

n is conventionally called the *winding number*. From Eqs. (6.12) and 6.13), plus the normalization condition on $\Psi(\mathbf{r})$ (see Sec. V.A), we see that unless the geometry of the trap [and hence $|\Psi(\mathbf{r})|^2$] departs very far from cylindrical symmetry, the value of $\langle\mathbf{L}\rangle$ in a state characterized by a given value of $n(\neq 0)$ in Eq. (6.12) has the order of magnitude

$$\langle\mathbf{L}\rangle \sim Nn\hbar\hat{\mathbf{z}}, \tag{6.14}$$

although this relation becomes an equality only for exact cylindrical symmetry (in which case it gives $\rho_s=\rho$ at $T=0$, just as in the noninteracting case). A similar argument shows that the "extra" kinetic energy in a state with $n\neq 0$ [associated with the angular term in the Laplacian in Eq. (6.9)] is of order $n^2\hbar^2/2mR^2$. From these conditions it follows that for any reasonable toroidal geometry there will be a finite range of ω around $\omega=0$ for which the effective Hamiltonian $\hat{H}_{\mathrm{eff}}$, Eq. (6.3), is minimized by the choice $n=0$. For finite ω the angular momentum of this state is not zero (except for exact cylindrical symmetry), but for reasonable geometries it is substantially less than the classical value $NmR^2\omega$. Thus, very generically, we expect the system to show a Hess-Fairbank effect.

In the simply connected case it is clear that if $\Psi(\mathbf{r})$ is everywhere finite, the winding number n must be zero for any closed circuit that stays within the volume occupied by the system. The simplest configuration that allows nonzero n is a vortex; if for illustration we consider a single-quantized $(n=1)$ vortex centered on the axis of rotation, then in terms of the standard cylindrical polar coordinates r, z, θ the order parameter has the generic form

$$\Psi(\mathbf{r})\equiv\Psi(\rho,z,\theta)=f(\rho,z,\theta)\exp[i\varphi(\theta)], \tag{6.15}$$

where the real functions f and φ satisfy the conditions

$$f(0,z,\theta)=0, \tag{6.16a}$$

$$\oint(\partial\varphi/\partial\theta)d\theta=2\pi \tag{6.16b}$$

if the circuit in Eq. (6.16b) encircles the line $\rho=0$ once in the clockwise direction. [In the case of approximate cylindrical symmetry, $\varphi(\theta)\approx\theta$.] More complicated arrays of vortices, not necessarily centered on the axis of rotation, are also possible.[32] All the generic considerations given above for the toroidal geometry apply with appropriate modifications also to the simply connected case, and in particular one always expects a Hess-Fairbank effect.

It should be emphasized that all the considerations addressed in this subsection relate to the thermodynamically stable state of the system, in general in the presence of rotation of the container. The quite different question of the metastability or not of certain excited states is taken up in the next subsection.

D. Metastability of superflow

1. General considerations

Let us turn at this point to the types of generic behavior possible for a system described by an effective Hamiltonian of the form (6.3). We shall take the angular velocity $\boldsymbol{\omega}$ along the z axis and denote by L the expectation value of the z component of angular momentum. We first consider the effective (ω-dependent) moment of inertia $I(\omega)$ defined by

$$I(\omega)\equiv\partial L/\partial\omega. \tag{6.17}$$

By varying ω around some initial ω_o $(\omega\equiv\omega_o+\delta\omega)$ and treating the term $-\delta\boldsymbol{\omega}\cdot\hat{\mathbf{L}}$ in Eq. (6.3) as a perturbation, we see that I is in fact the static response function corresponding to $\delta\boldsymbol{\omega}$. For a mechanically stable state all static response functions must be >0, and thus we conclude that $I(\omega)$ is positive for any stable state of the system.

Let us now consider the lab-frame free energy $F_{lab}\equiv\langle H_{lab}\rangle-TS$, whose minimization determines the possible (meta)stable states in the absence of rotation. From the condition that $L(\omega)$ is determined from the minimum of $F_{eff}\equiv F_{lab}-\boldsymbol{\omega}\cdot\mathbf{L}$, we find $\partial^2F_{lab}/\partial L^2=\partial\omega/\partial L=I^{-1}(\omega)$. Now it is clear that while $F_{lab}(L)$ always has a stable minimum[33] at $L=0$, the existence of one or more metastable minima at finite values of L requires $\partial^2F_{lab}/\partial L^2$ to be negative for some range of L. If L is a continuous function of ω, this cannot happen (see above). Consequently, we conclude that a sufficient condition for the absence of metastability is that the function $L(\omega)$ calculated by taking the (absolute) minimum of $F_{lab}-\boldsymbol{\omega}\cdot L$ be continuous.

It is somewhat more difficult to prove that the condition is necessary as well as sufficient. A zeroth-order argument is that if the function $L(\omega)$ is discontinuous, this must mean that L "jumps" as a function of ω, i.e., a macroscopically different state has become the ground state. Barring pathologies (of which one case is the noninteracting Bose gas in exactly cylindrical geometry; see below), it seems plausible that such a macroscopically different state will be metastable relative to the true ground state for at least some finite range of $\boldsymbol{\omega}$ (though not necessarily for $\boldsymbol{\omega}=0$.) This consideration is related to the fact that the winding number n is a topological invariant; that is, it cannot be changed unless the magnitude of the order parameter $\Psi(r)$ is suppressed to zero over an appropriate cross section of the terms, something that for positive g is resisted by the interaction term (see the next subsection).

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[32] However, the case $|n|>1$ is not of much practical interest, since such multiply quantized vortices are rather generically unstable against dissociation into several singly quantized ones.

[33] This follows, for a Bose system in arbitrary geometry, from the fact that the many-body ground-state wave function can always be chosen real.

2. A toy model

These considerations may be illustrated by means of a toy model, which, while it would be quite difficult to realize experimentally for the BEC alkalis, is nevertheless quite a useful guide to the behavior in more realistic cases. In particular, it illustrates rather straightforwardly the fact that hysteresis appears only for a sufficiently strong repulsion. Consider a narrow annulus with thickness $d \ll$ radius R, and with weak deviations from exact symmetry, and imagine it filled with a weakly interacting Bose gas at $T=0$ and rotated with angular velocity ω. More specifically, let ψ_o and ψ_1 denote, respectively, the lowest-lying s and p states (that is, the exact eigenstates of $\hat{L}_z$) of a single particle in the torus (with the dependence on the azimuthal and polar coordinates self-consistently determined). The overall phase of ψ_1 is chosen relative to ψ_0 so as to make V_o [Eq. (6.19) below] real and positive. Then define three characteristic energies, namely,

(a) the single-particle quantization energy

$$\hbar^2/mR^2 \equiv \hbar\omega_c, \tag{6.18}$$

(b) the asymmetry energy

$$V_o \equiv -\int \psi_1^*(\mathbf{r}) V_{ext}(\mathbf{r}) \psi_o(\mathbf{r}) d\mathbf{r} > 0, \tag{6.19}$$

where $V_{ext}(r)$ is the external potential, and

(c) the mean interaction energy per particle, in (say) the s-wave state, which is given by

$$g \equiv \frac{4\pi\hbar^2 N a_s}{m} \int d\mathbf{r} |\psi_o(\mathbf{r})|^4. \tag{6.20}$$

The conditions of weak asymmetry and interaction are then explicitly

$$|V_o| \ll \hbar\omega_c, \quad |g| \ll \hbar\omega_c, \quad 0 < \omega < \omega_c. \tag{6.21}$$

Note that g can have either sign.[34] Since under these conditions the promotion of particles to any states other than the s and p states is negligible, and since for weak asymmetry $|\psi_1(\mathbf{r})|^2 \cong |\psi_0(\mathbf{r})|^2$ almost everywhere, the effective Hamiltonian takes the form, apart from a constant,

$$\hat{H}_{eff} = -\hbar\,\delta\omega(a_1^+ a_1 - a_o^+ a_o) - V_o(a_o^+ a_1 + \mathrm{H.c.}) + g(a_o^+ a_o a_1^+ a_1), \tag{6.22}$$

where $\delta\omega \equiv (\omega - \frac{1}{2}\omega_c)$ (so $|\delta\omega| < \frac{1}{2}\omega_c$) and the last term is the difference of the interaction term [i.e., Eq. (6.20) with $\psi_o(\mathbf{r})$ replaced by $\psi(\mathbf{r})$] from its value in the pure s or p state. [Note carefully that this term enters only because of the factor of 2 (Sec. IV.D).]

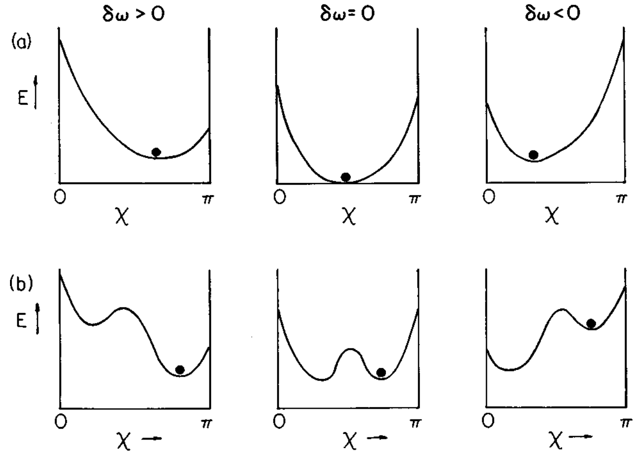

FIG. 2. The shape of the energy curve $E(\chi)$ as given by Eq. (6.24): (a) the nonhysteretic case $g < V_0$; (b) the hysteretic case $g > V_0$ (schematic). The zeros of energy are arbitrary. The heavy dot indicates the position (value of χ) of the system in an experiment in which $\delta\omega$ is swept from positive to negative values; note that, according to Eq. (6.25), the value of χ/π is a rough qualitative measure of the angular momentum per particle.

We look for a solution of the Gross-Pitaevskii type:

$$\Psi_N = \left(a_o^+ \cos\frac{\chi}{2} \exp(i\Delta\varphi/2) + a_1^+ \sin\frac{\chi}{2} \exp(-i\Delta\varphi/2) \right)^N |\mathrm{vac}\rangle. \tag{6.23}$$

It is clear that the only term dependent on $\Delta\varphi$ is that in V_o, and thus the optimum choice is to take $\Delta\varphi = 0$ [so that, by Eq. (6.19), $\Psi(\mathbf{r})$ is smallest, roughly speaking, where V_{ext} is the most repulsive]. The dependence of the energy and angular momentum per particle on χ is then given up to terms of relative order N^{-1} by

$$E(\chi)/N = \delta\omega \cos\chi - V_o \sin\chi + \frac{g}{2}\sin^2\chi, \tag{6.24}$$

$$L/N\hbar = \frac{1}{2}(1 - \cos\chi). \tag{6.25}$$

It is clear that the qualitative behavior of the curve $E(\chi)$, and thus the presence or absence of metastability (hysteresis), is determined by the ratio g/V_o (see Fig. 2). If this quantity is smaller than 1 (which of course is automatically the case for $g<0$) then $E(\chi)$ is monotonic for any value of ω and the stable solution for $\delta\omega = 0$ is $\chi = \pi/2$ (superposition of s and p states with equal weight). In this case, if we vary $\delta\omega$ as a function of time and assume that the system can exchange energy and angular momentum with its environment, it will follow the (unique) $L(\omega)$ curve smoothly. There is no difficulty with the fact that in going from the s state to the p state the winding number changes, because it is easily verified that at some stage in the process (when $\delta\omega = 0$, in fact) the condensate wave function has a node at some point in the torus (typically where V_{ext} is largest). Note, how-

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[34] In general, negative values of g are apt to lead to collapse in position space (see Dalfovo *et al.*, 1999, Sec. III.C), but for any given geometry it is possible to choose g small enough that this does not occur.

ever, that for small ω the first term $(-\hbar\omega_c \cos\chi)$ dominates the other two, so $\cos\chi \simeq 1$ and $L \simeq 0$; we do get a (nearly complete) Hess-Fairbank effect, though it is not complete (i.e., $\rho_s \neq \rho$) because of the term in $\sin\chi$.

The opposite case, $g/V_o > 1$, is more interesting. In this case, for $\delta\omega = 0$, there is still a stationary point of $E(\chi)$ at $\chi = \pi/2$, but it is a *maximum*; the minima occur at the pair of points $\chi = \sin^{-1}(V_o/g)$. If we now make $\delta\omega$ nonzero, one minimum is pushed up and the other down, and the barrier between them disappears entirely when

$$|\delta\omega|^{2/3} = g^{2/3} - V_o^{2/3}. \tag{6.26}$$

Thus, if for example we start rotating with $\omega = \omega_c$ and gradually decrease the rotation, the system will stay in the $\chi > \pi/2$ minimum not only in the regime where it is the globally stable one $(\omega > \omega_c/2)$ but also for a finite range of ω below $\omega_c/2$ where it is globally unstable. However, because of our choice (6.21) of the orders of magnitude of the parameters, there is no metastability in this case for $\omega = 0$. Note that in the context of the present discussion the case of the noninteracting Bose gas in an exactly cylindrical geometry $(g = 0,\ V_o = 0)$ is rather pathological: it shows a discontinuous $L(\omega)$ curve but no hysteresis.

The above argument needs to be supplemented in one important respect: In Eq. (6.23) it is implicitly *assumed* that all the relevant states of the system are of the Gross-Pitaevskii (coherent) type, i.e., involve only simple BEC. But what of the role of possible Fock states, that is, those of the form

$$\Psi_{Fock} \sim (a_o^+)^M (a_1^+)^{N-M} |\text{vac}\rangle, \tag{6.27}$$

where M and $N-M$ are both macroscopic (general BEC)? Actually it is straightforward to show that in the limit $N \to \infty$ the expectation value of the interaction term is identical to that in the Gross-Pitaevskii state with the same value of $\langle a_o^+ a_o \rangle$, while the expectation value of the asymmetry energy corresponding to Eq. (6.19) is zero. Thus for any given value of $\delta\omega$ the "best" Gross-Pitaevskii state [i.e., that corresponding to the choice $\Delta\varphi = 0$ and the best choice of χ in Eq. (6.23)] always does better than any Fock state. It is amusing that the fact that the interaction energy has a nonmonotonic behavior not only on the coherent path (6.23) but on the Fock path (6.27) is a direct consequence of the factor of 2 discussed at length in Sec. IV.

3. Further remarks

In real experiments with liquid helium, and probably though not certainly future experiments with the BEC alkali gases in a toroidal geometry, the (repulsive) interaction is typically strong enough that g is large compared to both $\hbar\omega_c$ and V_o (which may, however, be mutually comparable). Under these conditions, it is intuitively rather obvious that even for $\omega = 0$, not only the p state but many higher-ℓ states will be metastable. We get a rough idea of the degree of metastability by repeating the above argument replacing the p state by the state $\ell = n$, so that for $\omega = 0$ the coefficient of $\cos\chi$ in Eq. (6.24) becomes $n^2\hbar^2/2mR^2$. Then the term in V_o can be neglected to a first approximation, and we find (a) that the allowed values of L/N are always very close to $n\hbar$, and (b) that the condition for metastability of the state with winding number n when the container is stationary is $g > n^2\hbar^2/mR^2$. When rewritten in terms of the superfluid velocity $v_s \equiv n\hbar/mR$ of the metastable state and the velocity of sound $c_s \equiv \sqrt{g/m}$, this reads $v_s < c_s$, which is just the famous Landau criterion for the metastability of superfluid flow.

