Spinor Bose-Einstein condensates

Masahito Ueda
Department of Physics, University of Tokyo, Tokyo, Japan

ABSTRACT
Bose-Einstein (BE) condensation is a phenomenon in which a macroscopic number of particles occupy a single-particle state. Once a system undergoes BE condensation, a significant fraction of particles behave in lockstep, leading to a number of spectacular macroscopic quantum phenomena. This article delineates fundamental aspects of BE condensates with an emphasis on spin degrees of freedom. Here the gauge and spin degrees of freedom are coupled to produce a rich variety of spinor superfluidity and topological excitations.

1. Fundamentals of Bose-Einstein condensation

1.1. Scarcity of low-energy states

Broadly speaking, Bose-Einstein (BE) condensation signifies a macroscopic occupation of a single-particle state, be it in thermal equilibrium or out of equilibrium. Once BE condensation occurs, a macroscopic number of particles behave in exactly the same manner, thereby amplifying microscopic quantum effects to be observed in real life. However, this deceptively simple account of BE condensation raises several legitimate questions. For example, what drives a macroscopic number of particles into the same single-particle state? According to a purely energetic point of view, particles fall into the lowest energy state when the temperature is below the single-particle energy-level spacing $\Delta E$ between the ground and the first excited states. If so, the BE transition temperature would be $T_0 \sim \Delta E/k_B \sim \hbar^2/(2mk_B V^{\frac{2}{3}})$, where $\hbar$ is the Planck constant, $m$ is the mass of the particle, $k_B$ is the Boltzmann constant, and $V$ is the volume of the system. Surprisingly, Einstein proved that a system of $N$ ideal bosons in three dimensions undergo BE condensation at a vastly higher temperature $[1]$:

$$ T_c \sim T_0 N^{\frac{2}{3}} = \frac{\hbar^2}{2mk_BT_c}n^\frac{2}{3}, \quad (1) $$

where $n = N/V$ is the particle-number density. This result implies that BE condensation actually occurs when the average interparticle distance $d \sim n^{-\frac{1}{3}}$ becomes comparable with the thermal de Broglie length: the coherence length of de Broglie waves:

$$ d \sim \frac{\hbar}{\sqrt{mk_BT_c}}. \quad (2) $$

Below the critical temperature, the de Broglie waves begin to overlap and particles lose their identity. The crucial observation here is that the number of possible configurations of indistinguishable particles is exponentially smaller than that of distinguishable ones. For example, the number of ways to distribute $N$ particles into two boxes is $2^N$ for distinguishable particles and $N + 1$ for indistinguishable ones. Thus, below the critical temperature $T_c$, a significant fraction of particles have no other choice but to condense into the lowest single-particle state. Remarkably, this forced condensation can occur without recourse to interactions. In this sense, BE condensation is a genuinely quantum-statistical phase transition.

It is worthwhile to note that the number of single-particle states below $T_c$ is of the order of $N^\frac{2}{3} \sim 10^{14}$ for bulk superfluids and $N^\frac{2}{3} \sim 10^4$ for atomic-gas BE condensates. Considering this vast number of single-particle states below $k_B T_c$, one might well wonder why BE condensation should occur in just one state rather than many. The answer to this question is subtle and two different mechanisms to be discussed below are considered to make crucial contributions to the condensation into a single-particle state.
1.2. Multiparticle interference and bosonic stimulation

Let \( \Psi(\xi_1, \ldots, \xi_N) \) be a solution to the Schrödinger equation of \( N \) particles, where \( \xi_i \) is the label specifying the state of the \( i \)th particle. Since the many-body wave function \( \Psi \) of bosons must be symmetric under exchange of any two particles, we have

\[
\Psi(\xi_1, \ldots, \xi_N) = \frac{1}{\sqrt{N!}} \sum_{\sigma \in S_N} \Phi(\xi_{\sigma(1)}, \ldots, \xi_{\sigma(N)}),
\]

where \( \sigma \) is an element of the symmetry group \( S_N \) on a set \( \{1, \ldots, N\} \). Taking the absolute square of Equation (3), we have \( N! \) diagonal elements and \( N!(N! - 1) \) off-diagonal elements. Thus

\[
|\Psi(\xi, \ldots, \xi)|^2 = N! |\Phi(\xi, \ldots, \xi)|^2,
\]

which implies that the probability of \( N \) bosons to be found in the same single-particle state \( \xi \) is by a factor of \( N! \) larger than that of distinguishable particles. This effect, known as bosonic stimulation, is a consequence of multiparticle interference and lends strong support for a macroscopic occupation of a single-particle state. In fact, as the temperature is lowered and the thermal de Broglie length increases, an increasing number of particles can undergo multiparticle interference, leading to an eventual condensation into a single-particle state.

1.3. Role of repulsive interactions

Once a macroscopic number of particles undergo BE condensation, the repulsive interparticle interaction plays a key role in stabilizing a single BE condensate against fragmentation. To see this, let us consider a system of bosons interacting via a contact interaction:

\[
V = g \sum_{p \neq q} a_p^\dagger a_q^\dagger a_{p+q} a_{p-q},
\]

where \( g \) is the strength of the interaction and \( a_p^\dagger \) \((a_p)\) is the creation (annihilation) operator of a boson with momentum \( p \). Suppose now that \( N_0 \) and \( N_1 \) bosons undergo BE condensation in the zero momentum state and a nonzero momentum state, respectively, where \( N_0 + N_1 = N \) is the total number of bosons. Then the state of the system is \( |N_0, N_1\rangle \) and the expectation value of the interaction energy (5) is given by

\[
V = g[N_0(N_0 - 1) + N_1(N_1 - 1) + 4N_0N_1]
\]

\[
= g[N(N - 1) + 2N_0N_1].
\]

If the interaction is repulsive \((g > 0)\), the system costs an extensive Fock exchange energy \( 2gN_0N_1 \) compared with the case in which a BE condensate occupies only a single momentum state. Therefore a BE condensate with more than one macroscopically occupied state, which is called a fragmented condensate \([2]\), is energetically unfavorable.

