We study a two-component Bose gas with a symmetric spin-orbit coupling, and find that two atoms can form a bound state with any intra- or inter-species scattering length. Consequently, in the dilute limit, a stable condensation of diatomic molecules in the Bardeen-Cooper-Shrieffer (BCS) pairing state can be formed with weakly-attractive inter-species and repulsive intra-species interactions. This BCS paring state is energetically favored over Bose-Einstein condensation (BEC) of atoms at low densities, but as the density increases, there is a first-order transition from the BCS to BEC states.

**Introduction.**—Observation of BCS-BEC crossover in Fermi gases was a tremendous triumph in the research of ultracold quantum gases [1]. In contrast, although it was proposed around a century ago [2, 3], the BCS state of bosons has never been observed. The BCS state of a Bose gas with Feshbach resonance was theoretically studied [4–6], and it was found that this state is generally unstable in the attractive region or close to the resonance [7, 8]. In experiments, the lifetime of Feshbach molecules was too short for equilibrating into a BEC state [9, 10]. Here we propose that the BCS state with a Bose gas can be realized in a Bose with a three-dimensional (3D) spin-orbit coupling (SOC).

The SOC in cold atomic gases was experimentally realized in Bose gases in recent years [14, 15] and Fermi gases [16, 17]. In contrast to SOC of electrons, the SOC of cold atoms refers to the coupling between spin of the atomic internal states and momentum of the atom [18–21]. The experimental realization of SOC in cold atoms provides a new platform for studying spin-orbit-coupled many-body systems [22–24]. It can provide simulations of complex phenomena, such as the quantum spin Hall effect [19, 25], topological insulators and superconductors [26, 27], Majorana fermions [28] and spintronics [29]. So far most of experimental SOC was one-dimensional (1D), and more recently two-dimensional (2D) SOC was realized experimentally [30, 31]. Many theoretical work have been focused on phase diagrams of Bose gases with 1D and 2D SOC [32–37]. There have been proposals to generate 3D SOC in a Bose gas, which has attracted several theoretical studies [38–40].

The realization of SOC in cold atoms may offer the opportunity to realize the long-sought BCS pairing state of Bose atoms. A pairing condensation in a dilute Bose gas with 2D Rashba SOC and weak intra-species attraction can be stabilized by inter-species repulsion [41], but the intra-species attraction can also lead to phase separation which may become an experimental obstacle. In this work, we investigate the pairing state of Bose gas with an isotropic 3D SOC. First, we study the two-body bound state of Bose atoms with 3D SOC and find that the bound state can exist for arbitrary inter-species and intra-species scattering length, which is helpful in forming a BCS pairing state. Next, we study the molecular condensation in a dilute Bose gas with 3D SOC in the framework of the BCS theory. We find that this pairing state can be stable in the case with weak inter-species attraction and intra-species repulsion which avoids phase separation. As the atomic density increases, there is a first-order phase transition from the BCS pairing state to the atomic BEC. We discuss the experimental perspective of realizing the BCS pairing state of bosons and conclude in the end.

**Model.**—We study a two-component homogeneous Bose gas described by the Hamiltonian $H = H_0 + H_{int}$, where the single-particle Hamiltonian is given by

$$H_0 = \sum_{\mathbf{k}, \mathbf{p}, \rho, \rho'} c_{\mathbf{k}\rho}^\dagger \left[ \epsilon_{\mathbf{k}} + \frac{\hbar^2 \kappa}{m} \mathbf{k} \cdot \sigma_{\rho\rho'} \right] c_{\mathbf{k}\rho'}^\dagger,$$

and the interaction between atoms is given by

$$H_{int} = \frac{1}{2V} \sum_{\mathbf{k}, \mathbf{q}, \rho, \rho'} g_{\rho\rho'} c_{\mathbf{k}\rho}^\dagger c_{\mathbf{q}+\mathbf{k}\rho}^\dagger c_{\mathbf{k}-\mathbf{q}\rho'} c_{\mathbf{q}-\mathbf{k}\rho'}^\dagger c_{\mathbf{q}-\mathbf{k}\rho'}^\dagger c_{\mathbf{k}\rho'}^\dagger.$$

Here $\sigma_{\rho\rho'}$ are Pauli matrices, $m$ is the atomic mass, $\epsilon_{\mathbf{k}}$ is the annihilation operator of a Boson with wavevector $\mathbf{k}$ and spin component $\rho$, $\epsilon_{\mathbf{k}} = \hbar^2 k^2 / 2m$, $\kappa$ is the strength of isotropic 3D SOC, $V$ is the volume, $g_{\uparrow\downarrow} = g_{\downarrow\uparrow}$ is the intra-species coupling constant, and $g_{\uparrow\downarrow} = g_{\downarrow\uparrow}$ is the inter-species coupling constant. The single-particle Hamiltonian can be easily diagonalized, yielding two helicity branches of atomic excitations with eigenenergies $\epsilon_{\mathbf{k}} \pm \hbar^2 k^2 / m$.