Actually, the Landau prediction has been verified experimentally in ^{4}He only in the *prima facie* rather different case of the mobility of ions moving through the liquid (Allum *et al.*, 1977; for an analogous experiment in the alkali-gas case, see Chikkatur *et al.*, 2000); in a toroidal geometry the critical velocities observed in practice are often orders of magnitude less than the Landau value (see Donnelly, 1967, Sec. 2.9). It is suspected that in most cases the reason for the discrepancy has to do with the presence of a "tangle" of vortices formed in nonequilibrium processes during the quench through the BEC transition temperature. However, under favorable conditions it is possible to observe an apparently intrinsic decay of superflow even at velocities less than c_s (Kukich *et al.*, 1968). The classic paper on the theory of this process is that by Langer and Fisher (1967); they postulate that the mechanism involves the formation of a vortex ring and its thermally activated expansion (a process that is apparently not possible for the simple toy model discussed above). Related considerations have been given for the alkali gases by Mueller *et al.* (1998).

One further question concerns the possible role of the hyperfine degree of freedom. As regards the Hess-Fairbank effect, there seems no reason to assume that this makes any appreciable difference. However, as regards the question of metastability of superflow, Ho (1982) obtained the following surprising and beautiful result: Consider a system of bosons each with total atomic spin F and with a Hamiltonian that is invariant under spin rotation in a toroidal geometry which is approximately cylindrically symmetric. Then for any given value of the winding number n there exists a path that changes n by $2F$ and involves no energy barrier; i.e., under zero rotation no state with $n > F$ can be metastable. For further discussion of this result and its possible applications to the alkali gases, and also for further discussion of the Landau criterion, see Leggett (2000a).

E. Real-life BEC alkali gases in harmonic traps

The analysis of this section so far (which largely rests on concepts developed in the context of liquid helium) needs to be modified in two ways before it can be applied to a realistic alkali-gas problem (even if we neglect the hyperfine degree of freedom, on which see above). The first has to do with the geometry of realistic traps, which is usually of the anisotropic simple harmonic-oscillator type.[35] A number of papers in the literature have studied the properties of the solutions of Eq. (6.9) in such a geometry [with the rotation generally taken around the axis of the (not quite exact) cylindrical symmetry]; the most detailed known to me is that of Butts and Rokhsar (1999; see also, for example, Benakli *et al.*, 1999). In contrast to the case of a narrow annulus, in this geometry a major role is played by centrifugal effects; in fact, for a rotational velocity ω larger than the radial frequency ω_r of the trap, the gas flies apart. For $\omega<\omega_r$ the behavior is qualitatively reminiscent of the hysteretic regime of the toy model of Sec. VI.D: as ω inreases from zero, the equilibrium value of **L** jumps between different smooth curves $L_{\ell}(\omega)$ characterizing different numbers ℓ of vortices, which in general (for $\ell\neq 1$) are not situated at the center of the trap. As a result, the angular momentum per particle is in general not integral. For general ω there is usually some degree of hysteresis in the transitions between the states corresponding to different ℓ; however, for $\omega=0$ none of the finite-ℓ states is metastable, because it turns out always to be energetically advantageous to move a vortex out towards the edge of the condensate, where it eventually disappears. For details the reader is referred to Butts and Rokhsar (1999) and the references cited therein. For new effects which may arise when the healing length becomes comparable to or larger than the cloud size, see Wilkin and Gunn (2000).

The second respect in which the considerations developed so far in this section need qualification concerns the effects of the kinetics (see Sec. II.E). In liquid ^{4}He, a strongly interacting system, the characteristic time scale for collisions of an atom both with other atoms and (inelastically) with the container walls is so small that it has very little effect on the decay of a metastable state, which is totally dominated by energetic considerations. By contrast, in the alkali gases it is entirely conceivable that even though a particular process may be "downhill all the way" energetically, the unstable state still appears stable over times of the order of perhaps seconds, because of the difficulty of energy exchange (and also exchange of angular momentum) not just between atoms but, even more importantly, with the container. As an example, if we have created, by rotation, a vortex at the center of a harmonic trap and then, by stopping the rotation, rendered it unstable, it may still persist for macroscopically long times (Fedichev *et al.*, 1999; cf. Matthews *et al.*, 1999).

F. The experimental situation

Recently two experimental groups have reported the observation of vortices in a BEC alkali gas. Matthews *et al.* (1999) started with ^{87}Rb in a pure $F=1$, $m_F=-1$ state ($|1\rangle$) and used a two-photon microwave transition to produce superpositions of $|1\rangle$ and the state $F=2$, $m_F=+1$ ($|2\rangle$) (see Sec. VII.B). As mentioned in Sec. V, the equilibrium of such a binary combination in a harmonic trap corresponds to a ring or shell of $|1\rangle$ surrounding a core of $|2\rangle$. Following a suggestion of Williams and Holland (1999), Matthews *et al.* (1999) were able by an appropriate rotation and detuning of the laser field to produce a single vortex in an outer component that could be either $|1\rangle$ or $|2\rangle$ at will; the presence of the vortex was confirmed by measuring the relative phase of the two condensates as a function of angle by an appropriate $\pi/2$ pulse (see Sec. VII.E). As the authors observe, it is noteworthy that in this experiment, while the effective equilibrium geometry of the $|2\rangle$ species is essentially that of the harmonic trap, that of the $|1\rangle$ species resembles more the toroidal (annular) geometry of Sec. VI.D. It is therefore perhaps not surprising that the observed lifetime of a vortex in the $|1\rangle$ species was considerably longer than that of one in $|2\rangle$.

A second experiment, that of Madison *et al.* (2000), adopts a scheme closer to that envisaged in Secs. VI.B and VI.C, with a single species in a slightly anisotropic harmonic trap uniformly rotated. The vortices were detected by observing (after trap expansion) the "holes" in the density distribution due to their cores. As the angular velocity of rotation is varied from zero up to the radial trap frequency, Madison *et al.* report observation of first no vortices, then successively one, two, three, and four (at higher velocities the system flies apart); the general pattern is similar to the predictions of Butts and Rokhsar (1999). Very recently, the same group has made direct measurements of the angular momentum of the system as a function of the angular velocity of the trap (Chevy *et al.*, 2000) and in particular confirmed that below the critical value of ω for the entry of the first vortex the system appears to be at rest in the laboratory frame, as the above discussion would lead us to expect.

VII. BEC IN A TWO-STATE SYSTEM: JOSEPHSON-TYPE EFFECTS, PHASE DIFFUSION

In traditional condensed-matter physics, the term *Josephson effect* is used generically to refer to a situation in which a large number N of identical bosons are restricted to occupy the same two-dimensional single-particle Hilbert space. Well-known examples are the eponymous effect,[36] originally predicted by Josephson (1962) for superconductors, and the related effect which occurs when two baths of ^{4}He (or ^{3}He) are connected through a narrow channel, or superleak (Ander-

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[35] There are further complications when more than one hyperfine species is involved. See Sec. VI.F.

[36] It is a matter of purely historical interest that in the original realization of the Josephson effect in superconductivity (a) the "bosons" (Cooper pairs) are composite rather than elementary objects, and (b) the system is coupled to external current leads and therefore cannot be described by the Hamiltonian (7.5) as it stands. The closed problem described by Eq. (7.5) is actually conceptually simpler than the original version (and nowadays can be realized in a superconducting context, e.g., in mesoscopic systems).

son, 1966; Avenel and Varoquaux, 1988). I will call these effects "external," since the two single-particle states in question are spatially separated. A condensed-matter example of an "internal" Josephson effect, in which the two states differ in some internal (nongeometrical) quantum number, is the longitudinal nuclear magnetic resonance in superfluid ^{3}He-A (Leggett, 1975; Wheatley, 1975); in this particular case the relevant quantum number is the hyperfine (nuclear spin) index of a Cooper pair. A general review of the Josephson effect in these and other physical systems is given by Barone (1999).

In the context of the BEC alkali gases, the interest of the generic Josephson situation is twofold: it can serve as at least a starting model for a number of situations of practical experimental interest (see Sec. VII.B), but perhaps even more importantly, it provides a simple and sometimes exactly soluble toy model for the examination of questions (such as corrections to the Gross-Pitaevskii description, or the generation and destruction of BEC) that arise in a less tractable form in the general theory of BEC in a spatially nonuniform system.

A. General formulation: choice of basis

We consider a system of N identical bosons, each of which is restricted to occupy a Hilbert space spanned by two orthonormal eigenvectors $|1\rangle$ and $|2\rangle$, which for the moment we choose arbitrarily; we denote the corresponding single-particle creation operators a_1^+, a_2^+. The Hilbert space of the N-particle system is thus $N+1$ dimensional and spanned by the eigenvectors in the Fock basis

$$|M\rangle \equiv \left[\left(\frac{N}{2}+M\right)!\left(\frac{N}{2}-M\right)!\right]^{-1/2} \times (a_1^+)^{N/2+M}(a_2^+)^{N/2-M}|\text{vac}\rangle,$$

$$M=-N/2,-N/2+1\cdots N/2,\quad N \text{ even:}$$

$$=-N/2-1/2,-N/2+1/2\cdots N/2-1/2,\quad N \text{ odd,} \tag{7.1}$$

where $|\text{vac}\rangle$ denotes the vacuum; it is clear that M is the (nearest integer to)[37] half the difference in the numbers of particles in states 1 and 2. This model is then isomorphic to the $N+1$-dimensional representation of the group SU(2).

It is clear that for such a system the occurrence of BEC as defined in Sec. III.A is automatic; the only question is whether it is simple or general. A useful invariant measure of the *degree of simplicity* (coherence) of the BEC is the quantity

$$\eta \equiv 2N^{-2}\,\mathrm{Tr}\,\hat{\rho}_1^2-1, \tag{7.2}$$

where $\hat{\rho}_1$ is the (2×2) single-particle density matrix; η evidently takes values from 0 to 1.

A complete set of number-conserving Hermitian operators describing the N-particle system is the set

$$\hat{M}\equiv\frac{1}{2}(a_1^+a_1-a_2^+a_2),$$

$$\hat{Q}_1\equiv\frac{1}{2}(a_1^+a_2+a_2^+a_1), \tag{7.3}$$

$$\hat{Q}_2\equiv-\frac{1}{2}i(a_1^+a_2-a_2^+a_1)$$

and thus the Hamiltonian can be expressed as a function of these three operators. At this point it is convenient to make a definite choice of basis. In most Josephson-type problems there is an intuitively natural choice; for example, in an extended problem the natural basis is one in which $|1\rangle$ and $|2\rangle$ refer to the states physically localized in the two bulk reservoirs, while for an internal effect (see below) it is the two single-particle hyperfine eigenstates in the absence of laser coupling. Formally, we can often (though not always) select a basis by requiring (a) that any terms of fourth order in the $a_{1,2}^+$ that are not simply proportional to M^2 be small and not involve M, and (b) that there be no term linear in $\hat{Q}_2$ (this fixes the relative phase of the basis vectors $|1\rangle$ and $|2\rangle$). With this specification, the most general Hamiltonian can be written in the form (up to terms that are functions only of N and hence constant)

$$\hat{H}=\frac{1}{2}K\hat{M}^2-\Delta\mu\cdot\hat{M}-\mathcal{E}_J\hat{Q}_1+f(\hat{M},\hat{Q}_1,\hat{Q}_2) + \sum_{i,j=1,2}\xi_{ij}\hat{Q}_i\hat{Q}_j, \tag{7.4}$$

where f contains terms of third order and higher in its arguments and all ξ_{ij} are $\ll K$. In a number of cases of practical interest the last two terms can be either neglected or incorporated into a shift in the origin of $\hat{M}$ (see below), and in this case I shall call the resulting expression the "canonical Josephson Hamiltonian": explicitly (in the former case),

$$\hat{H}_{canon}=\frac{1}{8}K(a_1^+a_1-a_2^+a_2)^2-\frac{\Delta\mu}{2}(a_1^+a_1-a_2^+a_2) - \frac{\mathcal{E}_J}{2}(a_1^+a_2+a_2^+a_1). \tag{7.5}$$

We shall see below that the canonical form (7.5) lends itself to a particularly simple analysis, while preserving most (though not all) of the features of the most general problem. It is amusing that the $\hat{H}_{\text{eff}}$ used in Sec. VI.D [Eq. (6.22)] is, up to a constant, equivalent to Eq. (7.5)

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[37] This choice of definition for M, while technically convenient, means that some of the formulas below, which are written explicitly for even N, need correction by factors $\sim(N^{-1})$ for odd N. This affects none of the conclusions and will not be noted explicitly below.

although the interpretation of the various terms there is different from that discussed below.

B. Realizations in the BEC alkali gases

The scheme developed in Sec. VII.A can form, at least, a starting point for the discussion of two effects in the BEC alkali gases that may be reasonably characterized, respectively, as an external and internal Josephson effect. However, it should be emphasized that in each case the simple canonical Hamiltonian (7.5) is applicable, if at all, only for a very restricted region of the experimentally accessible parameter space.[38] Space precludes a discussion here of the issues involved in the justification of Eq. (7.5), so I shall simply state the results and some caveats, and refer the reader to Sols (1999), Leggett (1999a, 2000a), and references therein for further details; see also Meier and Zwerger (2000).

Let us start with the external effect. The simplest way to create the necessary "two-well" potential would seem to be to use the initial setup of the MIT interference experiment (Andrews *et al.*, 1997; see Sec. 7.5), with an elongated cylindrical trap split down the center by a strongly detuned laser beam, and to turn the laser power down to a value substantially less than that used in the published experiments[39] so that tunneling between the two wells becomes non-negligible. Very crudely speaking, we expect the single-particle tunneling matrix element to be of order $\hbar\omega_o \exp -B$, where ω_o is a typical in-well frequency and B an appropriate WKB exponent which is $\gg 1$ for a high laser barrier. One's immediate instinct is that it should be possible to handle the two-well problem by a simple application of the time-dependent Gross-Pitaevskii equation (see, for example, Ostrovskaya *et al.*, 2000), and indeed for sufficiently strong tunneling this is almost certainly a good approximation. However, it is of interest to consider also the opposite limit $B \gg 1$. In that case it is plausible to truncate the possible states of the atoms to a two-dimensional subspace corresponding to the self-consistent ground states in the two wells separately, which we identify with the basis states $|1\rangle, |2\rangle$ of Sec. VII.A. Then, provided that (a) any bias between the two wells is very small compared to the barrier height, and (b) the typical asymmetry M is very small compared to the total number N, it is possible to justify the canonical Hamiltonian (7.5), with $\mathcal{E}_J$ an appropriate single-atom tunneling amplitude through the barrier, $\Delta\mu$ the bias, and K essentially the "bulk modulus" $\partial\mu/\partial N$ for a single well, which up to a numerical factor is given by $\hbar\omega_o\lambda^2/N$ where λ is defined in Eq. (5.52). Once one goes to larger values of the bias and/or asymmetry, the generic two-state Hamiltonian (7.4) may still be a good approximation but the approximation of it by Eq. (7.5) is likely to fail badly, both for the (relatively well-known) reason that for the single well μ is a highly nonlinear function of N and for the (less widely appreciated but at least equally important) one that once M becomes comparable to N the relevant WKB integral B, and hence the tunneling amplitude $\mathcal{E}_J$, is substantially modified from its $M=0$ value.[40]

Turning now to the internal Josephson effect, the nearest approximation to this realized to date in the BEC alkali gases seems to be the experiments of Hall and co-workers (Hall, Matthews, Ensher, *et al.*, 1998; Hall, Matthews, Wieman, and Cornell, 1998) in which a set of ^{87}Rb atoms in a (single-well) magnetic trap were driven by a microwave coupling into a linear superposition of two different hyperfine states and the degree of phase coherence between them measured by a Ramsey-fringe technique (see below for details). To analyze this experiment along the lines of Sec. VII.A, we for the moment pretend that the equilibrium condensate wave function $\chi_o(\mathbf{r})$ is independent of the hyperfine index, and moreover note that, since the microwave source injects very large numbers of photons, the electromagnetic field can be treated as a completely classical object. Then we can identify the two basis states $|1\rangle$ and $|2\rangle$ of Sec. VII.A with (say) the $F=1$, $m_F=-1$ and $F=2$, $m_F=+1$ hyperfine states, respectively. Since the laser fields are strongly time dependent, it is useful in this case to consider the Hamiltonian in the rotating frame, that is, the frame in which the laser field is constant over the time of the pulse (see, for example, Cohen-Tannoudji, 1992). Within the standard rotating-wave approximation (*ibid.*) this Hamiltonian can then be cast, for any one pulse, into the canonical form (7.5), with the identifications

$$\Delta\mu = -\delta + (4N\pi\hbar^2/m)\tilde{\eta}\cdot(a_{11}-a_{22}), \tag{7.6}$$

$$\mathcal{E}_J = \hbar\Omega_R, \tag{7.7}$$

$$K = \frac{4\pi\hbar^2}{m}\tilde{\eta}(a_{11}+a_{22}-2a_{12}), \tag{7.8}$$

where

$$\tilde{\eta} \equiv \int |\chi_o(r)|^4\, dr. \tag{7.9}$$

In Eqs. (7.6) δ is the detuning of the lasers from resonance (appropriately corrected for the laser-induced shifts of the atomic levels), Ω_R is the standard two-photon Rabi frequency, and a_{ij} is the s-wave scattering amplitude of hyperfine species i and j (see Sec. IV.E; for details, see Leggett, 2000a).