Repulsive interactions also stabilize a single condensate against proliferation of single-particle excitations. Suppose that there is a single BE condensate of \( N_0(\geq 1) \) bosons. Then up to terms of the order of \( N_0 \), Equation (5) becomes

\[
V \simeq gM(N - 1) + g \sum_{q \neq 0} (2a_q^\dagger a_0^\dagger a_q + a_q^2 + a_{-q}^\dagger a_q^\dagger + a_0^\dagger a_q a_{-q}),
\]

where the second term on the right-hand side is the Fock exchange interaction between the BE condensate and single-particle excitations. The positive definiteness of this term tends to suppress single-particle excitations and this tendency is greater for larger \( N_0 \). The last two terms in Equation (7) are unique to BE condensed systems; they describe processes in which two BE condensed atoms collide to produce two particles with wave numbers \( q \) and \(-q\) and its reversed process. These pair creation and annihilation are phase-locked to a BE condensate and elementary excitations therefrom, which are called Bogoliubov quasiparticles, are therefore coherent and collective.

1.4. Off-diagonal long-range order

Suppose now that \( N_0 \) bosons share the same single-particle state \( \psi_0(\mathbf{r}) \). If this is the only macroscopically occupied state, \( N_0 \) should be the largest eigenvalue of the single-particle density matrix \( \rho(\mathbf{r}, \mathbf{r}') \) and \( \psi_0(\mathbf{r}) \) is the corresponding eigenfunction. Then the spectral decomposition of \( \rho(\mathbf{r}, \mathbf{r}') \) can be made as

\[
\rho(\mathbf{r}, \mathbf{r}') = N_0 \psi_0^\dagger(\mathbf{r}) \psi_0(\mathbf{r}') + \sum_i n_i \phi_i^\dagger(\mathbf{r}) \phi_i(\mathbf{r}'),
\]

where \( n_i \)'s are the other eigenvalues which are of the order of 1 and \( \phi_i \)'s are the corresponding eigenfunctions.

To understand the physical meaning of this result, let us recall that \( \rho(\mathbf{r}, \mathbf{r}') \) can be expressed in terms of the field operator \( \hat{\psi}(\mathbf{r}) \) as [3]

\[
\rho(\mathbf{r}, \mathbf{r}') = \langle \Psi | \hat{\psi}_0^\dagger(\mathbf{r}) \hat{\psi}(\mathbf{r}') | \Psi \rangle,
\]

where \( |\Psi\rangle \) denotes the many-body state of the system; if the system is in a mixed state, the right-hand side should be replaced by an appropriate quantum-statistical average. The right-hand side of Equation (9) can be interpreted as the transition amplitude that the system returns to the same state after one particle is removed at \( \mathbf{r}' \) and another added at \( \mathbf{r} \). The fact that \( \rho(\mathbf{r}, \mathbf{r}') \) remains to be of the order of \( N_0 \) for a large \( |\mathbf{r} - \mathbf{r}'| \) implies the presence of a long-range quantum-mechanical order since a
classical system would never return to the original state unless \( \mathbf{r} = \mathbf{r}' \). If one regards \( \rho(\mathbf{r}, \mathbf{r}') \) as a matrix element, it is off-diagonal for \( \mathbf{r} \neq \mathbf{r}' \). It follows from Equation (8) that a BE condensate exhibits an off-diagonal long-range order (ODLRO) since Equation (8) remains nonvanishing in the limit of \( |\mathbf{r} - \mathbf{r}'| \to \infty \), and the quantity \( \Psi(\mathbf{r}) = \sqrt{N_0}\psi(\mathbf{r}) \) plays the role of the order parameter of a BE condensate.

The possibility of a particle being transported over a long distance without changing the quantum-mechanical state of the system is reminiscent of superfluidity. While BE condensation and superfluidity occur simultaneously in many cases, they are neither necessary nor sufficient to each other. In fact, BE condensation occurs without the help of interactions [1], whereas superfluidity needs repulsive interaction for its stability. Superfluidity occurs in two dimensions via the Berezinskii-Kosterlitz-Thouless transition without accompanying BE condensation [4,5].

Writing the complex order parameter as \( \psi(\mathbf{r}) = |\psi(\mathbf{r})|e^{\text{i}\theta(\mathbf{r})} \), we find that the gradient of the phase gives the superfluid velocity:

\[
v_s = \frac{\hbar}{m} \nabla \theta. \tag{10}
\]

The vorticity, which is given by the rotation of \( v_s \), vanishes identically, and therefore a BE condensate of spinless bosons, which is called a scalar BE condensate, is irrotational. An important implication of the complex order parameter is that the superfluid phase (more precisely, the phase difference or the gradient of the phase) serves as a thermodynamic variable that is needed to describe thermodynamic properties of a superfluid system. It is the phase difference between different points that gives rise to an observable effect. The phase difference can be created by exchange of particles between these points without changing the total number of particles. Thus it is the relative rather than absolute U(1) gauge symmetry that is actually broken in a superfluid system.

A quantum-mechanical wave function must be single-valued, so must be the order parameter of a BE condensate. It then follows from Equation (10) that the circulation of the superfluid velocity is quantised in units of \( \hbar/m \) [6]:

\[
\oint \mathbf{v}_s d\mathbf{r} = \frac{\hbar}{m} \times \text{integer}. \tag{11}
\]

2. Spinor interactions

Atoms, in general, have electronic and nuclear spins which are coupled via a hyperfine interaction, and the combined spin–hyperfine spin \( f \) is a good quantum number at temperatures below mK. There is a relatively long-lived spin-1 manifold available for \( ^7\text{Li} \), \( ^{23}\text{Na} \), \( ^{41}\text{K} \), \( ^{87}\text{Rb} \), a spin-2 manifold for \( ^{87}\text{Rb} \) and a spin-3 manifold for \( ^{52}\text{Cr} \) [7,8]. Here the last one is purely electronic since \( ^{52}\text{Cr} \) has no nuclear spin. When the system is placed in a magnetic trap, every atomic spin is polarised along a local magnetic field. However, in an optical potential, the spin degrees of freedom are liberated and develop spin textures caused by spin-exchange interactions.

