

GROUND STATES AND DYNAMICS OF SPIN-ORBIT-COUPLED BOSE–EINSTEIN CONDENSATES*

WEIZHU BAO[†] AND YONGYONG CAI[‡]

Abstract. We study analytically and asymptotically, as well as numerically, ground states and dynamics of two-component spin-orbit-coupled Bose–Einstein condensates (BECs) modeled by the coupled Gross–Pitaevskii equations (CGPEs). In fact, due to the appearance of the spin-orbit (SO) coupling in the two-component BEC with a Raman coupling, the ground state structures and dynamical properties become very rich and complicated. For the ground states, we establish existence and nonexistence results under different parameter regimes and obtain their limiting behaviors and/or structures with different combinations of the SO and Raman coupling strengths. For the dynamics, we show that the motion of the center-of-mass is either nonperiodic or with different frequency than the trapping frequency when the external trapping potential is taken as harmonic and/or the initial data is chosen as a stationary state (e.g., ground state) with a shift, which is completely different from the case of a two-component BEC without the SO coupling, and obtain the semiclassical limit of the CGPEs in the linear case via the Wigner transform method. Efficient and accurate numerical methods are proposed for computing the ground states and dynamics, especially for the case of box potentials. Numerical results are reported to demonstrate the efficiency and accuracy of the numerical methods and show the rich phenomenon in the SO-coupled BECs.

Key words. Bose–Einstein condensate, spin-orbit coupling, coupled Gross–Pitaevskii equations, ground state, dynamics, Raman coupling

AMS subject classifications. 35Q55, 49J45, 65N06, 65N12, 65Z05, 81-08

DOI. 10.1137/140979241

1. Introduction. Spin-orbit (SO) coupling is the interaction between the spin and motion of a particle and is crucial for understanding many physical phenomena, such as quantum Hall effects [33] and topological insulators [17]. However, SO coupling observation in solid state matters is inaccurate due to the disorder and impurities of the system. Since the first experimental realization of Bose–Einstein condensates (BEC) in 1995 [1, 12], degenerate quantum gas has become a perfect candidate for studying quantum many-body phenomena in condensed matter physics. Such a system of quantum gas can be controlled with high precision in experiments. Very recently, in their pioneering work [25] Lin, Jiménez-García, and Spielman created an SO-coupled BEC with two spin states of ⁸⁵Rb: $|\uparrow\rangle = |F = 1, m_f = 0\rangle$ and $|\downarrow\rangle = |F = 1, m_f = -1\rangle$. Due to this remarkable experimental progress and its potential applications, SO coupling in cold atoms has received increased attentions in the atomic physics and condensed matter physics communities [14, 16].

At temperatures T much smaller than the critical temperature T_c , following the mean field theory [23, 25, 29, 34], an SO-coupled BEC is well described by the macro-

*Received by the editors July 25, 2014; accepted for publication (in revised form) January 6, 2015; published electronically March 19, 2015.

<http://www.siam.org/journals/siap/75-2/97924.html>

[†]Department of Mathematics and Center for Computational Science and Engineering, National University of Singapore, Singapore 119076 (matbaowz@nus.edu.sg, <http://www.math.nus.edu.sg/~bao/>). This author’s research was supported by Ministry of Education of Singapore grant R-146-000-196-112.

[‡]Beijing Computational Science Research Center, Beijing 100084, People’s Republic of China, and Department of Mathematics, Purdue University, West Lafayette, IN 47907 (yongyong.cai@gmail.com). This author’s research was partially supported by NSF grants DMS-1217066 and DMS-1419053.