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[38] This situation is to be contrasted with that obtained in traditional condensed-matter systems, where physical considerations generally restrict the motion to the regime when Eq. (7.5) is an excellent approximation.

[39] Subsequent experiments may in fact have attained this regime (see Rohrl *et al.*, 1997).

[40] It may be shown that in the WKB limit ($B \gg 1$) the M dependence of $\mathcal{E}_J$ resulting from this effect is much greater than the "kinematic" dependence explicitly appearing in Eq. (7.21) below.

The canonical Hamiltonian (7.5), with time-independent parameters given by Eqs. (7.6)–(7.9), is adequate to describe the behavior during a single monochromatic laser pulse. In real life, both the amplitude of the laser field and its phase $\zeta(t)$ in the rotating frame may vary in time.[41] In this case, if one wishes to use a time-independent choice of axes, it is necessary to generalize the term in $\mathcal{E}_J$ in Eq. (7.4) to read

$$-\mathcal{E}_J(t)[\cos\zeta(t)\cdot\hat{Q}_1-\sin\zeta(t)\hat{Q}_2] \\ [\equiv-\mathcal{E}_J(t)(e^{i\zeta(t)}a_1^+a_2+\text{H.c.})]. \tag{7.10}$$

The above schematic description is unfortunately still too simple to apply to most existing experiments. In real life not only is the external potential (and hence the condensate wave function, even in the absence of interactions) different for the two species, but according to the results of Sec. V.E the condensate wave functions will themselves be functions of M. In the adiabatic limit, where the Rabi frequency Ω_R is small compared to the characteristic inverse "rearrangement time" of the condensates, it should still be possible to use the generic two-state Hamiltonian (7.4) [but not Eq. (7.5)], with the dependence on M given simply by that of the global ground-state energy for that M value. However, in existing experiments (Hall, Matthews, Wieman, and Cornell, 1998) we are quite far away from the adiabatic limit.[42]

For completeness it should be mentioned that there is one other experiment in the literature that is sometimes described as being of the Josephson type (in our classification, of the external variety), namely, that of Anderson and Kasevich (1998), which detects the coherence between the output beams from an array of wells at different heights in the Earth's gravitational field. In this experiment the system is not closed, so it does not fall under the general scheme of Sec. VI.B, and I shall therefore not discuss it here. (The analysis is in fact quite straightforward and is given in the cited reference.)

C. Kinematics of the Josephson effect: the Rabi, Josephson, and Fock regimes

We first note that the three operators (7.3), which form a complete set for our system, satisfy the commutation relations of the angular momentum components J_i, and thus we have an exact mapping to the problem of a particle of (large) spin J in an arbitrary $\mathbf{J}$-dependent potential:

$$\hat{M}\rightarrow\hat{J}_z,\hat{Q}_1\rightarrow\hat{J}_x,\hat{Q}_2\rightarrow\hat{J}_y,N/2\rightarrow J. \tag{7.11}$$

With this mapping we see that in the internal Josephson effect the laser coupling given by Eq. (7.10) is equivalent to the application of a magnetic field along an axis in the xy plane whose orientation angle relative to the x axis is given by the phase $\zeta(t)$. This angular momentum representation of the BEC two-state system is exact and is sometimes quite helpful to one's intuition. Notice in particular that in a physical situation where the quantity M is well defined (or has small fluctuations relative to N), the quantity $\hat{J}_x^2+\hat{J}_y^2$ is fixed at the value $(N/2+1)-M^2$; thus, while the phase angle of the xy component of angular momentum may or may not be well defined (see below), its magnitude certainly is, and in particular for $M\cong 0$ is close to $N/2$. This feature is a direct result of the BEC; it is easy to see that in a system described by many different single-particle labels λ in addition to the two-state one (e.g., a noncondensed mixture of two hyperfine species) the angular momentum $\mathbf{J}$ whose components are defined by

$$J_i\equiv\sum_\lambda J_{i\lambda},\quad J_{x\lambda}\equiv\frac{1}{2}(a_{1\lambda}^+a_{2\lambda}+a_{2\lambda}^+a_{1\lambda}),\ \text{etc.} \tag{7.12}$$

does not have a corresponding property, since the different $\mathbf{J}_\lambda$ can interfere destructively.

Since the magnitude $N/2$ of the angular momentum is fixed, the motion is, intuitively speaking, described by only two variables corresponding to its direction, and it is tempting to ask whether they can be chosen to be canonically conjugate. The most obvious suggestion is to try to define an operator $\hat{\varphi}$ corresponding to the relative phase, i.e., in the angular momentum picture to the angle of $\hat{\mathbf{J}}$ in the xy plane, such that (a) $\hat{\varphi}$ is canonically conjugate to $\hat{J}_z$, i.e., it satisfies the commutation relation

$$[\hat{J}_z,\hat{\varphi}]=-i \tag{7.13}$$

and (b) the coherent (Gross-Pitaevskii) states, that is, states of the form

$$\Psi_N=(N!)^{-1/2}(\cos\chi e^{i\varphi/2}a_1^++\sin\chi e^{-i\varphi/2}a_2^+)^N|\text{vac}\rangle \tag{7.14}$$

(where we denote the polar angle by χ rather than the conventional θ to avoid subsequent confusion), are as nearly as possible eigenstates of $\hat{\varphi}$ with eigenvalue φ. Is this possible?

The difficulties that arise in defining a relative phase operator having the above properties are closely analogous to the well-known problems that arise in quantum optics in defining an absolute phase operator for a single-mode electromagnetic field; see, for example, Mandel and Wolf (1995), Sec. 10.7, and references cited therein. However, generally speaking, those problems become acute only when one is discussing states containing no or a few photons, and in our case it is important to remember that we are interested in large values of the total particle number N. Thus it is plausible that we will be able to define a satisfactory relative phase operator provided that (i) the amplitude, in the state we are considering, of states with $N/2-|M|\lesssim N^{1/2}$ is small, and (ii) we are prepared to neglect effects of relative order $N^{-1/2}$

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[41] For example, the experiments of Hall, Matthews, Wieman, and Cornell (1998) use two pulses of approximately equal amplitude but shifted by a phase φ in the rotating frame. In this case $\mathcal{E}_J(t)$ is of course zero outside the pulses, and we can take $\zeta(t)\equiv 0$ during the first pulse and $\equiv\varphi$ during the second.

[42] This is at least partly due to the anomalously small value of the quantity $(a_{11}+a_{22}-2a_{12})$ for ^{87}Rb and is not necessarily a generic characteristic of such experiments.

TABLE II. Correspondence between Josephson parameters in different superfluid systems.

System+effect	$\Delta\mu$	K	E_J
^{4}He/BEC gases, external	gravitational/magnetic potential	bulk modulus	tunneling through aperture/barrier
Superconducting grains	voltage	Coulomb interaction	tunneling through aperture/barrier
^{3}He, internal (longitudinal NMR)	external magn. field	spin polarizability	nuclear dipole force
BEC gases, internal (rotating frame)	detuning	difference in inter- and intra-species interaction	laser coupling

or smaller. Under these conditions, the most appropriate procedure[43] is probably an adaptation of that of Carruthers and Nieto[44] for the absolute case. Namely, we define our operator $\hat{E}\equiv\exp i\hat{\varphi}$ by

$$\hat{E}\equiv[(N/2-\hat{J}_z)(N/2+\hat{J}_z+1)]^{-1/2}(\hat{J}_x+i\hat{J}_y) \tag{7.15}$$

so that

$$\hat{E}^+\equiv(\hat{J}_x-i\hat{J}_y)[(N/2-\hat{J}_z)(N/2+\hat{J}_z+1)]^{-1/2}. \tag{7.16}$$

As in the quantum-optical case, the operator $\hat{E}\equiv e^{i\hat{\varphi}}$ so defined is not unitary, so that $\hat{\varphi}$ cannot be Hermitian. However, we can if desired define sine and cosine operators that are Hermitian (cf. Mandel and Wolf, 1995), and in any case the lack of unitarity in the present context is not too serious; we have in fact

$$\hat{E}\hat{E}^\dagger\equiv 1,\ \ \hat{E}^\dagger\hat{E}\equiv 1-|N/2\rangle\langle N/2|-|-N/2\rangle\langle -N/2|. \tag{7.17}$$

Thus, provided that the state we are considering has only a small component of the extreme states, $M=\pm N/2$, we may treat $\hat{\varphi}$ itself as effectively Hermitian. Further, it may be verified by direct calculation that we have (independent of this condition)

$$[\hat{J}_z,\hat{E}]\equiv[\hat{J}_z,\exp i\hat{\varphi}]=\exp i\hat{\varphi}, \tag{7.18}$$

which is consistent with Eq. (7.13), and furthermore that just as in quantum optics the large-amplitude coherent states are approximate eigenstates of the (absolute) phase operator, so in our case the coherent states of the form (7.14) satisfy the relation

$$\hat{E}\Psi_N=\exp i\varphi\cdot\Psi_N+\delta\cdot\Psi_\perp \tag{7.19}$$

when $\Psi_\perp$ is a normalized state orthogonal to Ψ_N and the amplitude δ is of order $N^{-1/2}$ provided that $|\sin\theta|\gg N^{-1/2}$ [i.e., condition (i) above is fulfilled]. Thus, subject to conditions (i) and (ii), our definition (7.15) of $\hat{\varphi}$ indeed satisfies the requirements (a) and (b). It is clear that to the same accuracy we can write the intuitively plausible relation

$$J_x\pm iJ_y=\sqrt{(N/2)^2-\hat{J}_z^2}\cdot\exp\pm i\hat{\varphi} \tag{7.20}$$

without worrying about the ordering of the operators $\hat{J}_z$ and $\hat{\varphi}$. While the above discussion could no doubt be expanded, it should be adequate for the purposes of this section. To conclude it, we note that a Fock (fixed-M) state can be generated (up to normalization) from a coherent state of the form (7.14) by multiplying by $\exp(-iM\phi)$ and integrating over ϕ from zero to 2π. That is, a Fock state can be regarded as a superposition of coherent states with random phase.

The commutation relation (7.13) together with the Hamiltonian $\hat{H}(\hat{M},\hat{\varphi})$ gives a complete description of our problem, which is now one dimensional. In the most general case the function $\hat{H}(\hat{M},\hat{\varphi})$ is arbitrary (within certain generic constraints such as Hermiticity, etc.), but for the canonical case described by Eq. (7.5) it takes a relatively simple form: using Eqs. (7.3) and (7.19) we have

$$\begin{aligned}\hat{H}&=-\Delta\mu\cdot\hat{M}+\frac{1}{2}K\hat{M}^2-E_J\sqrt{1-\frac{4\hat{M}^2}{N^2}}\cos\hat{\varphi},\\ E_J&\equiv N\mathcal{E}_J.\end{aligned} \tag{7.21}$$

The Hamiltonian (7.21) can be applied to a variety of Josephson-type situations both in the traditional superfluids (superconductors and the two isotopes of He) and in the BEC alkali gases. In Table II I tabulate the physical meaning of the various parameters for some of these cases. As we saw in the last subsection, in the case of the external Josephson effect in an alkali gas, the truncation of the general form (7.4) to the special case described by Eq. (7.5) and hence Eq. (7.21) is justified, if at all, only for small values of $\hat{M}$; the same is actually true for the external effect in ^{4}He, and even for the internal effect in ^{3}He, but in these cases the physical conditions are almost invariably such that this is the only relevant case.

The generic behavior of an alkali-gas BEC system described by the Hamiltonian (7.5) [or the equivalent formulation via Eq. (7.14)] and the commutation relation (7.11) has been discussed in a number of papers in the literature.[45] It is useful for our purposes to distinguish three principal regimes, which are characterized by different orders of magnitude of the ratio K/E_J, and to attach names to them (Leggett, 1999a):

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[43] A possible alternative approach (Javanainen and Ivanov, 1999) is to take over the definition of phase used by Pegg and Barnett (1988) to the two-state problem. While this automatically guarantees the Hermiticity of $\hat{\varphi}$, the relation to the coherent state (7.14) is not so direct.

[44] While these authors also discuss the status of an angle variable, it is the angle of a coordinate vector rather than of the angular momentum itself, and we therefore cannot simply take over their discussion verbatim.

[45] These include, for example, Milburn *et al.*, 1997; Smerzi *et al.*, 1997; Javanainen and Ivanov, 1999; Leggett, 1999a; Marino *et al.*, 1999; Raghavan *et al.*, 1999; Sols, 1999.

- (1) “Rabi,” $K/E_J \ll N^{-2}$,
- (2) “Josephson,” $N^{-2} \ll K/E_J \ll 1$,
- (3) “Fock,” $1 \ll K/E_J$.

We examine below the ways in which the behavior of the system differs qualitatively in these three regimes.

First, however, it is useful to enquire in what regime we are likely to find ourselves for the various realizations of the Josephson effect listed above. It turns out that the traditional superfluids lie overwhelmingly in the Josephson regime, though the Fock regime is attainable, for instance, in ultrasmall superconducting grains; the Rabi regime is never attainable. As regards the external effect in the BEC alkali gases, it follows from the consideration of Sec. VI.B that the Rabi regime is never attainable under conditions in which Eq. (7.20) remains valid. Since the order of magnitude of the quantity K is given by the single-well bulk modulus, while the Josephson energy E_J is exponentially sensitive to the barrier height (see, for example, Zapata *et al.*, 1998), it is relatively easy to adjust the latter so as to go continuously from the Josephson to the Fock regime; it appears probable that the initial state in the MIT interference experiment (Andrews *et al.*, 1997) corresponded to the extreme Fock limit (though see footnote 39).