The fundamental symmetry of interactions of spinful particles is dictated by quantum statistics. The many-body wave function of spin-\( f \) atoms acquires a phase factor of \((-1)^f\) under exchange of two atoms. By the same exchange, the orbital part of the wave function acquires a factor of \((-1)^I\), where \( L \) is the relative orbital angular momentum of the two atoms, and the spin part acquires a factor of \((-1)^{F+2f}\), where \( F \) is the total spin of the two atoms. To be consistent, we must have \((-1)^{2f} = (-1)^L \times (-1)^{F+2f}\). Hence \( L + F \) must be an even integer. At low temperature, s-wave scattering is a dominant scattering process for ultracold atoms, so that \( L = 0 \). The total spin \( F \) of two colliding atoms must therefore be even.

Let us first consider spin-1 identical bosons. Bose symmetry requires that the total spin \( F \) of two colliding bosons be 0 or 2. Let \( P_0 \) and \( P_2 \) be the projection operators for the collision channel into the total spin 0 and 2 sectors. Then we have the completeness relation

\[
P_0 + P_2 = I_1 \otimes I_2, \tag{12}
\]

where \( I_1 \) and \( I_2 \) are the identity matrices for the two particles.1 Let \( f_1 \) and \( f_2 \) be the spin vectors of two bosons. Then

\[
f_1 \cdot f_2 = \frac{1}{2} [(f_1 + f_2)^2 - f_1^2 - f_2^2] = \frac{1}{2} F(F+1)P_F - 2I_1 \otimes I_2, \tag{13}
\]

where \( P_F \) is the projector onto the total spin-\( F \) sector, and \( f_1^2 = f(f+1)I_1 = 2I_1 \) is used. Since \( F(F+1) = 0 \) and \( F = 0 \) and \( F = 2 \), respectively, we have

\[
f_1 \cdot f_2 = 3P_2 - 2I_1 \otimes I_2. \tag{14}
\]

It follows from Equations (12) and (14) that we obtain

\[
P_0 = \frac{1}{3} (I_1 \otimes I_2 - f_1 \cdot f_2), \tag{15}
\]

\[
P_2 = \frac{2}{3} (2I_1 \otimes I_2 + f_1 \cdot f_2).
\]

The interaction Hamiltonian for spin-1 bosons is thus constructed as

\[
V^{(f=1)} = \frac{g_0}{2} P_0 + \frac{g_2}{2} P_2 = \frac{c_0^{(1)}}{2} I_1 \otimes I_2 + \frac{c_1^{(1)}}{2} f_1 \cdot f_2, \tag{16}
\]
where $g_0$ and $g_2$ are the interaction strengths of the total spin-0 and 2 channels and $c_0^{(1)} := (g_0 + 2g_2)/3$ and $c_1^{(1)} := (g_2 - g_0)/3$. These interaction strengths are given in terms of the corresponding $s$-wave scattering lengths $a_0$ and $a_2$ as

$$g_F = \frac{4\pi\hbar^2}{m} a_F (F = 0, 2).$$  \hspace*{2cm} (17)

When all particles in a BE condensate share the same single-particle state $\psi_m(r)$ ($m = 1, 0, -1$), the interaction Hamiltonian (16) gives

$$V^{(f=1)} = \frac{1}{2} \int dr \left( c_0^{(1)} n(r)^2 + c_1^{(1)} f(r)^2 \right),$$  \hspace*{2cm} (18)

where

$$n(r) = \sum_{m=-f}^{f} |\psi_m(r)|^2$$

is the particle-number density, and

$$f_{\alpha}(r) = \sum_{m,n=-f}^{f} \psi_m^*(r)(S_{\alpha})_{mn}\psi_n(r) (\alpha = x, y, z)$$  \hspace*{2cm} (20)

is the $\alpha$ component of the spin-density vector $\mathbf{f}(r)$ with $S_{\alpha}$ being the $\alpha$ component of spin-1 matrices.

We next consider the case of spin-2 bosons. The total spin $F$ of two bosons must be 0, 2 or 4. Let $P_F$ ($F = 0, 2, 4$) be the projector onto the total spin-$F$ sector. Then the completeness relation is

$$P_0 + P_2 + P_4 = I_1 \otimes I_2.$$  \hspace*{2cm} (21)

Similarly to Equation (14), we have

$$\mathbf{f}_1 \cdot \mathbf{f}_2 = \frac{1}{2} \sum_{F=0,2,4} F(F+1)P_F - 6I_1 \otimes I_2$$

$$= 3P_2 + 10P_4 - 6I_1 \otimes I_2.$$  \hspace*{2cm} (22)

From Equations (21) and (22), we obtain

$$P_2 = \frac{4 - \mathbf{f} \cdot \mathbf{f} - 10P_0}{7}, \hspace{1cm} P_4 = \frac{3 + \mathbf{f} \cdot \mathbf{f} + 3P_0}{7}.$$  \hspace*{2cm} (23)

The interaction Hamiltonian for spin-2 bosons is thus given by

$$V^{(f=2)} = \frac{g_0}{2} P_0 + \frac{g_2}{2} P_2 + \frac{g_4}{2} P_4$$

$$= \frac{4g_2 + 3g_4}{14} I_1 \otimes I_2 + \frac{g_4 - g_2}{14} \mathbf{f}_1 \cdot \mathbf{f}_2$$

$$+ \frac{7g_0 - 10g_2 + 3g_4}{14} P_0.$$  \hspace*{2cm} (24)

When all particles in a BE condensate share the same single-particle state $\psi_m(r)$ ($m = 2, 1, 0, -1, -2$), the interaction Hamiltonian (24) leads to

$$V^{(f=2)} = \frac{1}{2} \int dr \left( c_0^{(2)} n(r)^2 + c_1^{(2)} f(r)^2 + c_2^{(2)} |\mathcal{A}(r)|^2 \right),$$  \hspace*{2cm} (25)

where $c_0^{(2)} := (4g_2 + 3g_4)/7$, $c_1^{(2)} := (g_4 - g_2)/7$, $c_2^{(2)} := (7g_0 - 10g_2 + 3g_4)/7$ and $\mathcal{A}(r)$ is the spin-singlet amplitude given by

$$\mathcal{A}(r) = \sum_{m_1,m_2=-2}^{2} \langle F = 0, M_F = 0 | f = 2, m_1; f = 2, m_2 \rangle$$

$$\times \psi_{m_1}(r)\psi_{m_2}(r),$$  \hspace*{2cm} (26)

where $\langle 0,0 | 2, m_1; 2, m_2 \rangle$ is the Clebsch-Gordan coefficient. This can be understood by recalling $P_0 = |F = 0, M_F = 0\rangle\langle F = 0, M_F = 0 |$. Substituting $\langle 0,0 | 2, m_1; 2, m_2 \rangle = \delta_{m_1,-m_2}(-1)^{m_1}/\sqrt{5}$ into Equation (26), we obtain

$$\mathcal{A}(r) = \frac{1}{\sqrt{5}} \sum_{m=-2}^{2} (-1)^{m}\psi_{m}(r)\psi_{-m}(r).$$  \hspace*{2cm} (27)

To prevent the system from collapsing, $c_0^{(f)}$ must be positive. Otherwise, the system can lower its energy by increasing its density to infinity. We therefore assume $c_0^{(f)} > 0$ in the following discussions.