**Two-body bound state.**—The wavefunction of a two-body bound state satisfies the eigenequation $H|\phi\rangle = E_\mathbf{q}|\phi\rangle$, where $\hbar \mathbf{q}$ is the center of mass momentum, and $E_\mathbf{q}$ is the eigenenergy. It can be generally written as

$$|\phi\rangle = \sum_{\mathbf{k}, \rho, \rho'} \psi_{\rho\rho'}(\mathbf{k}, \mathbf{q} - \mathbf{k}) c_{\mathbf{k}\rho}^\dagger c_{\mathbf{q}-\mathbf{k}\rho'}^\dagger |0\rangle.$$

Due to Bose statistics, the coefficients satisfy the symmetric condition $\psi_{\rho\rho'}(\mathbf{k}, \mathbf{k}') = \psi_{\rho\rho'}(\mathbf{k}', \mathbf{k})$. From the eigenequation, we obtain the following matrix equation

$$H_0 |\phi\rangle + \sum_{\mathbf{k}, \rho, \rho'} \left[ \frac{\hbar^2 \kappa}{m} \mathbf{k} \cdot \sigma_{\rho\rho'} \right] c_{\mathbf{k}\rho}^\dagger c_{\mathbf{k}\rho'}^\dagger |\phi\rangle = E_\mathbf{q} |\phi\rangle.$$
for the coefficients at $q = 0$

$$M_k \psi'_k = \frac{1}{V} G \sum_p \psi'_p,$$

where $\psi'_k$ is a four-component vector given by $\psi'_k = [\psi_{\uparrow\uparrow}(k, -k), \psi_{\downarrow\downarrow}(k, -k), \psi_{\uparrow\downarrow}(k, -k), \psi_{\downarrow\uparrow}(-k, k)]$, and $G$ is the matrix of coupling constants

$$G = \begin{pmatrix}
    g_{\uparrow\uparrow} & 0 & 0 & 0 \\
    0 & g_{\downarrow\downarrow} & 0 & 0 \\
    0 & 0 & g_{\uparrow\downarrow} & 0 \\
    0 & 0 & 0 & g_{\downarrow\uparrow}
\end{pmatrix}. \tag{5}$$

The matrix $M_k$ is given by

$$M_k = \begin{pmatrix}
    \epsilon_k & 0 & S^*(k_\perp) & -S^*(k_\perp) \\
    0 & \epsilon_k & -S(k_\perp) & S(k_\perp) \\
    S(k_\perp) & -S^*(k_\perp) & \epsilon_k - \frac{2\hbar^2 \kappa k_x}{m} & 0 \\
    -S(k_\perp) & S^*(k_\perp) & 0 & \epsilon_k + \frac{2\hbar^2 \kappa k_x}{m}
\end{pmatrix}, \tag{6}$$

where $\epsilon_k = E_0 - 2\epsilon_k$, $k_\perp$ is the projection of $k$ in the $x-y$ plane, and $S(k_\perp) = \hbar^2 \kappa (k_x + ik_y)/m$. Define a new vector

$$Q = \frac{1}{V} G \sum_k \psi'_k, \tag{7}$$

and from the eigenenergy we obtain

$$Q = \frac{1}{V} G \sum_k M_k^{-1} Q. \tag{8}$$

Thus the eigenenergy of the bound state satisfies the equation

$$\| 1 - \frac{1}{V} G \sum k M_k^{-1} \| = 0, \tag{9}$$

which has three nontrivial bound-state solutions, two due to the intra-species interaction and one due to inter-species interaction. Eigenenergies of these bound states satisfy the same equation

$$\frac{m}{4\pi \hbar^2 a_{pp'}} = \frac{1}{2V} \sum_k \left[ \frac{1}{\epsilon_k} + \frac{2}{E_0 - 2\epsilon_k} + \frac{16\epsilon_k \epsilon_{\kappa}}{(E_0 - 2\epsilon_k)^3 - 16\epsilon_k \epsilon_{\kappa}(E_0 - 2\epsilon_k)} \right], \tag{10}$$

where $a_{pp'}$ is the scattering length. In this derivation, the renormalization condition, $1/g_{pp'} = m/(4\pi a_{pp'} \hbar^2) = 1/(2V) \sum_k 1/\epsilon_k$, is used.