The most interesting case is that of the internal effect in the BEC alkali gases. Since in this case the Josephson coupling E_J is solely due to the action of the microwave pumps, we can trivially attain the Fock regime simply by switching the pumps off. As to the Rabi regime, from Eqs. (7.6) and the results of Sec. V.E we see that its attainment requires, crudely speaking, the condition $\Omega_R \gtrsim \overline{\omega}(N\epsilon a_s/d)^{2/5}$, where ϵ is the factor by which the difference $a_{11}+a_{22}-2a_{12}$ is reduced from a typical value a_s of the a_{ij}. Unfortunately, the expression on the right-hand side of this inequality is just of the order of the spatial rearrangement time, so that according to the discussion in Sec. VI.B the spatial degrees of freedom cannot be ignored. It seems that this was the situation during the pulse sequences in the experiment of Hall *et al.* (Hall, Matthews, Ensher, *et al.*, 1998; Hall, Matthews, Wieman, and Cornell, 1998).

Let us now examine the ways in which the behavior differs qualitatively in the three different regimes defined above, starting with the case of an unbiased system, $\Delta\mu=0$, and a starting value of M that is small compared to $N/2$. We then see that the main difference between the Rabi regime on the one hand and the Josephson (and Fock) regimes on the other lies in the source of the principal dependence on M: for the Rabi case this comes principally from the factor $\sqrt{1-(4\hat{M})^2/N^2}$ in the Josephson coupling energy (E_J), while for the Josephson and Fock cases it arises mostly from the explicit dependence of the interaction term $\frac{1}{2}K\hat{M}^2$. Consequently, in the extreme Rabi regime we can neglect the latter term and the behavior will be approximately that of a simple set of Bose-condensed two-level systems; conversely, far into the Josephson (or Fock) regime we can neglect the $\hat{M}$ dependence of the Josephson term, and the Hamiltonian then becomes simply that of a simple pendulum. Within this ($K/E_J \gg N^{-2}$) parameter regime the Josephson and Fock regimes are distinguished by the relative importance of quantum fluctuations, which may be measured (see below) by the rms value of φ in the ground state of Eq. (7.14); in the Josephson limit this is $\ll 1$, and as we shall see this means that the pendulum can for most (though not all) purposes be treated classically, while in the Fock limit it is $\gg 1$ (i.e., $\sim 2\pi$, since φ is by definition a periodic variable) and, conversely, the spread in $\hat{M}$ in the ground state is $\ll 1$, i.e., the ground state corresponds approximately to the Fock state (relative number eigenstate) $(a_L^\dagger)^{N/2}(a_R^\dagger)^{N/2}|\text{vac}\rangle$. Note that the simplicity parameter η defined in Eq. (7.2) is 1 in the extreme Rabi limit and close to 1 in both the Rabi and Josephson regimes, but 0 in the Fock limit for $M=0$. The same considerations may be applied qualitatively to the biased case, where $\Delta\mu \neq 0$, or to the case $|M| \sim N/2$ [but ($N/2 - |M| \gg N^{1/2}$)]; the obvious procedure in this case is to replace $\hat{M}$ by $\hat{M}' \equiv \hat{M} - M_{eq}$, where M_{eq} is the equilibrium value of M defined by $\Delta\mu/K$; evidently the commutation relation of M' with φ is still the canonical one, Eq. (7.11), and the Josephson coupling energy may be expanded in $\hat{M}$ around M_{eq} rather than around zero. The only point to watch is that if $\Delta\mu/K \gtrsim N/2$, so that the equilibrium value of $\hat{M}$ is close to $N/2$ (or if we start from such a state), then it will be impossible to neglect the $\hat{M}$ dependence of the Josephson coupling even if for $\Delta\mu=0$ we are well on the Josephson side.

To summarize the conclusions of the above discussion in slightly different language: The Rabi regime corresponds to a pendulum with a variable length depending on its angular momentum (see below and Marino *et al.*, 1999), while in the Josephson and Fock regimes the length is fixed. The Fock regime corresponds to a strongly quantum pendulum, while in the Rabi and Josephson regimes the behavior is (semi)classical. Accordingly, the theory of the Josephson effect in the Josephson parameter regime which corresponds to most of its traditional realizations in condensed-matter physics is just the theory of a simple classical pendulum (though see below). As we have seen, the external effect in the BEC alkali gases may correspond to either the Josephson or the Fock regime, and the internal effect to any of the three regimes, although in the Rabi regime the simple two-state model is inadequate.

The most detailed discussion known to me in the existing literature that covers the whole of the semiclassical region (Rabi and Josephson regimes) is that of Raghavan *et al.* (1999), while an extended discussion of the simple-pendulum region that allows for Fock-limit effects such as recurrences is given by Milburn *et al.* (1997). Here I shall concentrate on the Josephson and Fock regimes and just mention the extra effects that arise as we go towards the Rabi limit.

D. The Josephson regime: Josephson resonance and macroscopic quantum self-trapping

The general mapping of the Josephson effect to the problem of a pendulum is obtained by the replacements

$$\begin{aligned}
&\hat{\varphi}\to\hat{\theta}, && (7.22)\\
&\hat{M}\to\hat{L}/\hbar,\\
&N\to 2L_{max}/\hbar,\\
&E_J\to mg\ell,\\
&K\to(m\ell^2)^{-1}\equiv I^{-1},\\
&\Delta\mu\to A_\theta/\hbar,
\end{aligned}$$

where ℓ is the length of the pendulum and $\hat{\theta}$ the angle made with the vertical, and A_θ is a fictitious "vector potential," which couples to the angular momentum. Thus in the Josephson or Fock regimes we have in the pendulum analogy, adding for convenience a c-number term proportional to A_θ^2,

$$\hat{H}\to\frac{[\hat{L}-A_\theta(t)]^2}{2I}-mg\ell\cos\hat{\theta},$$

$$[\hat{L},\hat{\theta}]=-i\hbar. \qquad (7.23)$$

We specialize to the case of the Josephson regime and moreover assume $A_\theta\ll L_{max}$, i.e., the bias, if any, is such that the equilibrium value of M is much less than N ("nearly symmetric" case). We have dropped the $\hat{L}$ dependence of the potential term, so that the Hamiltonian is, as already noted, that of a simple (but in general driven) pendulum. For the moment we do not replace the quantum-mechanical commutator by a classical Poisson bracket.

Let us first put $A_\theta\equiv 0$ and study the quantum-mechanical ground state. We assume that the rms value of θ will be small and subsequently confirm that this is consistent. In that case, the Hamiltonian effectively reduces to that of a simple harmonic oscillator with frequency ω_J, thus $V(\theta)\cong\frac{1}{2}m\omega_J^2\theta^2$ where $\omega_J\equiv\sqrt{g/l}$, or in the language of our original problem $\hbar\omega_J\equiv\sqrt{E_J K}$; ω_J is known (because of its original realization in the superconducting problem) as the "Josephson plasma resonance frequency." The zero-point excursion in θ is of order $(\hbar/m\omega_J)^{1/2}$, which in the original language is simply $\sqrt{K/E_J}$. Provided therefore that we are indeed in the Josephson regime, the rms value of $\theta(=\varphi)$ is indeed $\ll 1$; in fact, we have $\varphi_{rms}\sim(K/E_J)^{1/4}$, $(M)_{rms}\sim(E_J/K)^{1/4}$; note that provided we are well out of the Rabi regime, this latter quantity is still much smaller than the value $(\sim N^{1/2})$ it would have for a Bose condensate of simple two-state systems—a point that is of crucial importance in discussing the nonequilibrium dynamics that arise when E_J changes as a function of time; see Sec. VII.E below.

The latter point may be put in a different way: The ground state of the interacting system is not a simple Gross-Pitaevskii state. Such a state may be written in the general case in the form (7.14), that is,

$$\begin{aligned}
\Psi_N&=[a_1^\dagger\cos\chi\exp(i\varphi/2)+a_2^\dagger\sin\chi\exp(-i\varphi/2)]^N|\text{vac}\rangle\\
&\equiv|\varphi\rangle. \qquad (7.24)
\end{aligned}$$

The ground state of the pendulum problem is not of this nature; rather, it is a coherent superposition of states $|\chi,\varphi\rangle$ with χ approximately $\pi/4$ but φ varying over a range of order φ_{rms}, i.e.,

$$\begin{aligned}
&\Psi_N=\int\psi(\varphi)|\varphi\rangle d\varphi,\\
&\psi(\varphi)\sim\exp-\frac{1}{4}(\varphi^2/\varphi_{rms}^2).
\end{aligned} \qquad (7.25)$$

We see therefore that once we introduce interactions the simple Gross-Pitaevskii description of the ground state cannot, strictly speaking, be consistent. Of course, provided we are well on the Josephson side of the Josephson-Fock boundary (so that $\varphi_{rms}\ll 1$) this does not usually matter very much, because typically physical quantities depend on φ only on the scale of unity (or π) and so the spread in φ does not affect them. However, as we have seen above, replacement of the true Ψ_N by the Gross-Pitaevskii form (7.24) (with $\chi,\varphi=0$) would lead to a serious overestimate of $\langle\hat{M}^2\rangle$ and thus of quantities such as the dephasing rate, which may depend on the latter (see Sec. VII.E).

The same remarks apply to the dynamics generated by the Hamiltonian (7.21). In the Josephson-Fock regime with $A_\theta=0$, the quantum-mechanical equations of motion for the operators $\hat{L}$ and $\hat{\theta}$ are

$$\dot{\hat{L}}=-\partial H/\partial\hat{\theta}=-mgl\sin\hat{\theta}, \qquad (7.26)$$

$$\dot{\hat{\theta}}=\partial H/\partial\hat{L}=\hat{L}/2I. \qquad (7.27)$$

Generally speaking, a necessary (and usually sufficient) condition to replace the operators $\hat{L}$ and $\hat{\theta}$ by the corresponding classical variables is that $\langle\sin\hat{\theta}\rangle\cong\sin\langle\hat{\theta}\rangle$, where the pointed brackets indicate averages over the quantum-mechanical wave function $\psi(\theta)$ [i.e., $\psi(\varphi)$]. Provided only that the spread of φ is not much greater in order of magnitude than the ground-state rms spread φ_{rms}, this condition is automatically fulfilled in the Josephson regime, and thus we can usually treat the dynamics semiclassically in this regime. However, this argument does not, as it stands, cover the case in which, for instance, the initial state is nearly a pure Fock state (eigenstate of $\hat{M}$) and thus has a spread $\sim 2\pi$ in φ, and further arguments are necessary in such a case to justify a semiclassical approximation; see Sec. IX.E.

Once we have established that in the Josephson regime the dynamics are (usually) those of a simple classical pendulum, we can immediately apply our classical intuition. However, because the most directly observable quantity in the BEC case (the quantity M, which can be measured, for example, by optical absorption techniques; see Sec. II) corresponds to the angular momentum rather than the displacement of the pendulum, the results are sometimes quite striking. Consider first the small oscillations about equilibrium; if for present purposes we neglect quantum fluctuations, the latter corresponds to $\varphi=0$ $(\theta=0)$. Taking the classical version of Eqs. (7.26) and (7.27), we see that the small oscillations are sinusoidal with the Josephson frequency $\omega_J \equiv (KE_J)^{1/2}$; they should in principle be observable as a sinusoidal oscillation of the atomic density between the two wells (or two hyperfine states).

A more interesting experiment is one in which we initially hold $\Delta\mu$ fixed at a small but finite value and then, at time zero, reduce it to zero. It is easy to verify that the equilibrium ground state for $t \leqslant 0$ has $\varphi = 0$ but $M = -\Delta\mu/K \neq 0$, i.e., in the pendulum analogy, it has finite canonical angular momentum [but zero angular velocity ω, since we recall that in the presence of a finite $A_\theta \omega$ is given not by L/I but by $(L - A_\theta)/I$]. For $t \geqslant 0$ the dynamics are given by the classical version of the (unforced, that is $A_\theta = 0$) Eqs. (7.26) and (7.27), i.e., the simple pendulum equations, but the initial condition is that $L(t=0+) = A_\theta$ (so that the pendulum is given an impulsive torque at $t=0$), or in the original BEC language $M(t=0+) = -\Delta\mu/K$. It is clear from our intuition regarding the classical pendulum that there is a critical value of $L(t=0+)$ or equivalently a critical value M_c of M, given by $M_c = \sqrt{2E_J/K}$ [note that in the Josephson region, by definition, this value is much greater than 1, and in fact much greater than $M_{rms} \sim (E_J/K)^{1/4}$, but much smaller than N.] For $M < M_c$ $(L < L_c)$ the pendulum performs simple librational (oscillatory) motion, which for $L \ll L_c$ is nearly simple harmonic at the Josephson plasma frequency ω_J. As M approaches M_c from below the motion becomes strongly anharmonic, and for $M > M_c$ the pendulum rotates instead of librating. It is clear that in the rotating state the angular momentum stays always positive definite,[46] and analogously, for the Josephson system M does the same, i.e., the system never reaches the equilibrium value (zero) of M (in the absence of damping). This behavior has been seen spectacularly in the longitudinal nuclear magnetic resonance of ^{3}He-A (Wheatley, 1975, Sec. VIII). In the case of the BEC alkali gases, it has not at the time of writing been seen experimentally but has been analyzed in the theoretical literature under the name "macroscopic quantum self-trapping."

There are a number of other interesting phenomena that can be seen in the semiclassical regime of the Josephson effect, particularly near the Rabi-Josephson boundary: see Smerzi *et al.* (1997) and Marino *et al.* (1999).

The question of dissipation in the Josephson effect is of considerable interest, both in its own right and as a possible guide to the more general characteristics of relaxation in a BEC system. However, to discuss it we clearly have to go beyond the simple conservative Hamiltonian (7.4), for instance, by introducing extra degrees of freedom corresponding to the normal component (see, for example, Ruostekoski and Walls, 1998; Zapata *et al.*, 1998; Meier and Zwerger, 2000). I shall therefore not attempt to discuss it here.

E. The Fock regime: phase diffusion

One advantage of studying BEC in a two-state system is that it allows us to formulate, in a very clean and unambiguous way, the problem of phase diffusion. In this context "phase" always means relative phase. For present purposes I shall consider only the very simplest possible case, a system that is for the duration of the relevant part of the experiment in the extreme Fock limit (i.e., the Josephson coupling E_J is simply set to zero) and where the initial (and conserved) expectation value of the relative number M is zero. The dispersion in M is for the moment taken to be $\ll N$ but otherwise arbitrary. Such a situation is realized in the "Ramsey-fringe" experiment of Hall, Matthews, Wieman, and Cornell (1998); in this case, the two states in question are two different hyperfine states of ^{87}Rb. A superposition state of the type (7.28) below is created by the initial $\pi/2$ two-photon pulse[47]; the system is then allowed to evolve freely $(E_J = 0)$ until a second $\pi/2$ pulse, arbitrarily phased with respect to the first. Finally, the number of atoms in each of the two hyperfine states is measured.

Consider initially a normalized Gross-Pitaevskii-type state of the form [a special case of Eq. (7.14)]

$$\Psi_N = \frac{[2^{-1/2}(e^{i\varphi/2}a_1^+ + e^{-i\varphi/2}a_2^+)]^N}{\sqrt{N!}}|\mathrm{vac}\rangle$$

$$\equiv \sum_M \sqrt{\frac{\frac{N}{2}+M!\frac{N}{2}-M!}{N!}}\exp iM\varphi|M\rangle. \quad (7.28)$$

In this state the dispersion of M is clearly of order $N^{1/2}$. It is convenient to introduce the operator

$$\hat{Q} \equiv \frac{2}{N}(\hat{Q}_1 + i\hat{Q}_2) \equiv a_1^+ a_2/(N/2) \quad (\cong \exp i\hat{\varphi}). \quad (7.29)$$

The Gross-Pitaevskii state (7.28) is an approximate eigenstate of $\hat{Q}$, with eigenvalue $\exp i\varphi$; equivalently, in the 3D angular momentum picture of Eqs. (7.11), the angular momentum lies in the xy plane at an angle φ with respect to the x axis (for example, if the magnetic field corresponding to the initial $\pi/2$ pulse lies along the x axis, $\mathbf{J}$ lies initially along the y axis).