scopic wave function $\Psi := \Psi(\mathbf{x}, t) = (\psi_1(\mathbf{x}, t), \psi_2(\mathbf{x}, t))^T := (\psi_1, \psi_2)^T$, which is governed by the coupled Gross–Pitaevskii equations (CGPEs) in three dimensions (3D)

$$(1.1) \quad \begin{aligned} i\hbar\partial_t\psi_1 &= \left[-\frac{\hbar^2}{2m}\nabla^2 + \tilde{V}_1(\mathbf{x}) + \frac{i\hbar^2\tilde{k}_0}{m}\partial_x + \frac{\hbar\tilde{\delta}}{2} + \sum_{l=1}^2 \tilde{g}_{1l}|\psi_l|^2 \right] \psi_1 + \frac{\hbar\tilde{\Omega}}{2}\psi_2, \\ i\hbar\partial_t\psi_2 &= \left[-\frac{\hbar^2}{2m}\nabla^2 + \tilde{V}_2(\mathbf{x}) - \frac{i\hbar^2\tilde{k}_0}{m}\partial_x - \frac{\hbar\tilde{\delta}}{2} + \sum_{l=1}^2 \tilde{g}_{2l}|\psi_l|^2 \right] \psi_2 + \frac{\hbar\tilde{\Omega}}{2}\psi_1. \end{aligned}$$

Here, t is time, $\mathbf{x} = (x, y, z)^T \in \mathbb{R}^3$ is the Cartesian coordinate vector, \hbar is the Planck constant, m is the mass of particle, $\tilde{\delta}$ is the detuning constant for Raman transition, \tilde{k}_0 is the wave number of Raman lasers representing the SO coupling strength, $\tilde{\Omega}$ is the effective Rabi frequency describing the strength of Raman coupling (i.e., an internal atomic Josephson junction), and $\tilde{g}_{jl} = \frac{4\pi\hbar^2 a_{jl}}{m}$ ($j, l = 1, 2$) are interaction constants with $a_{jl} = a_{lj}$ ($j, l = 1, 2$) being the s -wave scattering lengths between the j th and l th components (positive for repulsive interaction and negative for attractive interaction). $\tilde{V}_1(\mathbf{x})$ and $\tilde{V}_2(\mathbf{x})$ are given real-valued external trapping potentials whose profiles depend on different applications and on the setups of the experiments [25, 16]. Currently, in typical experiments the following harmonic potentials are commonly used [25, 16, 20, 21]:

$$(1.2) \quad \tilde{V}_j(\mathbf{x}) = \frac{m}{2} [\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 (z - \tilde{z}_j)^2], \quad j = 1, 2, \quad \mathbf{x} = (x, y, z)^T \in \mathbb{R}^3,$$

where $\omega_x > 0$, $\omega_y > 0$, and $\omega_z > 0$ are trapping frequencies in the x -, y -, and z -directions, respectively, and $\tilde{z}_1, \tilde{z}_2 \in \mathbb{R}$ are two given constants. The wave function Ψ is normalized as

$$(1.3) \quad \|\Psi\|^2 := \|\Psi(\cdot, t)\|_2^2 = \int_{\mathbb{R}^3} [|\psi_1(\mathbf{x}, t)|^2 + |\psi_2(\mathbf{x}, t)|^2] d\mathbf{x} = N,$$

where N is the total number of particles in the SO-coupled BEC.

In order to nondimensionalize the CGPEs (1.1) with (1.2), we introduce [6, 3]

$$(1.4) \quad \tilde{t} = t/t_s, \quad \tilde{\mathbf{x}} = \mathbf{x}/x_s, \quad \tilde{\psi}_j(\tilde{\mathbf{x}}, \tilde{t}) = N^{-1/2} x_s^{3/2} \psi_j(\mathbf{x}, t), \quad j = 1, 2,$$

where $t_s = \frac{1}{\omega_0}$ and $x_s = \sqrt{\frac{\hbar}{m\omega_0}}$ with $\omega_0 = \min\{\omega_x, \omega_y, \omega_z\}$ are the scaling parameters of dimensionless time and length units, respectively. Plugging (1.4) into (1.1), multiplying by $\frac{t_s^2}{m(x_s N)^{1/2}}$, and then removing all tildes, we obtain the following dimensionless CGPEs in 3D for a SO-coupled BEC:

$$(1.5) \quad \begin{aligned} i\partial_t\psi_1 &= \left[-\frac{1}{2}\nabla^2 + V_1(\mathbf{x}) + ik_0\partial_x + \frac{\delta}{2} + (g_{11}|\psi_1|^2 + g_{12}|\psi_2|^2) \right] \psi_1 + \frac{\Omega}{2}\psi_2, \\ i\partial_t\psi_2 &= \left[-\frac{1}{2}\nabla^2 + V_2(\mathbf{x}) - ik_0\partial_x - \frac{\delta}{2} + (g_{21}|\psi_1|^2 + g_{22}|\psi_2|^2) \right] \psi_2 + \frac{\Omega}{2}\psi_1, \end{aligned}$$

where $k_0 = \tilde{k}_0 x_s$, $\delta = \frac{\tilde{\delta}}{\omega_0}$, $\Omega = \frac{\tilde{\Omega}}{\omega_0}$, $g_{11} = \frac{4\pi N a_{11}}{x_s}$, $g_{12} = g_{21} = \frac{4\pi N a_{12}}{x_s}$, $g_{22} = \frac{4\pi N a_{22}}{x_s}$, $\gamma_x = \frac{\omega_x}{\omega_0}$, $\gamma_y = \frac{\omega_y}{\omega_0}$, and $\gamma_z = \frac{\omega_z}{\omega_0}$, and the dimensionless trapping potentials are

$$(1.6) \quad V_j(\mathbf{x}) = \frac{1}{2} (\gamma_x^2 x^2 + \gamma_y^2 y^2 + \gamma_z^2 (z - z_j)^2), \quad \mathbf{x} \in \mathbb{R}^3, \quad j = 1, 2,$$

with $z_1 = \frac{\tilde{z}_1}{x_s}$ and $z_2 = \frac{\tilde{z}_2}{x_s}$.

When the trapping potentials in (1.6) are strongly anisotropic, similar to the dimension reduction of the GPE for a BEC [6, 3, 10, 29], the CGPEs (1.5) in 3D can be formally reduced to two dimensions (2D) or one dimension (1D) for the disk-shaped or cigar-shaped BEC, respectively. For simplicity of notation, we assume $z_1 = z_2 = 0$ in (1.6). When we have $\gamma_z \gg \gamma_x$ and $\gamma_z \gg \gamma_y$, i.e., a disk-shaped condensate, by taking the ansatz [10, 6]

$$(1.7) \quad \psi_j(\mathbf{x}, t) = \psi_j^{2D}(x, y, t)e^{-i\gamma_z t/2}\gamma_z^{-1/4}w(\gamma_z^{1/2}z), \quad \mathbf{x} = (x, y, z)^T \in \mathbb{R}^3, \quad j = 1, 2,$$

with $w(z) = \pi^{-1/4}e^{-z^2/2}$, multiplying both sides of (1.5) by $w(\gamma_z^{1/2}z)$, and integrating over $z \in \mathbb{R}$, we can formally reduce the 3D CGPEs (1.5) into 2D [6, 3]. Similarly, when we have $\gamma_z \gg \gamma_x$ and $\gamma_y \gg \gamma_x$, i.e., a cigar-shaped condensate, we can formally reduce the 3D CGPEs (1.5) into 1D [6, 3, 10, 29].

In fact, the CGPEs (1.5) in 3D and the corresponding one- and two-dimensional effective equations can be written in a unified form [6, 3, 10, 29] in d -dimensions ($d = 1, 2, 3$) with ψ_j ($j = 1, 2$) being the d -dimensional wave function for $\mathbf{x} \in \mathbb{R}^d$ with $\mathbf{x} = x \in \mathbb{R}$, and $\beta_{jl} = \frac{\sqrt{\gamma_y\gamma_z}}{2\pi}g_{jl}$ for $d = 1$; $\mathbf{x} = (x, y)^T \in \mathbb{R}^2$, and $\beta_{jl} = \frac{\sqrt{\gamma_z}}{\sqrt{2\pi}}g_{jl}$ for $d = 2$; and $\mathbf{x} = (x, y, z)^T \in \mathbb{R}^3$ and $\beta_{jl} = g_{jl}$ ($j, l = 1, 2$) for $d = 3$ as