### 3. Spin-1 BE condensates

We first investigate properties of spin-1 BE condensates. For simplicity of discussions, we consider a spatially uniform system in the absence of an external magnetic field. In this case, the kinetic term can be ignored and the properties of the ground state are determined by the interparticle interaction.

It follows from Equation (18) that the magnetism of the ground state is determined by the sign of $c_1^{(1)} = 4\pi\hbar^2(a_2 - a_0)/m$, where $a_2$ ($a_0$) is the scattering length of the total spin-2 (spin-0) collision channel. For $a_2 > a_0$, it is energetically favorable for the spins of colliding bosons to be antiparallel. The ground state is therefore polar (see Section 3.1). For $a_2 < a_0$, the spin parallel configuration is energetically favorable. The ground state is therefore ferromagnetic. A BE condensate of spin-1 $^{87}$Rb atoms is ferromagnetic and a BE condensate of spin-1 $^{23}$Na atoms is polar [7,8].

#### 3.1. Polar phase

When $a_2 > a_0$, the ground-state energy is minimised when $|\mathbf{f}| = 0$. This condition is met by the nonmagnetic polar phase whose standard spinor is given by $\sqrt{m}(0,1,0)^T$, where $T$ denotes the transposition. A general order parameter is obtained by an arbitrary Euler
rotation of the standard spinor followed by the U(1) gauge transformation:

\[
\begin{pmatrix}
\Psi_1 \\
\Psi_0 \\
\Psi_{-1}
\end{pmatrix} = \sqrt{n} e^{i\theta} U(\alpha, \beta, \gamma) \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}
\]

where \(\theta\) is the gauge angle, and \(U(\alpha, \beta, \gamma) := e^{-iS_0}\alpha} e^{-iS_y\beta} e^{-iS_z\gamma}\) is the unitary operator for an Euler rotation with \(\alpha, \beta, \gamma\) being the Euler angles and \(S_y\) and \(S_z\) being the \(y\) and \(z\) components of spin-1 matrices. By letting the Euler angles depend on space, we can spatially vary the direction of the local spin density. As can be seen from Equation (28), the order parameter of the polar phase changes sign upon inversion in spin space about a direction perpendicular to the symmetry axis (i.e. \(\beta \rightarrow \pi - \beta\)). This is why this phase is called polar.

Substituting Equation (28) into the expression of the superfluid velocity

\[
v = \frac{\hbar}{2m} \sum_m [\nabla \Psi_m^* \Psi_m - (\nabla \Psi_m^*) \Psi_m],
\]

we obtain

\[
v^p = \frac{\hbar}{m} \nabla \theta.
\]

This is irrotational (\(\nabla \times \mathbf{v} = 0\)) like a scalar BE condensate. However, unlike the scalar case, the circulation is quantised in units of one half of \(\hbar/m\). To understand this, let us take the cylindrical coordinates \((r, \phi, z)\) and set \(\theta = \alpha = \phi/2\) and \(\beta = \pi/2\). Then Equation (28) becomes

\[
\begin{pmatrix}
\Psi_1 \\
\Psi_0 \\
\Psi_{-1}
\end{pmatrix} = \sqrt{n} e^{i\phi} \begin{pmatrix} e^{-i\phi/2} \\ 0 \\ e^{i\phi/2} \end{pmatrix}.
\]

If we circumnavigate a closed loop around the symmetry axis, \(\phi\) changes by \(2\pi\) and the gauge angle \(\theta = \phi/2\) changes by \(\pi\). Nevertheless, the single-valuedness of the order parameter is met because the spinor part changes its sign due to the change in \(\alpha = \phi/2\) by \(\pi\). This discrete coupling between spin and gauge at \(\theta = \pi\) is called the discrete spin-gauge symmetry. Since the single-valuedness of the order parameter is met by the gauge angle of \(\pi\) which is one half of the usual \(2\pi\), the circulation is quantised in units of \(\hbar/2m\)

\[
\oint \mathbf{v}^p \cdot d\mathbf{r} = \frac{\hbar}{2m} \times \text{integer},
\]

and the polar phase possesses a half-quantum vortex [9] which is also known as an Alice vortex or an Alice string [10]. Figure 1 displays a false-color representation of a half-quantum vortex whose spinor is given in Equation (31). Pairs of half-quantum vortices were created in a spin-1 \(^{23}\text{Na}\) BE condensate [11].

### 3.2. Ferromagnetic phase

When \(a_2 < a_0\), the ground-state energy is minimised when \(|\mathbf{f}| = 1\), and therefore the ground-state phase is ferromagnetic. The standard order parameter of the ferromagnetic phase is \(\sqrt{n}(1, 0, 0)^T\). A general order parameter can be obtained if we rotate it to an arbitrary direction in spin space and perform a gauge transformation by an arbitrary gauge angle \(\theta\):

\[
\begin{pmatrix}
\Psi_1 \\
\Psi_0 \\
\Psi_{-1}
\end{pmatrix} = \sqrt{n} e^{i\theta} U(\alpha, \beta, \gamma) \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}
\]

\[
= \sqrt{n} e^{i(\theta - \gamma)} \begin{pmatrix} e^{-i\alpha} \cos^2 \beta/2 \\ \frac{1}{\sqrt{2}} \sin \beta \\ e^{i\alpha} \sin^2 \beta/2 \end{pmatrix}.
\]