Before proceeding to calculate the subsequent development of the expectation value $\langle Q(t)\rangle$ of $\hat{Q}$, it is important to discuss the relation of this quantity to what is actually measured experimentally. At this point it may be helpful to make a brief digression to discuss the celebrated MIT interference experiment (Andrews *et al.*, 1997), since although the latter involves some complications that are not present in the toy version of the Ramsey-fringe experiments that I shall consider, the issues concerning the relation of what is calculated to

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[46] In the classical approximation.

[47] As discussed in Sec. VII.C, during the pulse itself the system is in the Rabi limit.

what is actually measured is essentially identical. The ensuing discussion is highly schematic and is essentially a synopsis of considerations already thoroughly discussed in the existing literature on this experiment (e.g., Javanainen and Yoo, 1996; Naraschewski *et al.*, 1996; Castin and Dalibard, 1997; Hegstrom, 1998); it makes no claim to any originality.

At the initial stage of the experiment, BEC is produced separately in two sets of atoms, confined in two separate traps; the number in each trap is macroscopic ($\sim 5\times 10^6$) and approximately, though in practice not exactly, equal. In the published experiments the (laser-induced) energy barrier between the two traps is so high that the probability of tunneling between them should be completely negligible, so that the system is firmly in the extreme Fock limit according to the classification of Sec. VII.C and, if we denote the single-atom ground state in the left and right wells by ψ_L and ψ_R, respectively, the initial many-body state should be schematically of the form

$$\Psi_N \sim [\psi_L(\mathbf{r})]^{N_L}[\psi_R(\mathbf{r})]^{N_R}, \quad N_L+N_R=N, \tag{7.30}$$

corresponding to a definite number N_L or N_R of atoms in the left or right well, or in the language of Sec. VII.A to a Fock state. The overlap of $\psi_L(\mathbf{r})$ and $\psi_R(\mathbf{r})$ is completely negligible. Next, the barrier is removed, so that the atoms can expand freely into the region between the two traps where they can overlap. At this stage, and before any measurement is made, a natural schematic description is of the form

$$\Psi_N \sim [\psi_L(\mathbf{r},t)]^{N_L}[\psi_R(\mathbf{r},t)]^{N_R}, \tag{7.31}$$

where $\psi_L(\mathbf{r},t)$ is the time-dependent state that evolves from $\psi_R(\mathbf{r})$ under the action of the time-dependent Gross-Pitaevskii equation.[48] In general, $\psi_L(\mathbf{r},t)$ and $\psi_R(\mathbf{r},t)$ will both be nonzero in the overlap region between the wells. The final step is to measure, by optical means, the atomic density $\rho(\mathbf{r},t)$ in this region, and the interesting question is: Do we see fringes (density oscillations) corresponding to interference between the two condensates?

If we had started not from the Fock state (7.30) but from a coherent state of the form

$$\Psi_N \sim [a\psi_L(\mathbf{r})+b\psi_R(\mathbf{r})]^N \quad (|a|\sim|b|), \tag{7.32}$$

then after the expansion we would have schematically instead of Eq. (7.31) the state

$$\Psi_N \sim [a\psi_L(\mathbf{r},t)+b\psi_R(\mathbf{r},t)]^N. \tag{7.33}$$

In such a state the expectation value of the density $\rho(\mathbf{r},t)$ is

$$\langle\rho(\mathbf{r},t)\rangle_{coh} = |N[|a|^2|\psi_L(\mathbf{r},t)|^2+|b|^2|\psi_R(\mathbf{r},t)|^2 + 2\,\mathrm{Re}\{ab\,\psi_L^*(\mathbf{r},t)\psi_R(\mathbf{r},t)\}], \tag{7.34}$$

and since the functions $\psi_L(\mathbf{r},t)$ (obtained by solving the time-dependent Gross-Pitaevskii equation) correspond approximately, at least locally, to oppositely propagating plane waves of relatively well-defined wavelength λ, the last term in Eq. (7.34) produces density oscillations of period $\lambda/2$, leading to the corresponding fringes in the optical transmission pattern. Note that if the initial conditions on each run of the experiment are identical (something that would be difficult to achieve in practice) then not only the spacing but the "offset" (absolute position) of the fringe pattern should be reproducible from run to run.

Now, what happens if the initial state is (as it almost certainly was in the published experiments) the Fock state (7.30)? If we carry out a direct calculation of $\langle\rho(\mathbf{r},t)\rangle$ on the basis of the many-body wave function (7.31), we find the rather disappointing result

$$\langle\rho(\mathbf{r},t)\rangle_{Fock} = N_L|\psi_L(\mathbf{r},t)|^2+N_R|\psi_R(\mathbf{r}t)|^2 \tag{7.35}$$

with no interference term. Yet the photographs obtained in the experiments show spectacular interference fringes! (See Andrews *et al.*, 1997, Fig. 2.)

The resolution of the apparent paradox lies in the observation that the predictions of quantum mechanics always refer to statistical averages over many experimental runs. In condensed-matter physics one is used to the idea that when the quantity one is measuring is macroscopic and is the sum of contributions from many microscopic entities (in this case, the atoms) then it is usually adequate to replace averages over runs by averages over atoms, i.e., to assume that the result obtained on any one run will be close to the run-averaged result. But this assumption may fail spectacularly if there is a strong degree of correlation between the atoms—and the phenomenon of BEC represents in some sense the strongest correlation conceivable, since every atom must be doing exactly the same thing at the same time! Indeed, when applied to the experiment of Andrews *et al.* (1997) the quantum-mechanical prediction (7.35) is entirely correct—but all that it tells us is that if we take a photograph of the density distribution on each individual run of many runs and then lay the photographs on top of one another, the pattern will be correctly described by Eq. (7.35). It tells us nothing (much) about what we will see in each individual photograph, and to find this out it is necessary to calculate higher-order correlation functions such as the quantity

$$P(\mathbf{r}\mathbf{r}':t) \equiv \langle\rho(\mathbf{r},t)\rho(\mathbf{r}',t)\rangle. \tag{7.36}$$

If we calculate P on the basis of the wave function (7.31), we find that it has strong oscillations as a function of $z-z'$, with period $\lambda/2$ (where z is the relevant coordinate, roughly speaking that corresponding to the axis separates the two wells). Thus the conditional probability that if one sees a high atomic density at position z one will also see a high density at a point $n\lambda/2$ away [and a low one at $(n+1/2)\lambda/2$] is high. One can evidently extend the argument to higher correlation functions, and the net result is that quantum mechanics makes a unique prediction about the fringe spacing but

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[48] This result is of course only approximate, and in particular ignores important questions concerning the effect of interatomic interactions in the overlap region (which fortunately turns out to be fairly negligible), but it will be adequate for our present purpose.

no prediction about the offset. What this means is that on each run we expect to see a definite fringe pattern, with spacing $\lambda/2$ but with random offset. This is exactly what is seen in the experiments. When the photographs from many different experiments are superimposed, the randomness of the offsets means that the average density thus seen conforms to Eq. (7.35), i.e., shows no fringes. An alternative way of describing the situation that may make the analogy to the Ramsey-fringe case clearer is that any Fock state of the form (7.30) may be represented as a linear superposition of coherent states of the form (7.32) with equal amplitudes for each value of the relative phase of a and b, and that according to Eq. (7.34) measurement of the atomic density constitutes a measurement of this relative phase; then according to the measurement axioms of quantum mechanics such a measurement must have a definite outcome, but that outcome is random from run to run and unpredictable in advance. [For a further discussion of this point in the general Josephson context, see Hegstrom and Sols (1995), and for the specific application to BEC alkali gases see the references cited above.]

Returning now to the Ramsey-fringe experiment, the second $\pi/2$ pulse, at time t, corresponds to application of a pulsed magnetic field along some axis in the xy plane rotated relative to that of the first pulse by some phase shift δ, and this is then followed by a measurement (by optical absorption) of the relative population of states $|1\rangle$ and $|2\rangle$, i.e., of J_z. Suppose first that at time t the system is still in an eigenstate of $\hat{Q}$ with eigenvalue $\exp i[\varphi+\theta(t)]$, i.e., the angular momentum has simply precessed around the z axis through an angle $\theta(t)$. Then it is clear that on each run of an ensemble of experiments involving the same initial conditions and the same time difference t, the measured value of J_z will be reproducible and equal to $\cos[\varphi(t)-\delta]$, $[\varphi(t)\equiv\varphi+\theta(t)]$ [cf. the predictions above for the coherent case described by Eq. (7.32)].

However, in general we shall find that the behavior of $\langle\hat{Q}(t)\rangle$ does not correspond to a unique precession. What does this mean for the expected experimental results? We have seen in Sec. VII.C that provided the system behaves as a simple BEC two-state system, the operator $J_x^2+J_y^2$ always has under these conditions a value of approximately $(N/2)^2$, which means that the magnitude of $Q(t)$, could it be directly observed in the experiment, should always be 1:

$$\langle\hat{Q}^\dagger(t)\hat{Q}(t)\rangle=1. \tag{7.37}$$

On the other hand, the calculation below will show that in general

$$|\langle\hat{Q}(t)\rangle|^2=\eta(t)<1, \tag{7.38}$$

where to obtain the equality we used the definition (7.2) of the degree of coherence $\eta(t)$, Eq. (7.29), and the fact that $\langle J_z\rangle=0$. What this means is that on any given run of the experiment the system behaves "as if" the (vector) angular momentum lies in the xy plane and has its full magnitude $N/2$, but with a phase angle $\theta(t)$ that is not necessarily well defined and whose apparent value may therefore vary from run to run (see the discussion above of the MIT interference experiment). Then, if the probability of the system realizing a given value of θ at time t is $P_t(\theta)$, the probability of obtaining a given value of $J_z[\equiv\frac{1}{2}(n_1-n_2)]$ after a second pulse at time t with phase angle δ relative to the first will be proportional to $P_t(\theta_o)$ where $\cos(\theta_o-\delta)=J_z$, and the expectation value of J_z will be

$$\langle J_z\rangle=\text{const}\int d\theta\, P_t(\theta)\cos(\theta-\delta). \tag{7.39}$$

Consider a series of experiments such that we first select a given value of t and of δ, measure the value of J_z on each of an ensemble of runs with this t and thus a value of $\langle J_z\rangle(t)$, then choose a new value of t (but the same δ) and repeat the procedure, and so on. The possible behavior varies between two extreme cases:

(a) If $\theta(t)$ is well defined and processes with angular frequency ω, then the value $J_z\equiv\frac{1}{2}i\langle(n_1-n_2)\rangle$ measured on each run of the ensemble of experiments conducted with time delay t is unique and given by the expression

$$J_z(t)\equiv\langle J_z(t)\rangle=(N/2)\cos(\omega t-\delta). \tag{7.40}$$

(b) If $\theta(t)$ is completely random (ill defined), then the value of J_z measured on a given run of the relevant ensemble should vary at random from $-N/2$ to $+N/2$, and the run-averaged value of $\langle J_z\rangle(t)$ should be zero. In the intermediate case $\langle J_z\rangle(t)$ should be given, crudely speaking, by a formula of the type $A(t)(N/2)\cos(\omega t-\delta)$ where the envelope function $A(t)$, which under appropriate conditions is slowly varying over a period $2\pi/\omega$, is less than 1 and is equal under the stated conditions to $|\langle\hat{Q}(t)\rangle| =\eta^{1/2}(t)$.

Let us now turn to the calculation of $\langle\hat{Q}(t)\rangle$, and thus of $\eta(t)$. Consider an initial state that is a generalization of Eq. (7.22), namely,

$$\Psi_N(0)=\sum_M \lambda_M \exp(iM\varphi)|M\rangle, \tag{7.41}$$

where the coefficients λ_M are real, positive, slowly varying between neighboring values of M, such that the dispersion in M is $\ll N$, and satisfy the normalization condition $\Sigma_M\lambda_M^2=1$. These conditions are satisfied, for example, by a normalized Gaussian distribution with width $\ll N$ (but $\gg 1$). Because of the slow variation condition, $\Psi_N(0)$ is an approximate eigenstate of $\hat{Q}$ with eigenvalue $\exp i\varphi$, and $\eta(0)=1$.

Consider now the time evolution of $\langle\hat{Q}\rangle$ and hence of η. For orientation let us first consider the case in which all interactions are small, so that the Hamiltonian is simply $-\Delta\mu\cdot M$. In the following, it is convenient to work in the rotating frame as defined by the initial and final $\pi/2$ pulses, so that $\Delta\mu$ is fairly small. It is immediately clear that the phase accumulated over time t by the state $|M\rangle$ is just $\Delta\mu \cdot Mt$, so that the many-body state at time t is just of the form (7.28) with φ replaced by $\varphi + \Delta\mu \cdot t$. Thus we have

$$\langle \hat{Q}(t) \rangle = \exp i(\varphi + \Delta\mu t) \tag{7.42}$$

and $\eta(t)$ stays equal to unity for all t.

Next let us consider the effect of a term in $\hat{H}$ of the form $\frac{1}{2} K \hat{M}^2$. The effect of this is to add to the evolution of the state $|M\rangle$ an extra phase $-\frac{1}{2} K M^2 t$. However, since all contributions to $\langle \hat{Q} \rangle$ come from the matrix elements between states $|M\rangle$ and $|M+1\rangle$, it is the derivative of this expression that enters $\langle \hat{Q}(t) \rangle$:

$$\langle \hat{Q}(t) \rangle = \exp i(\varphi + \Delta\mu t) \sum_M \lambda_M^2 \exp - iKMt. \tag{7.43}$$

Suppose the initial packet is a Gaussian of width $(\Delta M)_o$, i.e.,

$$\lambda_M \sim \frac{1}{\Delta M_o} \exp - M^2/4(\Delta M)_o^2. \tag{7.44}$$

Then the initial time dependence of $\langle \hat{Q}(t) \rangle$ can be obtained by replacing the sum over M by an integral:

$$\langle Q(t) \rangle = \exp i(\varphi + \Delta\mu \cdot t) \exp - K^2 (\Delta M)_o^2 t^2 \tag{7.45}$$

and so

$$\eta(t) = \exp - 2K^2 (\Delta M)_o^2 t^2. \tag{7.46}$$

Thus the degree of coherence $\eta(t)$ falls to zero over a time scale (call it τ_{decoh}) of the order of $\hbar/(K \cdot \Delta M_o)$. Since in an experiment of the JILA type $\Delta M_o \sim N^{1/2}$ and K is proportional, in a harmonic trap, to $N^{-3/5}$, [see Eq. (7.7)], we see that τ_{decoh} actually increases with N, though only as $N^{1/10}$. Since, as we have seen, K is of order E times the mean-field energy, which is typically of order 20 kHz, we see that for a sample of, say, 10^6 atoms τ_{decoh} can be of the order of a few seconds.[49]

The transition from a sum over M to an integral, however, obscures one phenomenon that is of potential interest, namely, that of *recurrences*. We see from Eq. (7.43) that at times which are exact multiples of $\hbar/K \equiv t_{rec}$ all the different states $|M\rangle$ come back into phase, and $\eta(t)$ recovers its original value of unity. The quantity t_{rec} is longer than τ_{decoh} by a factor $(\Delta M_o)^{-1}$, and thus for the JILA experiment would be of the order of hours and almost certainly unobservable.[50]

All the above assumes not only isolation of the system from any "environment" but neglect of processes such as recombination and trap evaporation. What happens if we relax these assumptions?