$$(1.8) \quad \begin{aligned} i\partial_t\psi_1 &= \left[-\frac{1}{2}\nabla^2 + V_1(\mathbf{x}) + ik_0\partial_x + \frac{\delta}{2} + (\beta_{11}|\psi_1|^2 + \beta_{12}|\psi_2|^2) \right] \psi_1 + \frac{\Omega}{2}\psi_2, \\ i\partial_t\psi_2 &= \left[-\frac{1}{2}\nabla^2 + V_2(\mathbf{x}) - ik_0\partial_x - \frac{\delta}{2} + (\beta_{21}|\psi_1|^2 + \beta_{22}|\psi_2|^2) \right] \psi_2 + \frac{\Omega}{2}\psi_1, \end{aligned}$$

where

$$(1.9) \quad V_1(\mathbf{x}) = V_2(\mathbf{x}) = \begin{cases} \frac{1}{2}(\gamma_x^2x^2 + \gamma_y^2y^2 + \gamma_z^2z^2), & d = 3, \\ \frac{1}{2}(\gamma_x^2x^2 + \gamma_y^2y^2), & d = 2, \\ \frac{1}{2}\gamma_x^2x^2, & d = 1, \end{cases} \quad \mathbf{x} \in \mathbb{R}^d.$$

For other potentials, such as box potential, optical lattice potential, and double-well potential, we refer the reader to [6, 25, 16, 20, 21, 29] and references therein. Thus, in the subsequent discussion, we will treat the external potentials $V_1(\mathbf{x})$ and $V_2(\mathbf{x})$ in (1.8) as two general real-valued functions and β_{jl} ($j, l = 1, 2$) satisfying $\beta_{12} = \beta_{21}$ as arbitrary real constants. In addition, without loss of generality, we assume $V_1(\mathbf{x}) \geq 0$ and $V_2(\mathbf{x}) \geq 0$ for $\mathbf{x} \in \mathbb{R}^d$ in the rest of this paper. The dimensionless CGPEs (1.8) conserve the total mass or normalization, i.e.,

$$(1.10) \quad N(t) := \|\Psi(\cdot, t)\|^2 = \int_{\mathbb{R}^d} [|\psi_1(\mathbf{x}, t)|^2 + |\psi_2(\mathbf{x}, t)|^2]d\mathbf{x} \equiv \|\Psi(\cdot, 0)\|^2 = 1, \quad t \geq 0,$$

and the energy per particle,

$$(1.11) \quad \begin{aligned} E(\Psi) &= \int_{\mathbb{R}^d} \left[\sum_{j=1}^2 \left(\frac{1}{2}|\nabla\psi_j|^2 + V_j(\mathbf{x})|\psi_j|^2 \right) + \frac{\delta}{2}(|\psi_1|^2 - |\psi_2|^2) + \Omega \operatorname{Re}(\psi_1\bar{\psi}_2) \right. \\ &\quad \left. + ik_0(\bar{\psi}_1\partial_x\psi_1 - \bar{\psi}_2\partial_x\psi_2) + \frac{\beta_{11}}{2}|\psi_1|^4 + \frac{\beta_{22}}{2}|\psi_2|^4 + \beta_{12}|\psi_1|^2|\psi_2|^2 \right] d\mathbf{x}, \end{aligned}$$

where \bar{f} and $\operatorname{Re}(f)$ denote the conjugate and real part of a function f , respectively. In addition, if $\Omega = 0$ in (1.8), the mass of each component is also conserved, i.e.,

$$(1.12) \quad N_j(t) := \|\psi_j(\mathbf{x}, t)\|^2 = \int_{\mathbb{R}^d} |\psi_j(\mathbf{x}, t)|^2 d\mathbf{x} \equiv \|\psi_j(\mathbf{x}, 0)\|^2, \quad t \geq 0, \quad j = 1, 2.$$