For this spinor, the local spin density is calculated to give

\[
\mathbf{f} = n(\sin \beta \cos \alpha, \sin \beta \sin \alpha, \cos \beta).
\]
Thus $\alpha$ and $\beta$ are the azimuthal and polar angles of the local spin. We note that the gauge angle $\theta$ and the rotation angle $\gamma$ appear as a linear combination in Equation (33). This continuous spin-gauge symmetry implies that if the local spin rotates about its symmetry axis, the system responds to it by flowing a supercurrent. To understand this, let us calculate the superfluid velocity by substituting Equation (33) in Equation (29):

$$\mathbf{v}^F = \frac{\hbar}{m} [\nabla (\theta - \gamma) - \cos \beta \nabla \alpha]. \quad (35)$$

From Equation (35), we have

$$\mathbf{v}^F - \frac{\hbar}{m} (1 - \cos \beta) \nabla \alpha = \frac{\hbar}{m} \nabla (\theta - \gamma - \alpha). \quad (36)$$

Taking the line integral of both sides along a closed loop $C$, we obtain

$$\oint_C \mathbf{v}^F \, d\mathbf{r} - \frac{\hbar}{m} \oint_C (1 - \cos \beta) \nabla \alpha \cdot d\mathbf{r} = \frac{\hbar}{m} \times \text{integer}. \quad (37)$$

The first term on the left-hand side is the circulation of the superfluid velocity along a closed loop $C$. The second term is the contribution from the Berry phase inside $C$. The Berry phase is a geometric phase accumulated in the parameter space of the Hamiltonian when the system undergoes an adiabatical cycle [12,13]. Here the parameter space is spanned by the Euler angles. Equation (37) shows that the difference between the circulation and the Berry-phase contribution is quantised in units of $\hbar/m$ for a ferromagnetic BE condensate.

It follows from Equation (35) that spatial variations of the Euler angles produce a superflow. Due to the last term in Equation (35), however, the superfluid velocity is not irrotational. In fact, taking the rotation of Equation (35), we obtain

$$\nabla \times \mathbf{v}^F = \frac{\hbar}{m} \sin \beta \nabla \beta \times \nabla \alpha. \quad (38)$$

The origin of the nonzero vorticity is a spin texture. The right-hand side can be rewritten in terms of the normalised spin-density vector $\mathbf{\hat{f}} := \mathbf{f}/n$ as

$$\nabla \times \mathbf{v}^F = \frac{\hbar}{2m} \sum_{i,j,k=x,y,z} \epsilon^{ijk} \hat{f}_i \nabla \hat{f}_j \times \nabla \hat{f}_k, \quad (39)$$

where $\epsilon^{ijk}$ is a completely antisymmetric tensor of rank three which takes on 1 for $(i,j,k) = (x,y,z), (y,z,x),(z,x,y)$, $-1$ for $(i,j,k) = (x,z,y), (y,x,z),(z,y,x)$, and 0 otherwise. The relation (39) is known as the Mermin-Ho relation [14]. The Mermin-Ho relation shows that the spin texture – spatial variations of the spin direction – can provide a source of vorticity. In fact, if the spin density does not vary over space, the right-hand side of Equation (39) vanishes. Since continuous variations of the spin density generates vorticity, the associated vortex is nonsingular and coreless. To illustrate this fact, let us consider a situation in which the system is confined in a cylinder of radius $R$ and employ the cylindrical coordinates $(r, \phi, z)$. Since the origin of the gauge angle $\theta$ is arbitrary, we choose it such that $\theta - \gamma = \alpha = \phi$ in Equation (33). Then we have

$$\begin{pmatrix} \Psi_1 \\ \Psi_0 \\ \Psi_{-1} \end{pmatrix} = \sqrt{n(r)} \begin{pmatrix} \cos^2 \beta(r) \\ \frac{\epsilon^{np}}{\sqrt{2}} \sin \beta(r) \\ \epsilon^{np} \sin^2 \frac{\beta(r)}{2} \end{pmatrix}. \quad (40)$$

The expectation value of the spin density is given by

$$\mathbf{f} = n(\sin \beta(r) \cos \phi, \sin \beta(r) \sin \phi, \cos \beta(r)). \quad (41)$$

If we set $\beta(0) = 0$ on the symmetry axis and $\beta(R) = \pi/2$ on the wall of the cylinder, the spin points in the positive $z$ axis on the symmetry axis and flares out toward the cylindrical wall and points perpendicular to the wall on the boundary. This type of spin texture is called the Mermin-Ho vortex [14]. If we take $\beta(R) = \pi$ instead, the spin points downward on the wall. This type of spin texture is called the Anderson-Toulouse vortex [15]. Both of these vortices are coreless and nonsingular, and they have nonzero circulations due to the Berry phase contributed from spin textures. This can be seen by substitution of $\theta - \gamma = \alpha = \phi$ in Equation (36):

$$\mathbf{v}^F = \frac{\hbar}{m} (1 - \cos \beta) \nabla \phi. \quad (42)$$

This shows that the superfluid velocity is purely due to the Berry phase. It follows that

$$\oint_C \mathbf{v}^F \, d\mathbf{r} = \begin{cases} \frac{\hbar}{m} \text{ Mermin–Ho vortex } (\beta = \frac{\pi}{2}) ; \\ \frac{2\hbar}{m} \text{ Anderson–Toulouse vortex } (\beta = \pi). \end{cases} \quad (43)$$

It should be noted that the quantization of circulation discussed here is due to the imposed boundary condition and does not originate from nontrivial topology of the order parameter manifold.

### 3.3. Bose antiferromagnet

When $a_2 > a_0$, antiparallel spin configuration is energetically favorable. Let us examine the ground state for this...
case under the situation in which the system is confined in a tight potential so that the kinetic degrees of freedom is frozen (single-mode approximation). We also assume that the number of particles is even (if it is odd, we should simply add an unpaired boson to the system). Let $A^\dagger$ be the creation operator of a spin-singlet boson pair. It can be constructed as

$$A^\dagger = \sum_{m_1,m_2=-1}^1 \langle F=0,m_F=0 \mid f=1,m_1;f=1,m_2 \rangle \times a_{m_1} a_{m_2}^\dagger,$$

$$= \frac{1}{\sqrt{3}} (a_2^\dagger - a_1^\dagger a_{-1}^\dagger). \quad (44)$$

The many-body state with total spin 0 can be constructed as

$$|S=0\rangle \propto (A^\dagger)^N |\text{vac}\rangle. \quad (45)$$

This is the desired many-body state for a Bose antiferromagnet [16]. Unlike the mean-field counterpart (see Equation (28)), there is no symmetry breaking in the spin sector and all magnetic sublevels are equally populated.