To the extent that the environment can be modeled by a classical random field which couples linearly to $\hat{M}$ [$H_{sys-env} \sim \hat{M} V(t)$, where $V(t)$ is random], it is clear that it gives rise to dephasing such that

$$\eta(t) = \left| \overline{\exp - i \int_o^t V(t) dt/\hbar} \right|^2, \tag{7.47}$$

where the bar indicates an average over the form of $V(t)$; the same should be true within a quantum-mechanical description of the environment, if the coupling is of the form $\hat{M}\hat{\Omega}$ with $\hat{\Omega}$ some operator of the latter and the average is replaced by a trace. A second example of dephasing that may be important in practice is the uncertainty, in a given experimental run, in the value of N and hence in the constant K. Finally, a more subtle example is recombination (Sinatra and Castin, 1998). Let us suppose for the moment that a single ℓ-body recombination process takes place at definite time $t-T$ (where t is, as above, the time of the second $\pi/2$ pulse and is fixed by the experimenter). The effect of this recombination is to replace each of the coefficients $C_M(t-T)$ of the state $|M\rangle$ by $C_{M+m}(t-T)$. This means that the relative phase of neighboring C_M at time t is of the form

$$\begin{aligned} \Delta\varphi_M &= (\Delta\mu - KM)(t-T) + [\Delta\mu - K(M-\ell)]T \\ &= (\Delta\mu - KM)t + \ell KT, \end{aligned} \tag{7.48}$$

i.e., it adds an M-independent term to $\Delta\mu_M$, whose value is determined by the unknown time T. The argument can obviously be generalized to the case of many recombinations; although it is classical in the sense that the decays are conceived as taking place at definite (but random) times, it seems extremely probable that a fully quantum-mechanical treatment would give the same result.

All the above considerations are confirmed quantitatively in an elegant calculation due to Sinatra and Castin (1998). If λ^{-1} is the characteristic time for the first recombination to occur, they find, for the quantity we have called $\hat{Q}(t)$, the result for $t \ll t_c$ [their Eq. (64)]

$$|\langle \hat{Q}(t) \rangle| = \exp - \frac{\chi^2 t^2}{8} \left(\frac{1}{(\Delta\varphi)_0^2} + \frac{4}{3} \ell^2 \lambda t \right), \tag{7.49}$$

where $(\Delta\varphi)_0^2$ is the mean-square spread in relative phase (as they define it) in the initial state. Since this quantity is proportional to $(\Delta M)_0^{-2}$ and the χ in Eq. (7.49) is proportional to our K, it is clear that the first factor in the brackets is identical in structure to that in Eq. (7.45), while the second indicates the effect of averaging over the recombination processes. Note that since in a JILA-type experiment $(\Delta\varphi)_o^2 \sim N^{1/2}$, the second term becomes comparable to the first only at times ($\sim N\lambda^{-1}$) so long that the whole sample has already decayed appreciably.

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[49] Note that had we started with a wave packet (such as the ground state of a harmonic well) that had a finite spread in φ and hence a value of $(\Delta M)_o$ much smaller than $N^{1/2}$, the decoherence time would have been much longer. Cf. Leggett and Sols, 1998; Javanainen and Wilkins, 1997.

[50] Inclusion in $\hat{H}$ of cubic and higher terms in $\hat{M}$ will tend to reduce the amplitude of the recurrences even for an isolated system, but a dimensional estimate shows that the effect is at most of order unity and may be smaller.

In the real-life JILA experiments, an important role is played by the spatial rearrangement processes following the initial $\pi/2$ pulse. These processes are discussed by Sinatra *et al.* (1999) and their effect on the phase coherence is noted by Sinatra and Castin (1998); the latter conclude that an important role is played by the dephasing due to uncertainty in the initial value of N, and that when this is taken into account the agreement of theory and experiment is reasonable.

VIII. THE BOGOLIUBOV APPROXIMATION

Let us confine ourselves for the moment to the case of a spinless gas at zero temperature. Then we have seen in Sec. V that in the dilute limit appropriate to the alkalis a very reasonable description of most of the properties, whether time dependent or not, is given by the Gross-Pitaevskii (Hartree) ansatz (5.14) for the many-body wave function, i.e., a simple product of single-particle functions with no two-particle or higher correlations (though see footnote 18). Now in fact it is clear that Eq. (5.14) can be regarded as the first of a sequence of trial functions, of which the next is one that builds in two- but not three-particle or higher correlations:

$$\Psi_N(\mathbf{r}_i\cdots\mathbf{r}_N:t)=\mathcal{S}\prod_{i<j}^{N}\varphi(\mathbf{r}_i,\mathbf{r}_j:t),\tag{8.1}$$

where $\mathcal{S}$ denotes the operation of symmetrization between the particles. Just as in the Gross-Pitaevskii approximation all particles occupy the same single-particle state, in the approximation (8.1) all *pairs* of particles occupy the same two-particle state. Equation (8.1) is nothing but the particle-number-conserving version of the celebrated *Bogoliubov approximation*. In the literature this approximation is, almost without exception, introduced either by explicitly relaxing the constraint of particle number conservation, as in the original work of Bogoliubov (1947), or by writing down and analyzing operator equations of motion. In my view neither of these techniques adequately exhibits the simple underlying structure (8.1) of the many-body wave function, so I shall take in this section a more direct approach. First, however, I give some motivation for going beyond the Gross-Pitaevskii approximation for the many-body ground state.

A. Inconsistency of the Gross-Pitaevskii approximation

Consider a system of N spinless bosons in free space. A direct way of seeing that the Gross-Pitaevskii ground state cannot be the true ground state of the system is to use the sum rules obeyed by the density fluctuation operator

$$\rho_{\mathbf{q}}\equiv V^{-1}\sum_i e^{i\mathbf{q}\cdot\mathbf{r}_i}\equiv V^{-1}\sum_p a^\dagger_{\mathbf{p}+\mathbf{q}/2}a_{\mathbf{p}-\mathbf{q}/2}.\tag{8.2}$$

The potential term in the Hamiltonian can be written in the form const $\Sigma_{\mathbf{q}}\rho_{\mathbf{q}}\rho_{-\mathbf{q}}$, and thus commutes with $\rho_{\mathbf{q}}$; this allows us to derive the "f-sum rule"

$$\sum_{\ell}(E_{\ell}-E_0)|\langle\ell|\rho_{\mathbf{q}}|0\rangle|^2=n\hbar^2q^2/2m\tag{8.3}$$

($n\equiv N/V$). Moreover, since the energy per unit volume in the Gross-Pitaevskii ground state is simply $\frac{1}{2}U_0n^2$, the compressibility χ_0 is just U_0^{-1}; writing out the second-order perturbation-theory expression for χ_0, we have

$$\sum_{\ell}|\langle\ell|\rho_q|0\rangle|^2(E_{\ell}-E_0)^{-1}=n/2U_0.\tag{8.4}$$

We can now use the Cauchy-Schwartz inequality to derive from Eqs. (8.3) and (8.4) the result

$$\langle\rho_q\rho_{-q}\rangle_0\equiv\sum_{\ell}|\langle\ell|\rho_q|0\rangle|^2\leqslant(n^2\hbar^2q^2/2mU_0)^{1/2}\equiv nq\xi\tag{8.5}$$

[where we used definition (5.6) of the healing length ξ]. However, we can also evaluate the quantity $\langle\rho_q\rho_{-q}\rangle_0$ directly:

$$\begin{aligned}\langle\rho_{\mathbf{q}}\rho_{-\mathbf{q}}\rangle_0&\equiv\sum_{\mathbf{pp}'}\langle a^\dagger_{\mathbf{p}+\mathbf{q}/2}a_{\mathbf{p}-\mathbf{q}/2}a^\dagger_{\mathbf{p}'-\mathbf{q}/2}a_{\mathbf{p}'+\mathbf{q}/2}\rangle_0\\&=\sum_{\mathbf{p}}\langle n_{\mathbf{p}+\mathbf{q}/2}\rangle_0\langle 1-n_{\mathbf{p}-\mathbf{q}/2}\rangle_0=n.\end{aligned}\tag{8.6}$$

For $q\xi\leqslant 1$ the relations (8.4) and (8.5) are clearly mutually inconsistent, and the only possible conclusion is that the Gross-Pitaevskii ground state cannot be the true ground state of the many-body system.

Some insight as to what has gone wrong may be obtained from our experience in Sec. VII.D with the two-state system in the Josephson regime. We saw there that in the presence of a term in the energy proportional to M^2, it is energetically advantageous to allow the relative phase of the condensate to fluctuate somewhat around its mean value, thereby lowering $\langle M^2\rangle$, which would otherwise be $\sim N$. In a similar way, in the bulk system, one would like to build in fluctuations so as to reduce the value of $\langle\rho_{\mathbf{q}}\rho_{-\mathbf{q}}\rangle$.

Another way of looking at what is essentially the same point is that, as we saw in Sec. IV.C, the total interaction energy is proportional to the sum over i and j of the quantity $|\Psi(r_{ij}\overset{\sim}{\rightarrow}0)|^2$, and it is therefore energetically favored to reduce the latter. It is intuitively plausible to expect that the distance in $|r_{ij}|$ over which the distortion from the simple Gross-Pitaevskii ansatz occurs will be, just as in the case of repulsion by a single-particle potential such as a hard wall, of the order of the healing length ξ, and we shall see that this is correct.

B. The Bogoliubov ground state in the translation-invariant case

Consider the case of a system moving in a constant external potential and subject to periodic boundary conditions, so that the ground-state wave function of the condensate is simply a zero-momentum plane wave (i.e., $\chi_0=$const). The upshot of the arguments of Sec. VIII.A is that we need to modify the Gross-Pitaevskii ground state so as to build in the effects of long-wavelength ($q\xi \lesssim 1$) density fluctuations. Now, the simplest way (indeed the only way) of creating a density fluctuation of wave vector q starting from the Gross-Pitaevskii ground state is to take a particle out of the state 0 ($\equiv \chi_0$) and put it into a state q. However, a single process of this kind would violate conservation of momentum. The simplest momentum-conserving procedure is to create *pairs* of density fluctuations of opposite momentum, i.e., to operate on the Gross-Pitaevskii ground state with the operator $a_q^\dagger a_{-q}^\dagger a_0 a_0 \equiv \hat{\Lambda}_q$. Thus we should expect that a good approximation to the true many-body ground state might be of the generic form

$$\Psi_N \sim \text{const} \sum_{\{n_j\}} c_{\{n_j\}} \prod_j \hat{\Lambda}_{q_j}^{n_j} |0\rangle, \tag{8.7}$$

where $|0\rangle$ is the Gross-Pitaevskii ground state and the $c_{\{n_j\}}$ are arbitrary complex coefficients.

Actually, however, the ansatz (8.7) turns out to be more general than we need; it can in fact be proved (Leggett, 1999b: the proof is too cumbersome to be given here) that in the limit $N \to \infty$ and small depletion (see below) the member of the class (8.7) that minimizes the energy is actually a member of a subclass, namely, the subclass of states corresponding to the ansatz (8.1). In second-quantized notation the latter reads in general, apart from normalization,

$$\Psi_N = (N!)^{-1/2} \left(\int \int d\mathbf{r}\, d\mathbf{r}' \times K(\mathbf{r}\mathbf{r}') \psi^\dagger(\mathbf{r}) \psi^\dagger(\mathbf{r}') \right)^{N/2} |\text{vac}\rangle, \tag{8.8}$$

and for the translation-invariant case we must have $K(\mathbf{r}\mathbf{r}') = K(\mathbf{r} - \mathbf{r}')$. Then, taking out the macroscopically occupied zero-momentum state explicitly and taking Fourier transforms, we have (still apart from normalization)

$$\Psi_N = N!^{-1/2} \left(a_0^\dagger a_0^\dagger - \sum_{\mathbf{q}>0} c_q a_q^\dagger a_{-q}^\dagger \right)^{N/2} |\text{vac}\rangle, \tag{8.9}$$

where the minus sign is introduced for subsequent convenience. Equation (8.9) is the ground state of a translation-invariant Bose system with fixed particle number N in the Bogoliubov approximation.[51]

It remains only to determine the coefficients c_q. To do this, we argue as follows: It is clear that the only terms in the second-quantized Hamiltonian that have nonzero expectation values in the state (8.9) are (ignoring terms of relative order N^{-1})

(a) the kinetic-energy terms

$$K = \sum_{q \neq 0} \epsilon_q a_q^\dagger a_q, \tag{8.10a}$$

(b) the Hartree terms

$$H_H = \frac{1}{2} \frac{U_0}{V} \sum_{qq'} a_q^\dagger a_{q'}^\dagger a_{q'} a_q = \frac{1}{2} \frac{N^2}{V} U_o, \tag{8.10b}$$

(c) the Fock terms

$$H_F = \frac{1}{2} \frac{U_0}{V} \sum_{q \neq q'} a_q^\dagger a_{q'}^\dagger a_{q'} a_q, \tag{8.10c}$$

(d) the "pairing" terms

$$H_P = \frac{1}{2} \frac{U_0}{V} \sum_{q \neq q'} a_q^\dagger a_{-q}^\dagger a_{-q'} a_{q'}. \tag{8.10d}$$

In the following I shall assume that the total "depletion" of the condensate, that is, the quantity $N^{-1} \Sigma_{q \neq 0} \langle a_q^\dagger a_q \rangle$, is much smaller than 1 (this will be confirmed below); this then allows us consistently to neglect, in Eqs. (8.10c) and (8.10d), all terms except those in which either $\mathbf{q}$ or $\mathbf{q}'$ is zero. Then if we take the zero of energy at the Gross-Pitaevskii value $\frac{1}{2} N^2 U_0 / V$, the Hamiltonian reduces to a sum of contributions from different values of $\mathbf{q}$:

$$\hat{H} = \sum_q \hat{H}_q, \tag{8.11}$$

$$\hat{H}_q \equiv \mathcal{E}_q a_q^\dagger a_q + \frac{1}{2} \frac{U_0}{V} (a_q^\dagger a_{-q}^\dagger a_0 a_0 + \text{H.c.}), \tag{8.12}$$

where

$$\mathcal{E}_q \equiv \epsilon_q + n_0 U_0, \quad n_0 \equiv N_0 / V \approx N/V. \tag{8.13}$$

To calculate $\langle H_q \rangle$ over the wave function (8.9) for any given $\mathbf{q}$, we make a binomial expansion of Eq. (8.9):

$$\Psi_N = N!^{-1/2} \sum_{m=0}^{N/2} C_m^{N/2} (a_0^\dagger a_0^\dagger - c_q a_q^\dagger a_{-q}^\dagger)^m \times \left(\sum_{k \neq q,0} - c_k a_k^\dagger a_{-k} \right)^{N/2-m} |\text{vac}\rangle, \tag{8.14}$$

with $C_m^{N/2}$ the binomial coefficient, and note that the second factor contributes only an overall probability factor to $\langle H_q \rangle$. Moreover, we can check that the only values of m contributing appreciably in Eq. (8.14) are close to N. Since the value of $\langle H_q \rangle$ for the normalized state corresponding to m is only weakly sensitive to m (see below), it follows that it is legitimate, in calculations of $\langle H_q \rangle$, to replace the full wave function (8.9) by the expression, now correctly normalized,

$$\Psi_{(q)} = (N!)^{-1/2} (1 - |c_q|^2)^{1/2} (a_0^\dagger a_0^\dagger - c_q a_q^\dagger a_{-q}^\dagger)^{N/2} |\text{vac}\rangle \quad (|c_q| < 1). \tag{8.15}$$

It is now extremely straightforward to calculate the quantity $\langle H_q \rangle \equiv \langle \Psi_{(q)} | \hat{H}_q | \Psi_{(q)} \rangle$, where $\hat{H}_q$ is given by

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[51] For related number-conserving formulations see, for example, Girardeau *et al.* (1959) and Gardiner (1997), and for the standard (number-nonconserving) approach see Huang (1987), Chap. 13.