The binding energy of the bound state is defined as $E_b = -E_0 - \epsilon_\kappa$, where $\epsilon_\kappa = \hbar^2 \kappa^2/2m$ is the lowest energy of a single atom with SOC. In FIG. 1 the binding energy is plotted against the inverse of the scattering length. Since the relation between the binding energy and the corresponding scattering length is the same in all scattering channels, we drop the subscripts and denote the scattering length as $a$ in this plot. As the scattering length decreases, the binding energy increases monotonously. The binding energy vanishes when the scattering length $a$ approaches negative zero $0^-$, signaling that the resonance position is shifted from where $a$ diverges to $0^-$ and the bound state can exist with any value of $a$. In the limit of $a \to 0^-$, we obtain the asymptotic form $E_b \sim \hbar^2 \kappa^4 a^2/(9m)$; at $1/a = 0$, the binding energy is given by $E_b = (2\sqrt{3} - 3)\hbar^2 \kappa^2/(3m)$; when $\kappa a \to 0^+$, the binding energy recovers the result in the case without SOC, $E_b \sim \hbar^2/(ma^2)$.

The reason for the bound state existing for all values of the scattering length with the resonance position shifted to $0^-$ is the special single-particle density of states (DOS) due to SOC. With SOC, the DOS at the lowest atom energy $\epsilon_\kappa = \hbar^2 \kappa^2/2m$ is a constant, in sharp contrast to the case without SOC where DOS vanishes near the lowest atom energy. As a result, the r.h.s. of Eq. (10) has infrared divergence at $E_0 = -2\epsilon_\kappa$ which guarantees a solution for any scattering length, whereas without SOC such infrared divergence is absent and the bound state only exists with positive scattering length.

**BCS state of a Bose gas with SOC.**—In a Bose gas with an isotropic SOC, pairing of two atoms, i.e. the tendency of two atoms forming a diatomic molecule, may lead to the formation of molecular condensation at low temperatures. This condensed state can be described by the BCS pairing theory. To avoid the possibility of phase separation, here we consider the case with repulsive intra-species interactions and attractive inter-species interaction. In this case the binding energy of the diatomic molecule in the inter-species channel is much smaller and this type of molecules are much easier
to generate. Thus we consider pairing between atoms with different spins only, with order parameter given by \( \Delta = (g_{\uparrow \uparrow}/V) \sum_k \langle c_{-k \uparrow} c_{k \downarrow} \rangle \). In general, the phase of the order parameter can be tuned arbitrarily under \( U(1) \) transformation, and in the following for simplicity we choose \( \Delta > 0 \).

We study a spin-balanced Bose gas with an isotropic SOC at zero temperature in the mean-field approximation, where in addition to pairing the Hartree-Fock contributions are also included. The mean-field Hamiltonian of this system is given by

\[
H_{MF} = \frac{1}{2} \sum_k (B_k^\dagger H_k B_k - 2 \xi_k) - \frac{\Delta^2}{g_{\uparrow \downarrow}} V - (2 g_{\uparrow \downarrow} + g_{\uparrow \uparrow}) n^2 V,
\]

(11)

where \( \xi_k = \epsilon_k + 2 g_{\uparrow \uparrow} n + g_{\uparrow \downarrow} n - \mu, B_k^\dagger \) is the field operator with four components \([c^\dagger_{k \uparrow}, c_{-k \uparrow}, c^\dagger_{k \downarrow}, c_{-k \downarrow}] \), \( n \) is the atom density of one spin component, and \( \mu \) is the chemical potential. The matrix \( H_k \) is given by

\[
H_k = \begin{pmatrix}
\xi_k + \hbar^2 n k^2 /m & 0 & S^*(k_{\perp}) & \Delta \\
0 & \xi_k - \hbar^2 n k^2 /m & \Delta & -S(k_{\perp}) \\
S(k_{\perp}) & \Delta & \xi_k - \hbar^2 n k^2 /m & 0 \\
\Delta & -S^*(k_{\perp}) & 0 & \xi_k + \hbar^2 n k^2 /m
\end{pmatrix}.
\]

(12)

The mean-field Hamiltonian Eq. (11) can be diagonalized by the generalized Bogoliubov transformation. We obtain two branches of quasi-particles with excitation energies given by

\[
\epsilon_{k \pm} = \sqrt{\xi_k^2 - \Delta^2 + \left( \hbar^2 n /m \right)^2 \pm 2 \hbar^2 n k^2 /m \sqrt{k^2 \xi_k^2 - \Delta^2 k^2}}.
\]

(13)