### 3.4. Fragmented BE condensates

In spinor BE condensates, the concept of fragmentation plays an important role. According to Penrose and Onsager [17], the system exhibits BE condensation if the largest eigenvalue of the one-particle reduced density matrix is extensive, i.e. proportional to the size of the system. The number of such extensive eigenvalues is one for most superfluid systems. If there is more than one extensive eigenvalue, the BE condensate is said to be fragmented [18,19].

The three conditions must be met for a fragmented BE condensate to be realised. First, the system must possess an exact symmetry that allows degeneracy between different macroscopically occupied single-particle states. Second, the interaction between the degenerate single-particle states must be attractive to gain the Fock exchange energy. Otherwise, the coexistence of multiple BE condensate costs the Fock exchange energy and a single BE condensate that minimises it would be selected. Third, the system must be mesoscopic to avoid collapse or symmetry breaking into a single condensate.

Classic examples of fragmented BE condensates include a rotating scalar BE condensate with an attractive contact interaction in a harmonic trap [20], and a Bose antiferromagnet [20–22] discussed in Section 3.3, where the interaction in the spin-singlet channel is effectively attractive in the sense that the interaction in the spin-singlet channel is less repulsive than that in the spin-triplet channel.

However, fragmented BE condensates are very fragile against symmetry-breaking perturbations. To understand this, suppose that a BE condensate is fragmented into two states 1 and 2 that are equally populated. This fragmented state can be expressed in terms of a linear superposition of single coherent BE condensates as follows:

$$|\psi(\phi)\rangle := \frac{1}{\sqrt{2^N N!}} (e^{i\phi} c_1^\dagger + e^{-i\phi} c_2^\dagger)^N |\text{vac}\rangle. \quad (47)$$

where $c_1^\dagger$ and $c_2^\dagger$ are the creation operators of bosons in states 1 and 2, respectively. Thus the fragmented state may be interpreted as a superposition state of single coherent BE condensates $|\psi(\phi)\rangle$.

Let us now consider a symmetry-breaking perturbation $V = (t c_1^\dagger c_2^\dagger + t^\ast c_2^\dagger c_1^\dagger)$ which mixes the two states. The expectation value of $V$ over the fragmented BE condensate (46) is zero, whereas that over $|\psi(\phi)\rangle$ is given by $|t|N \cos(2\phi - \delta)$ ($t = |t|e^{i\phi}$), which is minimised at $\phi = (\pi + \delta)/2$. Thus, even an infinitesimal perturbation $V$ (of the order of $1/N$) would break the symmetry over $\phi$ in Equation (46) and drive the fragmented BE condensate into a single coherent BE condensate $|\psi(\phi)\rangle$, where $\phi$ distributes randomly as $t$ varies randomly depending on experimental situations.

Another example is a Bose antiferromagnet discussed in Section 3.3. Here the many-body wave function $|S=0\rangle$ can be expressed as a linear superposition of single coherent BE condensates as

$$|S=0\rangle \propto \int \frac{d\mathbf{n}}{4\pi} (\mathbf{n} \cdot \mathbf{A})^N |\text{vac}\rangle, \quad (48)$$

where $\mathbf{n}$ is a three-dimensional unit vector and

$$A_x := -\frac{a_1 - a_{-1}}{\sqrt{2}}, \quad A_y := i\frac{a_1 + a_{-1}}{\sqrt{2}}, \quad A_z := a_0. \quad (49)$$

We note that the state $(\mathbf{n} \cdot \mathbf{A})^N |\text{vac}\rangle$ describe a polar state whose quantization axis is parallel to $\mathbf{n}$. For this fragmented state, the symmetry-breaking perturbation is a magnetic field that breaks the degeneracy among magnetic sublevels and drives the system into a single BE condensate whose $\mathbf{n}$ aligns with the magnetic field.

A fragmented BE condensate was experimentally realised in a mesoscopic spin-1 $^{23}$Na gas of about 100
atoms [23]. The system was confined in a tight potential so that a single-mode approximation is valid. As an external magnetic field was reduced, the system underwent a transition from an antiferromagnetic configuration \((1/\sqrt{2}, 0, 1/\sqrt{2})\) to an equally populated fragmented state \((1/3, 1/3, 1/3)\) by forming spin-singlet bosonic pairs.

4. Spin-2 BE condensates

The interaction Hamiltonian of a spin-2 BE condensate is given by Equation (25) which involves the particle density \(n\), the spin density \(\mathbf{f}\) and the spin-singlet pair amplitude \(\mathcal{A}\). Compared with the spin-1 case, where the coefficient of the spin-density term alone determines the ground-state phase, the spin-singlet term competes with the spin-density term in determining the magnetism of a spin-2 BE condensate.

When \(c_1^{(2)} < 0\) and \(c_2^{(2)} > 0\), the system minimises its energy for \(|\mathbf{f}| = 2\) and \(|\mathcal{A}| = 0\). The ground-state phase is ferromagnetic and its properties are basically the same as those of the ferromagnetic phase of a spin-1 BE condensate.

When \(c_1^{(2)} > 0\) and \(c_2^{(2)} < 0\), the system minimises its energy by setting \(|\mathbf{f}| = 0\) and maximizing \(|\mathcal{A}|\). This state is sometimes called polar in analogy with the spin-1 case. However, as we see later, the order parameter does not change sign upon inversion in spin space. Therefore this phase should more appropriately be called nematic.

When \(c_1^{(2)} > 0\) and \(c_2^{(2)} > 0\), neither a spin-parallel ferromagnetic nor spin-antiparallel nematic state is energetically favorable, and spin frustration arises. It turns out that three bosons form a spin-singlet trio and trio bosons undergo BE condensation. This phase is called cyclic [20–22].

There is only one relatively long-lived spin-2 BE condensate realised for \(^{87}\)Rb [7,8]. The ground state of this atomic species has not yet been decided but it is believed to be slightly on the nematic side of the phase boundary between the nematic and cyclic phases [24]. We now discuss properties of these two phases.

4.1. Nematic phases

There are two types of nematic phases that are relevant for a spin-2 BE condensate: the uniaxial nematic phase and the biaxial nematic phase. The former possesses one symmetry axis, and the latter has two symmetry axes.