Finally, by introducing the change of variables

$$(1.13) \quad \psi_1(\mathbf{x}, t) = \tilde{\psi}_1(\mathbf{x}, t)e^{i(\omega t + k_0 x)}, \quad \psi_2(\mathbf{x}, t) = \tilde{\psi}_2(\mathbf{x}, t)e^{i(\omega t - k_0 x)}, \quad \mathbf{x} \in \mathbb{R}^d,$$

with $\omega = \frac{-k_0^2}{2}$ in the CGPEs (1.8), we obtain for $\mathbf{x} \in \mathbb{R}^d$ and $t > 0$

$$(1.14) \quad \begin{aligned} i\partial_t \tilde{\psi}_1 &= \left[-\frac{1}{2}\nabla^2 + V_1(\mathbf{x}) + \frac{\delta}{2} + \beta_{11}|\tilde{\psi}_1|^2 + \beta_{12}|\tilde{\psi}_2|^2 \right] \tilde{\psi}_1 + \frac{\Omega}{2}e^{-i2k_0 x} \tilde{\psi}_2, \\ i\partial_t \tilde{\psi}_2 &= \left[-\frac{1}{2}\nabla^2 + V_2(\mathbf{x}) - \frac{\delta}{2} + \beta_{21}|\tilde{\psi}_1|^2 + \beta_{22}|\tilde{\psi}_2|^2 \right] \tilde{\psi}_2 + \frac{\Omega}{2}e^{i2k_0 x} \tilde{\psi}_1. \end{aligned}$$

For any $\Omega \in \mathbb{R}$, the CGPEs (1.14) conserve the normalization (1.10), i.e., $N(t) = \|\tilde{\Psi}(\cdot, t)\|^2 \equiv \|\tilde{\Psi}(\mathbf{x}, 0)\|^2 = 1$ for $t \geq 0$ with $\tilde{\Psi} = (\tilde{\psi}_1, \tilde{\psi}_2)^T$ and the energy per particle,

$$(1.15) \quad \begin{aligned} \tilde{E}(\tilde{\Psi}) &= \int_{\mathbb{R}^d} \left[\sum_{j=1}^2 \left(\frac{1}{2}|\nabla \tilde{\psi}_j|^2 + V_j(\mathbf{x})|\tilde{\psi}_j|^2 \right) + \frac{\delta}{2} \left(|\tilde{\psi}_1|^2 - |\tilde{\psi}_2|^2 \right) + \Omega \operatorname{Re}(e^{i2k_0 x} \tilde{\psi}_1 \bar{\tilde{\psi}}_2) \right. \\ &\quad \left. + \frac{\beta_{11}}{2}|\tilde{\psi}_1|^4 + \frac{\beta_{22}}{2}|\tilde{\psi}_2|^4 + \beta_{12}|\tilde{\psi}_1|^2|\tilde{\psi}_2|^2 \right] d\mathbf{x}. \end{aligned}$$

In fact, different proposals resulting in different theoretical models have been proposed in the literature for realizing SO-coupled BECs in experiments [30, 25, 16, 34, 13, 18]. Based on these proposed mean field models, including the CGPEs (1.8), ground state structures and dynamical properties of SO-coupled BECs have been theoretically studied and predicted in the literature, including spin-1 ground states [32], phase transition [18], spin vortex structure [13, 26, 27], motion of the center-of-mass [36], Bogoliubov excitation [37], etc. To the best of our knowledge, only the model described by the CGPEs (1.8) has been realized experimentally for an SO-coupled BEC [25, 16, 34]. Other models have not yet been realized in experiments. Thus, we will present our results on ground states and dynamics of SO-coupled BECs based on the CGPEs (1.8). We remark that our methods and results are still valid for other theoretical models for SO-coupled BECs found in the literature [30, 16, 34, 13, 18].

For the CGPEs (1.8), when $k_0 = 0$, i.e., a two-component BEC without SO coupling and without/with Raman coupling corresponding to $\Omega = 0/\Omega \neq 0$, ground state structures and dynamical properties have been studied theoretically in the literature [4, 11, 24, 5, 28, 35]. When the SO coupling is taken into consideration, i.e., $k_0 \neq 0$, when $\Omega = 0$, it can be easily removed from the CGPEs (1.8) via (1.13), and thus the SO coupling has no essential effect on the system. Therefore, in order to observe the effect of the SO coupling, Ω must be chosen nonzero. To the best of our knowledge, in the literature there exist very few mathematical results to the CGPEs (1.8) when $k_0 \neq 0$ and $\Omega \neq 0$. The main aim of this paper is to mathematically study the existence of ground states and their structures, as well as dynamical properties of SO-coupled BECs based on the CGPEs (1.8), and to propose efficient and accurate methods for numerically simulating ground states and dynamics.