The energy gap, i.e. the smallest energy, of these excitations is given by \( \epsilon_0 = \sqrt{\xi_0^2 - \Delta^2} \). For finite \( k \), these excitation energies are isotropic in the \( k_x-k_y \) plane, but anisotropic in the \( k_x-k_z \) plane. In the limit \( \Delta \to 0 \), they recover the non-interacting form, \( \epsilon_k \pm \hbar k \kappa /m \). For fixed \( k \), the excitation energy of the lower branch \( \epsilon_{k-} \) is between \( \sqrt{\xi_k^2 - \hbar^2 k \kappa^2/m^2 - \Delta^2} \) at \( k_z = 0 \) and \( \sqrt{\xi_k^2 - \Delta^2} - \hbar k \kappa /m \) at \( k_z = 0 \), while the excitation energy of the upper branch is between \( \sqrt{\xi_k^2 - \Delta^2 + \hbar k \kappa /m} \) and \( \sqrt{(\xi_k + \hbar k \kappa /m)^2 - \Delta^2} \). The gap between the lower and the upper excitation branches is given by \( 2 \hbar k \kappa /m \) at \( k_z = 0 \).

The anisotropy of quasi-particle excitation energies is a consequence of spin-momentum locking due to SOC and pairing. In the absence of pairing, the momentum and spin of a quasi-particle are locked, either parallel or antiparallel due to SOC. With pairing between spin-up and spin-down atoms, if the quasi-particle momentum is in \( z \) direction, the spin-momentum locking is still present, and the excitation energy of the lower-branch quasi-particle is at minimum for fixed \( k_z \); if the quasi-particle momentum is in \( x-y \) plane, the spin-momentum locking is lost and the excitation energy of the lower-branch quasi-particle is at maximum. The energy dependence of the upper-branch quasi-particle is simply opposite.

The pairing order parameter \( \Delta \) and the chemical potential \( \mu \) can be self-consistently solved together numerically. We find that the mean-field solution always exists in the dilute limit \( n \to 0 \). As shown in Fig. 2, the order parameter increases monotonically with the inverse of the inter-species scattering length \( 1/a \). In the limit \( a \to 0^- \), the order parameter \( \Delta \) vanishes; in the opposite limit \( a \to 0^+ \), \( \Delta \) diverges. The increase of the pairing order parameter with \( 1/a \) is consistent with relation between the binding energy \( E_b \) of a diatomic molecule and \( 1/a \).

**Phase transition.**—The pairing state is always stable in the dilute limit with enough repulsive intra-species interaction. As the density increases, the pairing order parameter increases, which reduces the energy gap of the quasi-particle excitation, contrary to the fermion case. When the density increases to a critical value, the excitation gap vanishes. Beyond the critical point, the pairing state do not exist and the system is likely turned...
FIG. 3. (color online) Energy comparison between atomic and molecular condensates at $\kappa a_{\uparrow \uparrow} = 0.37$ and $\kappa a_{\downarrow \downarrow} = -0.082$. The atomic BEC state is denoted by ABEC, and the pairing state, or the molecular BEC state is denoted by MBEC. The solid line is the energy density of the MBEC state, $E_{g1}$. The dashed line is the energy density of the ABEC state, $E_{g2}$. The excitation gap of MBEC state vanishes at $n \approx 1.9 \times 10^{-4} \kappa^{-3}$. The transition from MBEC to ABEC takes place around $n \approx 1.75 \times 10^{-4} \kappa^{-3}$.

into a BEC state of atoms. We compare the energy density of pairing state $E_{g1}$ and the energy density of atomic BEC state $E_{g2}$ [23], as shown in FIG. 3 and find that when the excitation gap of the pairing state vanishes, the atomic BEC state energy is always smaller than the pairing state energy, $E_{g1} > E_{g2}$, indicating that even before that gap closes, the system has already turned into the atomic BEC state and this transition is a first-order phase transition.

Discussion and Conclusion. If the isotropic SOC can be created experimentally, the BCS-BEC transition may be observed under current experimental conditions. For an ultra-cold Bose gas with density about $2 \times 10^{17} m^{-3}$ and the isotropic SOC with $\kappa = 8.2 \times 10^6 m^{-1}$, the first-order phase transition from MBEC to ABEC state take place at the inter-species scattering length about $-10nm$ and intra-species scattering length about $46nm$. The MBEC state can be observed at smaller inter-species scattering lengths.

In summary, we study a two-component Bose gas with an isotropic SOC and find that two atoms can form a bound state with any intra- or inter-species scattering lengths due to the SOC effect on DOS. In the dilute limit, a stable BCS pairing state can be formed with attractive inter-species and repulsive intra-species interactions. The excitation energies of the pairing state are anisotropic. As the density increases, there is a first-order transition from the BCS to BEC states.

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