The standard order parameter of the uniaxial nematic phase is \(\xi_0^{UN} = (0, 0, 1, 0, 0)^T\). A general order parameter can be obtained via an Euler rotation \(U(\alpha, \beta, \gamma)\) using spin-2 matrices and multiplying it by the gauge factor

\[
e^{i\theta} [7]:
\]

\[
\begin{pmatrix}
\Psi_2 \\
\Psi_1 \\
\Psi_0 \\
\Psi_{-1} \\
\Psi_{-2}
\end{pmatrix} = \sqrt{n} e^{i\theta} U(\alpha, \beta, \gamma)
\begin{pmatrix}
0 \\
0 \\
0 \\
1 \\
0
\end{pmatrix}
\]

\[
= \frac{\sqrt{6n}}{4} e^{i\theta}
\begin{pmatrix}
e^{-2i\alpha} \sin^2 \beta \\
-e^{-i\alpha} \sin 2\beta \\
\sqrt{\frac{2}{3}} (2 - 3 \sin^2 \beta) \\
e^{i\alpha} \sin 2\beta \\
e^{2i\alpha} \sin^2 \beta
\end{pmatrix}.
\] (50)

Substituting this in Equation (29), we obtain the superfluid velocity as

\[
\mathbf{v}^{UN} = \frac{\hbar}{m} \nabla \theta.
\] (51)

Unlike the spin-1 polar phase, the order parameter (51) does not change sign under inversion in spin space. Therefore the spin degrees of freedom are not coupled with the U(1) gauge and the circulation is quantised in units of the usual \(\hbar/2m\) rather than \(\hbar/2m\) for the spin-1 polar phase (see Equation (32)).

The standard spinor of the biaxial nematic phase is \(\xi_0^{BN} = (1/\sqrt{2}, 0, 0, 0, 1/\sqrt{2})^T\). Unlike the spin-1 case, this state is not connected to the uniaxial nematic state \((0, 0, 1, 0, 0)^T\) by any rotation in spin space because the symmetries of these two states are different. There is only one symmetry axis for a uniaxial nematic state but there are two for a biaxial nematic state. Since two rotations about different axes do not commute in general, the biaxial nematic phase exhibits non-Abelian properties in the collision dynamics of vortices [25].

Whereas \(\xi_0^{UN}\) and \(\xi_0^{BN}\) are not related to each other by any rotation in spin space, these two standard spinors can continuously be connected to each other by a single parameter \(\eta\) as

\[
\Psi^N(\eta) = \left(\frac{\sin \eta}{\sqrt{2}}, 0, \cos \eta, 0, \frac{\sin \eta}{\sqrt{2}}\right)^T.
\] (52)

It can be shown by direct substitution of Equation (52) in Equation (25) that the energy of the system is degenerate with respect to \(\eta\) [26]. Since \(\eta\) is not related to the symmetry of the Hamiltonian, the degeneracy with respect to \(\eta\) does not lead to a conserved current. Furthermore, since this degeneracy is not due to the symmetry of the Hamiltonian, it is lifted by zero-point fluctuations of the Bogoliubov vacuum, which results in a first-order quantum phase transition between the uniaxial nematic phase with \(c_1^{(2)} > 0\) and the biaxial nematic phase for \(c_1^{(2)} < 0\) [27,28]. In high-energy physics, this phenomenon is
known as the vacuum alignment and the mode that connects between the two degenerate vacua is called a quasi-Nambu-Goldstone mode [29].

### 4.2. Cyclic phase

The standard order parameter of the cyclic phase is \( \zeta_0^{\text{cyclic}} = (1/2, 0, -i/\sqrt{2}, 0, 1/2)^T \) which shows neither spin-singlet pair amplitude nor magnetisation, and breaks time-reversal symmetry.

Since there is no spin-singlet pair amplitude, one may wonder how the cyclic phase can be nonmagnetic. Here not two but three bosons form spin-singlet trio and the trio bosons undergo BE condensation [26]. In fact, if we rotate the system about the (1,1,1) axis in spin space through angle \( \pi/3 \) the iso-triplet state is given by \( \sum_{m=-1}^1 |m\rangle \langle m| = I \), where \( I \) is the identity operator. For two particles, the completeness relation reads

\[ I_1 \otimes I_2 = \sum_{m_1=-1}^1 |m_1\rangle \langle m_1| \otimes \sum_{m_2=-1}^1 |m_2\rangle \langle m_2| =: \sum_{m_1, m_2=-1}^1 |m_1, m_2\rangle \langle m_1, m_2|. \]

By operating this completeness relation from the right side of \( P_0 + P_2 \), we have

\[ P_0 + P_2 = \sum_{m_1, m_2} (P_0 + P_2) |m_1, m_2\rangle \langle m_1, m_2|. \]

The total spin of two identical bosons must be either 0 or 2, so that \( P_0 + P_2 \) should act as the identity operator for any spin state of two bosons: \( (P_0 + P_2) |m_1, m_2\rangle = |m_1, m_2\rangle \).
We thus obtain
\[ P_0 + P_2 = \sum_{m_1, m_2 = -1}^{1} |m_1, m_2 \rangle \langle m_1, m_2 | = I_1 \otimes I_2. \]

**Disclosure statement**

No potential conflict of interest was reported by the author.

**Notes on contributor**

*Masahito Ueda* is Professor in the Department of Physics at the University of Tokyo. He obtained his PhD from the University of Tokyo in 1991. After that he worked for six years at NTT Basic Research Laboratories, for six years at Hiroshima University, and then for eight years at Tokyo Institute of Technology, until he joined the University of Tokyo in 2008. He is interested in atomic, molecular and optical physics, and the foundational problems in quantum mechanics, thermodynamics, until he joined the University of Tokyo in 1991. After that he worked for six years at Hiroshima University, and then for eight years at Tokyo Institute of Technology, for six years at Hiroshima University of Tokyo in 1991. After that he worked for six years at Hiroshima University, and then for eight years at Tokyo Institute of Technology, until he joined the University of Tokyo in 2008. He is interested in atomic, molecular and optical physics, and the foundational problems in quantum mechanics, thermodynamics, and machine learning. In particular, he has developed ways to study information thermodynamics and non-Hermitian physics.