Eq. (8.12). Omitting the simple algebra, I just quote the result[52] for the total Hamiltonian $\hat{H}$:

$$\langle H\rangle = \sum_{\mathbf{q}\neq 0} \{\mathcal{E}_q \sinh^2\theta_q - n_0 U_0 \sinh\theta_q \cosh\theta_q\}, \tag{8.16}$$

where I have introduced the notation $c_q \equiv \tanh\theta_q$. Minimization of Eq. (8.16) with respect to θ_q gives $\tanh(2\theta_q) = n_0 U_0/\mathcal{E}_q$, or equivalently

$$c_q = \frac{1}{n_0 U_0}(\mathcal{E}_q - E_q) \quad (>0), \tag{8.17}$$

where for subsequent convenience we introduced the notation

$$\begin{aligned} E_q &\equiv (\mathcal{E}_q^2 - n_0^2 U_0^2)^{1/2} \equiv [\epsilon_q(\epsilon_q + 2n_0 U_0)]^{1/2} \\ &\equiv \left[\hbar^2 c_s^2 q^2 + \left(\frac{\hbar^2 q^2}{2m}\right)^2\right]^{1/2}. \end{aligned} \tag{8.18}$$

Insertion of Eq. (8.17) into Eq. (8.9) completely determines the many-body ground state, which, moreover, from Eq. (8.16) has the energy (relative to the Gross-Pitaevskii ground state)

$$\langle H\rangle_0 = \sum_{q\neq 0} \frac{1}{2}(E_q - \mathcal{E}_q). \tag{8.19}$$

The expression (8.19) is actually linearly divergent as it stands for large q; for the resolution of this difficulty, see below.

The above derivation, which is simply the particle-conserving version of Bogoliubov's original argument, relies on the pairing of the plane-wave states $\mathbf{q}, -\mathbf{q}$, which are not identical but are related by time reversal. With a view to the generalization to inhomogeneous systems (Sec. VIII.D), it is interesting to note that we could equally well have paired atoms in the same state (in this case sine or cosine waves). In fact, an alternative way of writing the ansatz (8.9) for the many-body wave function is

$$\Psi_N = N!^{-1/2}\left(a^{\dagger}{}_0 a_0^{\dagger} - \sum_{q>0} c_q (a_{qc}^{\dagger} a_{qc}^{\dagger} + a_{qs}^{\dagger} a_{qs}^{\dagger})\right)^{N/2} |\mathrm{vac}\rangle, \tag{8.20}$$

where $a_{q,s}^{\dagger}$ and $a_{q,c}^{\dagger}$ create particles in sine and cosine states; e.g., the normalized amplitude of $a_{q,c}^{\dagger}|\mathrm{vac}\rangle$ at $\mathbf{r}$ is $2^{1/2}\cos\mathbf{q}\cdot\mathbf{r}$. The algebra then proceeds exactly as above, the only difference being that if one considers, in the formula analogous to Eq. (8.15), only (say) the sine contribution, the normalization factor is $(1-|c_q|^2)^{1/4}$ rather than $(1-|c_q|^2)^{1/2}$. However, Eq. (8.16) and all subsequent formulas follow unchanged, with the sum over (all) $\mathbf{q}$ replaced by a sum over the positive half-space. The coefficients c_q are numerically equal to those in Eq. (8.9), and, needless to say, the results of Sec. III.C are unaffected.

C. Properties of the Bogoliubov ground state: elementary excitations

Once one has the correct form (8.17) of the coefficients c_q in the many-body ground state (8.9), the calculation of the correlations and the elementary excitations is straightforward and the algebra involved is closely parallel to that encountered in the "textbook" (particle-nonconserving) approach (see, for example, Huang, 1987, Chap. 13); I therefore simply quote the results below without derivation.

[*Note added in proof.* At a very late stage in the processing of this manuscript, I have realized that because of ambiguities in the precise definition of the "Gross-Pitaevskii" state (cf. footnote 18), both the (counterintuitive) sign of the right-hand side of Eq. (8.23) and the precise interpretation of Eq. (8.24) deserve considerably more detailed discussion than given here. (For some of the issues involved, see e.g., Cherny and Shanenko, 2000.) I thank Willi Zwerger for correspondence which drew my attention to this.]

(1) The depletion of the Gross-Pitaevskii ground state, that is, the quantity $\zeta \equiv N^{-1}\Sigma_q\langle a_q^{\dagger} a_q\rangle$, is given by the formula

$$\zeta = \frac{8}{3\sqrt{\pi}}(n_0 a_s^3)^{1/2}. \tag{8.21}$$

Since in published experiments on the alkali gases the right-hand side of Eq. (8.21) has never been much greater than 0.01, it is for most purposes an excellent approximation to ignore the depletion, i.e., set $n_0 = n$.

(2) In evaluating $\langle H_0\rangle$ one must beware of double-counting that part of the two-particle interaction energy that has already been taken into account in defining the s-wave scattering length (see Sec. IV.C). The result of this consideration is to subtract from the summation in Eq. (8.19) a term $-n_0^2 U_0^2/2\epsilon_q$, after which the sum is convergent and equal to the expression

$$\langle H\rangle_0 = \frac{64}{15\sqrt{\pi}} N(n_0 U_0)\cdot(n_0 a_s^3)^{1/2}. \tag{8.22}$$

Thus the correction (8.19) to the Gross-Pitaevskii ground-state energy is a fraction of order the depletion ζ of the latter, and thus again negligible in the alkali gases under most current conditions.

(3) The correction to the two-particle correlation $\langle\rho(\mathbf{r})\rho(\mathbf{r}')\rangle \sim |\Psi(r_{ij}\overset{\sim}{\rightarrow} 0)|^2$ also involves a subtraction to avoid double-counting the single-pair effects. Once this is done, the result is

$$\frac{\delta\langle\rho(\mathbf{r})\rho(\mathbf{r}')\rangle}{n_0^2} = -\mathrm{const}(n_0 a_s^3)^{1/2} F(|\mathbf{r}-\mathbf{r}'|/\xi), \tag{8.23}$$

where $F(x)$ tends to 1 for $x\rightarrow 0$ and to zero for $x\rightarrow\infty$. Thus the quantity $|\Psi(r_{ij}\overset{\sim}{\rightarrow} 0)|^2$ is reduced

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[52] To obtain Eq. (8.13) we replaced matrix elements such as $\sqrt{N_0(N_0+1)}$ by N_0. Note that the sum over q now goes over *all* nonzero q.

by a factor of order ζ from its Gross-Pitaevskii value $n(\approx n_0)$ and the effect on the two-particle wave function extends out to a distance of the order of the healing length ξ, as anticipated.

(4) Consider the operator α_q^+ defined by

$$\alpha_q^\dagger \equiv N_0^{-1/2}(u_q a_q^\dagger a_0 + v_q a_0^\dagger a_{-q}), \tag{8.24}$$

$$u_q \equiv \cosh\theta_q, \quad v_q \equiv \sinh\theta_q, \quad (\tanh\theta_q \equiv c_q). \tag{8.25}$$

It may be verified by direct calculation that when applied to the ground state (8.15) [with the c_q given their ground state values (8.25)], α_q^+ generates an excited state with momentum $\hbar\mathbf{q}$ and energy E_q given by Eq. (8.15), while its Hermitian conjugate α_q gives zero. Consequently, for weak excitation the Hamiltonian can be written, relative to the Bogoliubov ground-state value (8.19), in the simple form (Bogoliubov, 1946)

$$\hat{H} = \sum_q E_q \alpha_q^\dagger \alpha_q . \tag{8.26}$$

In the particle-nonconserving approach the quantities $N_0^{-1/2} a_0, N_0^{-1/2} a_0^\dagger$ are commonly replaced by 1.

(5) Finally, consider the superfluid density $\rho_s(0)$ (see Sec. VI). This quantity is no longer simply related to the condensate number N_o; in fact, inspection of the arguments of Sec. VI.C indicates that since, in the Hess-Fairbank effect in a cylindrical geometry for small but finite ω, the condensate remains in its original (s) state and the virtual Bogoliubov excitations are created out of it with zero total (angular) momentum, the latter contribute nothing to the circulating current, which remains zero. If so, then according to the definition in Sec. VI the superfluid fraction ρ_s/ρ should remain unity even though N_o is no longer equal to N. This result is in fact correct, not only within the Bogoliubov approximation but for arbitrary interaction strength, provided only that perturbation theory starting from the free Bose gas converges (Gavoret and Nozières, 1964; see also Leggett, 1998).

At finite but low temperature $[T \equiv (k_B\beta)^{-1} \ll T_c]$ the condensate is still not much depleted and the number $\langle n_q\rangle \equiv \langle \alpha_q^\dagger \alpha_q\rangle$ of Bogoliubov quasiparticles is given by the Bose distribution with E_q given by Eq. (8.15),

$$\langle n_q\rangle = [\exp(\beta E_q) - 1]^{-1}, \tag{8.27}$$

and a famous argument due to Landau (see Huang, 1987, Chap. 13) gives for the normal density $\rho_n(T) \equiv \rho - \rho_s(T)$

$$\rho_n(T) = \frac{1}{3}\sum_q (\hbar q)^2 (dn_q/dE_q). \tag{8.28}$$

For $T \ll nU_o$ this expression is proportional to T^4, while for $nU_o \ll T \ll T_c$ it has the same temperature dependence as $(1 - N_o/N)$, namely $T^{3/2}$. For $T \sim T_c$ the depletion is substantial and the theory becomes more complicated.

D. The inhomogeneous case

The case of a system moving in a spatially varying potential is considerably more complicated, because (a) there is no *a priori* choice for the condensate wave function $\chi_0(\mathbf{r})$ and one cannot assume *a priori* that it will retain its original (Gross-Pitaevskii-level) form in the presence of pairing, and (b) there is in general no simple analog of the orthogonality of the states $\mathbf{k}$ and $-\mathbf{k}$ to one another and to 0. As a result of (a), the class of wave functions for the many-body system that is considered in the Bogoliubov approximation is actually a subclass of the general class (8.1) of paired states, and thus may not correspond to the absolute minimum of the energy within this class; however, this effect may be shown to be of higher order in na_s^3 than the $(na_s^3)^{1/2}$-level effects considered in the Bogoliubov approximation and will therefore not be discussed here.

As regards point (b), it is important to realize[53] that despite those complications the many-body ground state can still be written[54] in a form that is the obvious generalization of Eq. (8.17), namely,

$$\Psi_N = (N!)^{-1/2}\left(a_o^\dagger a_o^\dagger - \sum_m \frac{1}{2} c_m a_m^\dagger a_m^\dagger\right)^{N/2} |\mathrm{vac}\rangle, \tag{8.29}$$

where the single-particle states m are orthogonal to one another and to the state 0, and, if one were interested in the ground-state energy and the structure of Ψ_N, one could proceed by a generalized version of the argument of Sec. VIII.B.[55] However, it turns out that in general there is no simple relationship between the basis vectors m appearing in Eq. (8.29) and the elementary excitations of the system, and an alternative approach is therefore standard in the literature. For the details of the derivation I refer the reader to Fetter (1999) and merely quote the principal results.

Relaxing (for the only time in this review) our insistence on exact particle number conservation,[56] we write the Bose destruction operator in the form $\hat{\psi}(\mathbf{r}) = \hat{a}_0\chi_0(\mathbf{r}) + \hat{\varphi}(\mathbf{r})$, expand the Hamiltonian up to second order in $\hat{\varphi}(\mathbf{r})$, and treat the quantity $\hat{a}_0\hat{a}_0$ as a c number with a value equal to N_0. In this way we obtain an effective Hamiltonian that is bilinear in $\hat{\varphi}$ and $\hat{\varphi}^\dagger$ and of the general form

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[53] To my knowledge, the first place in the literature where this is (implicitly) pointed out is a paper by Fetter (1972), which is probably less well known in the BEC community than it deserves to be.

[54] Provided it is real, which will be true if the Hamiltonian is invariant under time reversal.

[55] I hope to discuss this question further elsewhere.

[56] For explicitly number-conserving formulations of the ensuing argument and that of Sec. VIII.E, see Gardiner (1996) or Castin and Dum (1997).

$$\hat{H}=\int d\mathbf{r}\,\hat{\varphi}^{\dagger}(\mathbf{r})\left\{-\frac{\hbar^2}{2m}\nabla^2+V_{ext}(\mathbf{r})+2N_0|\chi_0(\mathbf{r})|^2\right\}\hat{\varphi}(\mathbf{r})+(N_0U_0[\chi_0(\mathbf{r})]^2\hat{\varphi}^{\dagger}(\mathbf{r})\hat{\varphi}^{\dagger}(\mathbf{r})+\mathrm{H.c.}).\tag{8.30}$$

One then shows that the expression (8.30) can be diagonalized (and minimized) by the substitution

$$\hat{\varphi}(r)=\sum_j\,[\alpha_j u_j(\mathbf{r})+\alpha_j^{\dagger}v_j(\mathbf{r})]\tag{8.31}$$

where the functions $u_j(\mathbf{r}), v_j(\mathbf{r})$ satisfy the celebrated Bogoliubov–de Gennes equations

$$\left(-\frac{\hbar^2}{2m}\nabla^2+V_{ext}(\mathbf{r})+2N_0|\chi_0(\mathbf{r})|^2-\mu\right)u_j(\mathbf{r})+N_0U_0\chi_0^2(\mathbf{r})v_j^*(\mathbf{r})=E_ju_j(\mathbf{r}),\tag{8.32a}$$

$$\left(-\frac{\hbar^2}{2m}\nabla^2+V_{ext}(\mathbf{r})+2N_0|\chi_0(\mathbf{r})|^2-\mu\right)v_j(\mathbf{r})+N_0U_0[\chi_0^*(\mathbf{r})]^2u_j(\mathbf{r})=-E_jv_j(\mathbf{r}).\tag{8.32b}$$

Equations (8.32) do not specify the normalization of the u_j and v_j, and it is convenient to choose the latter so that

$$\int\,[|u_j(\mathbf{r})|^2-|v_j(\mathbf{r})|^2]dr=1.\tag{8.33}$$

With this choice the operators $\alpha_j,\alpha_j^{\dagger}$ satisfy the standard Bose commutation relations,

$$[\alpha_j,\alpha_k]=[\alpha_j^{\dagger},\alpha_k^{\dagger}]=0,\quad[\alpha_j,\alpha_k^{\dagger}]=\delta_{jk},\tag{8.34}$$

and the effective Hamiltonian takes the form

$$\hat{H}=\sum_j\,E_j\alpha_j^{\dagger}\alpha_j+E_0,\tag{8.35}$$

$$E_0=-\sum_j\,E_j\int\,|v_j(r)|^2\,dr.\tag{8.36}$$

The u_j's and v_j's satisfy the orthogonality properties [with the normalization (8.33)]

$$\int\,d\mathbf{r}[u_j^*(\mathbf{r})u_k(\mathbf{r})-v_j^*(\mathbf{r})v_k(\mathbf{r})]=\delta_{jk},\tag{8.37a}$$

$$\int\,d\mathbf{r}[u_j^*(\mathbf{r})v_k(\mathbf{r})-u_k^*(\mathbf{r})v_j(\mathbf{r})]=0,\tag{8.37b}$$

$$\int\,d\mathbf{r}[u_j(\mathbf{r})\chi_0(\mathbf{r})-v_j\chi_0^*(\mathbf{r})]=0.\tag{8.37c}$$

Note that in general a given u_j is not orthogonal to the corresponding v_j, nor are either of them separately to χ_0. However, there are many cases of practical interest in which this is likely to be true to a good approximation; for example, if $\chi_0(\mathbf{r})$ is slowly varying in the semiclassical limit one can choose u and v to have the approximate forms

$$u_j(\mathbf{r})\sim A_j(\mathbf{r})\exp\left(i\int\,k_j(\mathbf{r})d\mathbf{r}\right),\tag{8.38a}$$

$$v_j(\mathbf{r})\sim B_j(\mathbf{r})\exp\left(-i\int\,k_j(\mathbf{r})d\mathbf{r}\right),\tag{8.38b}$$

where the functions A_j, B_j, and k_j are slowly varying functions of $\mathbf{r}$, and the fast oscillation of the phase then means that u_j and v_j are indeed approximately orthogonal to one another and to the slowly varying function $\chi_0(\mathbf{r})$.