**References**

[1] Einstein A. Quantentheorie des einatomigen idealen gases. (Zweite Abhandlung). Akademie-Vorträge: Sitzungsberichte der Preußischen Akademie der Wissenschaften. 1925;1914:245–257.

[2] Nozières P. Some comments on Bose-Einstein condensation. In: Bose-Einstein condensation. Cambridge: Cambridge University Press; 1995.

[3] Ueda M. Fundamentals and new frontiers of Bose-Einstein condensates. Phys Rev Lett. 2000;84(6):1066–1069.

[4] Nozières P, Saint James D. Particle vs. pair condensation in Bose-Einstein condensates. Phys Rev Lett. 1988;84(18):4031–4034.

[5] Berezinskii VL. Destruction of long range order in one-dimensional and two-dimensional systems having a continuous symmetry group. I. Classical systems. Sov Phys JETP. 1971;32:493–500; ibid. 1972;34:610.

[6] Kosterlitz JM, Thouless DJ. Ordering, metastability and phase transitions in two-dimensional systems. J Phys C. 1976;36(11):594–597.

[7] Kawaguchi Y, Ueda M. Spinor Bose-Einstein condensates. Phys Rev Lett. 2010;105:230406.

[8] Stamper-Kurn DM, Ueda M. Spinor bose gases: symmetries, magnetism, and quantum dynamics. Rev Modern Phys. 2013;85(3):1191–1244.

[9] Zhou F. Spin correlation and discrete symmetry in spinor Bose-Einstein condensates. Phys Rev Lett. 2001;87(8):080401.

[10] Leonhardt U, Volovik GE. How to create an Alice string (half-quantum vortex) in a vector Bose-Einstein condensate. Experimental Theoretical Phys Lett. 2000;72(2):46–48.

[11] Seo SW, Kwon WJ, Kang S, et al. Half-Quantum vortices in an antiferromagnetic spinor Bose-Einstein condensate. Phys Rev Lett. 2016;115:015301.

[12] Solem JC, Biedenharn LC. Understanding geometrical phases in quantum mechanics: an elementary example. Foundations Phys. 1993;23(2):185–195.

[13] Xia D, Chang M-C, Niu Q. Berry phase effects on electronic properties. Rev Mod Phys. 2010;82(3):1959–2007.

[14] Mermin ND, Ho T-L. Circulation and angular momentum in the A phase of superfluid Helium-3. Phys Rev Lett. 1976;36(11):594–597.

[15] Anderson PW, Toulouse G. Phase slippage without vortex cores: vortex textures in superfluid He 3. Phys Rev Lett. 1977;38(9):508–511.

[16] Law CK, Hu P, Bigelow NP. Quantum spins mixing in spinor Bose-Einstein condensates. Phys Rev Lett. 1998;81(24):5257–5261.

[17] Penrose O, Onsager L. Bose-Einstein condensation and liquid Helium. Phys Rev. 1956;104(3):576–584.

[18] Nozières P, Saint James D. Particle vs. pair condensation in attractive Bose liquids. J Physique. 1982;43(7):1133–1148.

[19] Mueller EJ, Ho T-L, Ueda M, et al. Fragmentation of Bose-Einstein condensates. Phys Rev A. 2006;74(3):033612.

[20] Wilkin NK, Gunn JMF, Smith RA. Do attractive bosons condense? Phys Rev Lett. 1998;80(11):2265–2268.

[21] Koashi M, Ueda M. Exact eigenstates and magnetic response of Spin-1 and Spin-2 Bose-Einstein condensates. Phys Rev Lett. 2000;84(6):1066–1069.

[22] Law CK, Pu H, Bigelow NP. Quantum spins mixing in spinor Bose-Einstein condensates. Phys Rev A. 2000;62(6):063612.

[23] Xu X, Chang M-C, Niu Q. Berry phase effects on electronic properties. Rev Mod Phys. 2010;82(3):1959–2007.

[24] Anderson PW, Toulouse G. Phase slippage without vortex cores: vortex textures in superfluid He 3. Phys Rev Lett. 1977;38(9):508–511.

[25] Wilkin NK, Gunn JMF, Smith RA. Do attractive bosons condense? Phys Rev Lett. 1998;80(11):2265–2268.

[26] Koashi M, Ueda M. Exact eigenstates and magnetic response of Spin-1 and Spin-2 Bose-Einstein condensates. Phys Rev Lett. 2000;84(6):1066–1069.

[27] Ho T-L, Yip SK. Fragmented and single condensate ground states of Spin-1 Bose gas. Phys Rev Lett. 2000;84(18):4031–4034.

[28] Evrard B, Qu A, Dalibard J, et al. Observation of fragmentation of a spinor Bose-Einstein condensate. Science. 2001;299:1340–1343.

[29] Klausen NN, Bohn JL, Greene CH. Nature of spinor Bose-Einstein condensates in rubidium. Phys Rev A. 2001;64:053602.

[30] Kobayashi M, Kawaguchi Y, Nitta M, et al. Collision dynamics and rung formation of non-Abelian vortices. Phys Rev Lett. 2009;103:115301.

[31] Ueda M, Koashi M. Theory of Spin-2 Bose-Einstein condensates: Spin correlations, magnetic response, and excitation spectra. Phys Rev A. 2002;65:063602.

[32] Song JL, Semenoff GW, Zhou F. Uniaxial and Biaxial Spin nematic phases induced by quantum fluctuations. Phys Rev Lett. 2007;98:160408.

[33] Turner AM, Barnett R, Demler E, et al. Nematic order by disorder in Spin-2 Bose-Einstein condensates. Phys Rev Lett. 2007;98:190404.

[34] Uchino S, Kobayashi M, Nitta M, et al. Quasi-nambu-goldstone modes in Bose-Einstein condensates. Phys Rev Lett. 2010;105:230406.

[35] Semenoff GW, Zhou F. Discrete symmetries and 1/3-quantum vortices in condensates of F = 2 cold atoms. Phys Rev Lett. 2007;98:100401.

[36] Ueda M. Topological aspects in spinor Bose-Einstein condensates. Rep Prog Phys. 2014;77:122401.

[37] Ueda M. Quantum equilibration, thermalization and prethermalization in ultracold atoms. Nature Rev Phys. 2020;2:669–681.