E. Time-dependent Bogoliubov–de Gennes equations: connection with the time-dependent Gross-Pitaevskii equation

In accordance with the considerations of Sec. VIII.B, it is convenient at this stage to redefine the Bogoliubov quasiparticle operators α_j^{+} [currently defined simply by the inversion of Eq. (8.31) and its Hermitian conjugate] so as to make them explicitly particle conserving:

$$\alpha_j^{\dagger}\equiv N_0^{-1/2}\left(a_0\int\,d\mathbf{r}\;u_j(\mathbf{r})\hat{\varphi}^{\dagger}(\mathbf{r})+a_0^{+}\int\,d\mathbf{r}\;v_j(\mathbf{r})\hat{\varphi}(\mathbf{r})\right).\tag{8.39}$$

According to Eq. (8.35), states of the general form (up to normalization)

$$\prod_j\,(\alpha_j^{\dagger})^{n_j}|0\rangle,\tag{8.40}$$

where $|0\rangle$ is the Bogoliubov ground state, are energy eigenstates and thus time independent. However, superpositions of such states will in general have a nontrivial time dependence. In particular, consider a linear superposition of the ground state and a small admixture of different states each containing a single quasiparticle of index j. The time-dependent wave function has the general form

$$\Psi_N(t)=\lambda^{-1/2}\left(1+\sum_j\,\epsilon_j\alpha_j^{\dagger}e^{-iE_jt/\hbar}\right)|0\rangle,\tag{8.41}$$

$$\lambda\equiv1+\sum_j\,|\epsilon_j|^2,\quad(\epsilon_j\ll1,\forall j).\tag{8.42}$$

On the other hand, let us go back to the time-dependent Gross-Pitaevskii equation (5.13), which we recall describes (in the case $N_0=\mathrm{const}$) the evolution of the condensate wave function $\chi_0(\mathbf{r}t)$. As we saw in Sec. V.C, if we linearize this equation around the static Gross-Pitaveskii ground state, we find that we get Eq. (5.16), with $\Psi_0(rt)\equiv\exp-i\mu t/\hbar\cdot\Psi_0(\mathbf{r})$, where $\Psi_o(r)\equiv\sqrt{N_o}\chi_o(r)$ is the ground-state form of the order parameter. But it is now a straightforward exercise (see, for example, Castin and Dum, 1998; Dalfovo *et al.*, 1999) to show that quite generally Eq. (5.16) is diagonalized by expanding $\delta\Psi(\mathbf{r}t)$ and $\delta\Psi^*(\mathbf{r}t)$, respectively, in terms of the Bogoliubov functions $u_j(\mathbf{r}), v_j(\mathbf{r})$. In fact,

$$\delta\Psi(\mathbf{r}t)=\sum_j\,\tilde{\epsilon}_j[u_j(\mathbf{r})e^{-iE_jt/\hbar}+v_j^*(\mathbf{r})e^{iE_jt/\hbar}],\tag{8.43}$$

suggesting a close relation with Eq. (8.41). [Equations (5.19) and (5.20) correspond to the special case of Eq. (8.42) with only one pair u_j, v_j nonzero.] In fact, if on the wave function (8.41) we evaluate the quantity $\langle \varphi^\dagger(\mathbf{r}) a_0\rangle(t)$ [where $\varphi^\dagger(\mathbf{r})$ is the part of the field operator $\psi^\dagger(r)$ orthogonal to χ_0], we find an expression identical to Eq. (8.43) (with $\epsilon_j \to \tilde{\epsilon}_j$; Castin and Dum, 1998). Thus *there is a one-one correspondence between the single-quasiparticle Bogoliubov eigenstates and the small oscillations of the condensate*. [In the free-space case we could already see this by a comparison of Eqs. (5.23) and (8.18).]

This correspondence should not surprise us: it is a characteristic feature of systems that are in some sense "quasiclassical." Consider, for example, our old friend the simple harmonic oscillator. We can do one of two things: (a) starting from a classical-approximation ground state, $\psi_0(x) \sim \delta(x)$, we can replace the argument x by $x - x_0(t)$, where $x_0(t)$ satisfies the classical equation of motion with a small amplitude [much less than $(\hbar/m\omega_0)^{1/2}$]; (b) we can start from the true quantum-mechanical ground state $\psi_0(x)$ and mix in a small amount of the first excited state $\psi_1(x)$. With a suitable correspondence of the parameters, these two procedures, which are the analogs of Eqs. (5.13) and (8.41), respectively, give precisely the same value for the physical observable $\langle x(t)\rangle$ [namely, $A\cos(\omega t)$]. However, it is clear that they correspond to quite different assumptions about the actual form of the wave functions. In the same way, despite the coincidence of their predictions for the quantity $\langle \varphi^\dagger(\mathbf{r}) a_0\rangle$, the *ansätze* (5.13) and (8.41) correspond to totally different assumptions about the actual many-body wave function (and hence different predictions for other possibly observable quantities).

The above discussion refers to small disturbances around the ground state. The question of the application of the Bogoliubov approximation to situations in which the condensate wave function is itself strongly time dependent is a good deal more delicate, and for the reasons sketched in Sec. IX.E, I shall not attempt to discuss it here.

F. The multicomponent case

In view of the weight given in the first seven sections of this review to the case of several co-existing hyperfine species, it seems appropriate to sketch very briefly the generalization of the considerations of the present section to this case. In fact, this generalization is rather obvious: one simply starts from the Hamiltonian

$$\hat{H} = \sum_{\alpha\beta} \int d\mathbf{r}\, \psi^\dagger_\alpha(\mathbf{r}) \left(-\delta_{\alpha\beta} \frac{\hbar^2}{2m} + V^{(ext)}_{\alpha\beta}(\mathbf{r}) \right) \psi_\beta(\mathbf{r}) \tag{8.44}$$

$$+ \frac{1}{2} \sum_{\alpha\beta\gamma\delta} U_{\alpha\beta\gamma\delta} \int \psi^\dagger_\alpha(\mathbf{r}) \psi^\dagger_\beta(\mathbf{r}) \psi_\gamma(\mathbf{r}) \psi_\delta(\mathbf{r})\, d\mathbf{r} \tag{8.45}$$

and expands about the Gross-Pitaevskii solution discussed in Sec. V.D, similarly to what is done in Sec. VIII.D:

$$\hat{\psi}_\alpha(\mathbf{r}) \to \Psi_\alpha(\mathbf{r}) + \hat{\varphi}_\alpha(\mathbf{r}). \tag{8.46}$$

Note that when we do this, the terms of the form, for example,

$$\Psi^*_\alpha(\mathbf{r}) \Psi^*_\beta(\mathbf{r}) \hat{\varphi}_\beta(\mathbf{r}) \hat{\varphi}_\alpha(\mathbf{r}) \tag{8.47}$$

contain *inter alia* the zero-temperature momentum-exchange contributions mentioned at the end of Sec. V.D.

Of course, if we are interested only in obtaining the elementary excitation spectrum, it is probably easier simply to linearize the time-dependent Gross-Pitaevskii equation (5.35) around the ground state (since we expect that the correspondence between the solutions of this equation and the elementary excitations will go through just as in the spinless case discussed in the last subsection). This is done for example by Ho (1998) and Ohmi and Machida (1998). Discussion of the Bogoliubov theory as such for the multicomponent case has, to the best of my knowledge, been limited to the spatially uniform case (Colson and Fetter, 1978; Huang and Gou, 1999).

IX. FURTHER TOPICS

In this section I very briefly list and comment on a number of topics in the theory of the BEC alkali gases that I have had to omit from the main body of this review, either for sheer lack of space or because I believe the theory is still in a state of flux and therefore feel unable to say anything definitive. The list is not complete, and in particular does not include some important topics, such as the collective excitations of a gas in a harmonic trap, which are extensively discussed in the review of Dalfovo *et al.* (1999; see also Griffin, 2000).

A. Attractive interactions

For some systems, in particular ^{7}Li and ^{85}Rb in low magnetic fields, the s-wave scattering length is negative and thus, by the arguments of Sec. IV, the effective interatomic interaction is attractive. Under these conditions it is believed that the system will be unstable against collapse in real space not only in free space but in a harmonic trap provided that the total number of atoms exceeds a critical value (see Dalfovo *et al.*, 1999, Sec. III.C); this seems consistent with existing experiments on ^{7}Li (Bradley *et al.*, 1997) and on ^{85}Rb (Cornish *et al.*, 2000). However, the kinetics of the collapse process and the nature of the final state are controversial. See, for a theoretical consideration, Kagan *et al.* (1998) and Sackett *et al.* (1998).

B. Optical properties

Most of the properties of the BEC alkali gases that are associated with genuinely "optical" transitions (i.e., visible-wavelength, as distinct from the microwave transitions discussed in Sec. VII.D) are believed to be sensitive primarily to the behavior of the local atomic density, and therefore do not require separate consideration. However, we have already seen one exception (Sec. IV.F). A second involves the phenomenon of super-radiance (see Inouye *et al.*, 1999). There may be other phenomena associated with spontaneous emission, which as we have seen is usually totally negligible for microwave transitions but need not be so in the optical regime. In this context some intriguing proposals related to the considerations of Sec. VII.E have been made (Javanainen, 1996); to date there has been no experimental realization.

C. Coexistence of three hyperfine species

Under very special circumstances it is possible to tune the parameters in a trap so that not only can three or more different hyperfine species coexist in it (Stenger *et al.*, 1998a) but collisions of the type $|1\rangle+|-1\rangle\rightarrow|0\rangle+|0\rangle$, in which the initial and final hyperfine states are different, can exactly or approximately conserve energy. Law *et al.* (1998) pointed out that in the case of exact degeneracy the ground state need not necessarily be of the simple Gross-Pitaevskii type but could represent a sort of spatially extended pseudomolecule, in which pairs of atoms condense into a state with, for example, total spin zero but no definite single-atom spin. However, it was subsequently pointed out by Ho and Yip (2000) that this kind of state is extremely fragile and that even tiny perturbations, such as magnetic field gradients, would be likely to restabilize the Gross-Pitaevskii ground state. This is currently a very active area of discussion.

D. The ‘‘atom laser’’

While the experiment of Andrews *et al.* (1997) demonstrates that it is certainly possible to produce two beams of atoms that either have a definite relative phase or acquire one on measurement, there has been to date no realization of the precise atomic analog of an optical laser, that is, roughly speaking, a continuous-output beam with a well-defined direction, frequency, intensity, and phase. Many theoretical papers have been devoted to the design of such an atom laser and an analysis of its likely properties; for an up-to-date review, see Ballagh and Savage (2000). It should be noted that the discussion of the phase coherence properties of an atom laser does not require us to introduce the concept of absolute phase (though this is often done in the literature), any more than does the discussion of, for instance, weak-localization effects in solids in the context of the simple one-electron Schrödinger equation; in each case it is the relative phase at different times that is at issue. The points raised in these discussions have much in common with the problem of diffusion of relative phase discussed in Sec. VII.D, and are also closely connected with the next issue.

E. Kinetics, damping, relaxation, etc.

Probably the most glaring omission in the main body of this review has been any discussion of the strongly nonequilibrium dynamics of a Bose-Einstein condensate (except in the special case of the two-state system discussed in Secs. VII.D and VII.E); this despite the fact that this problem is ubiquitous in the interpretation of experimental work (e.g., on the kinetics of the condensation process, the damping of collective excitations, and the decay of vortex states). The reason for the omission is partly sheer lack of space, but partly also that despite a proliferation of theoretical work in this area in the last four years, I still do not feel that the situation is entirely clear. The problem is not just one of uncertainty about how well particular approximation schemes work in practice for particular experimental setups; there also seem to me to be major conceptual issues that are not completely resolved. One particularly glaring issue is how far it is necessary to maintain the conceptual distinction between a situation in which one has complete or nearly complete Bose condensation but the state is highly chaotic and thus fluctuates randomly from run to run, and one in which there is genuinely no condensation. In neither case does the single-particle density matrix, as calculated by the standard techniques, possess an eigenvalue of order N (in the first case because it essentially predicts the average behavior over runs), and it is therefore tempting to assume that in practice the distinction is meaningless; however, the analysis of the MIT interference experiments shows that in that context an analysis based on the single-particle density matrix can be highly misleading (Javanainen and Yoo, 1996; see also Hegstrom, 1998). This issue is rendered increasingly urgent by the increasing popularity in the BEC field of the so-called ‘‘phase-space technique,’’ in which the density matrix of an arbitrary initial state is expressed as a sort of pseudomixture of Gross-Pitaevskii-type states, each individually possessing BEC but with wildly varying condensate wave functions, the time evolution of the latter calculated, and the results put together to describe the behavior of the real system (see Steel *et al.*, 1999, and for an early application of similar ideas to the kinetics of condensation, Kagan *et al.*, 1994). My suspicion is that, as so often happens in physics, we are dealing here with a trick that is extremely computationally convenient and gives physically correct results provided our measurements are in some sense sufficiently coarse grained, but may be subtly misleading under special circumstances. However, I feel at present unable to say anything clearly on this topic, and thus in accordance with the motto on my title page must ‘‘keep silent’’ and merely refer the reader to what I regard as some of the most important recent papers on this general question (as distinct from applications to specific experimental situations): Castin and Dum (1998), Kagan and Svistunov (1998), Lopez-Arias and Smerzi (1998), Drummond and Corney (1999), Steel *et al.* (1999), Stoof (1999), Walser *et al.* (1999), Carusotto *et al.* (2000), and Gardiner and Zoller (2000).

F. Late-breaking developments

The first draft of this review was completed in January 2000, and over the intervening year there have been a number of interesting developments, some but not all of which are mentioned in the main text. Of these developments, probably the one that will most obviously require us to extend the conceptual basis outlined in this review is the attainment of unprecedentedly high values of the "gas parameter" na^3 in experiments conducted close to a Feshbach resonance (Cornish *et al.*, 2000) and the production of diatomic molecules in an alkali-gas condensate by photoassociation (Wynar *et al.*, 2000). These two developments, which from a theoretical standpoint are closely related, pose a major challenge to theory and will very likely require us to go considerably beyond the simple contact-interaction approximation of Sec. IV. For some relevant considerations, see Holland *et al.* (2000) and Heinzen *et al.* (2000) and references cited therein.

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