The paper is organized as follows. In section 2, we establish existence and non-existence results of ground states under different parameter regimes and obtain their limiting behaviors and/or structures with different combinations of the SO and Raman coupling strengths. In section 3, we present efficient and accurate numerical methods for computing ground states and dynamics of SO-coupled BECs and report

ground states for different parameter regimes. In section 4, we derive dynamical properties on the motion of the center-of-mass and compare them with numerical results. In section 5, we obtain the semiclassical limit of the CGPEs in the linear case via the Wigner transform method. Finally, some conclusions are drawn in section 6. Throughout the paper, we adopt the standard notation of Sobolev spaces.

2. Ground states. The ground state $\Phi_g := \Phi_g(\mathbf{x}) = (\phi_1^g(\mathbf{x}), \phi_2^g(\mathbf{x}))^T$ of a two-component SO-coupled BEC based on (1.8) is defined as the minimizer of the energy functional (1.11) under the constraint (1.10); i.e., find $\Phi_g \in S$ such that

$$(2.1) \quad E_g := E(\Phi_g) = \min_{\Phi \in S} E(\Phi),$$

where S is defined as

$$(2.2) \quad S := \left\{ \Phi = (\phi_1, \phi_2)^T \in H^1(\mathbb{R}^d)^2 \mid \|\Phi\|^2 = \int_{\mathbb{R}^d} (|\phi_1(\mathbf{x})|^2 + |\phi_2(\mathbf{x})|^2) d\mathbf{x} = 1 \right\}.$$

Since S is a nonconvex set, the problem (2.1) is a nonconvex minimization problem. In addition, the ground state Φ_g is a solution to the following nonlinear eigenvalue problem, i.e., Euler–Lagrange equation of the problem (2.1):

$$(2.3) \quad \begin{aligned} \mu\phi_1 &= \left[-\frac{1}{2}\nabla^2 + V_1(\mathbf{x}) + ik_0\partial_x + \frac{\delta}{2} + (\beta_{11}|\phi_1|^2 + \beta_{12}|\phi_2|^2) \right] \phi_1 + \frac{\Omega}{2}\phi_2, \\ \mu\phi_2 &= \left[-\frac{1}{2}\nabla^2 + V_2(\mathbf{x}) - ik_0\partial_x - \frac{\delta}{2} + (\beta_{12}|\phi_1|^2 + \beta_{22}|\phi_2|^2) \right] \phi_2 + \frac{\Omega}{2}\phi_1 \end{aligned}$$

under the normalization constraint $\Phi \in S$. For an eigenfunction $\Phi = (\phi_1, \phi_2)^T$ of (2.3), its corresponding eigenvalue (or chemical potential in the physics literature) $\mu := \mu(\Phi) = \mu(\phi_1, \phi_2)$ can be computed as

$$(2.4) \quad \mu = E(\Phi) + \int_{\mathbb{R}^d} \left(\frac{\beta_{11}}{2}|\phi_1|^4 + \frac{\beta_{22}}{2}|\phi_2|^4 + \beta_{12}|\phi_1|^2|\phi_2|^2 \right) d\mathbf{x}.$$

Similarly, the ground state $\tilde{\Phi}_g = (\tilde{\phi}_1^g, \tilde{\phi}_2^g)^T \in S$ of (1.14) is defined as follows: Find $\tilde{\Phi}_g \in S$ such that

$$(2.5) \quad \tilde{E}_g := \tilde{E}(\tilde{\Phi}_g) = \min_{\tilde{\Phi} \in S} \tilde{E}(\tilde{\Phi}).$$

We notice that the ground state $\Phi_g = (\phi_1^g, \phi_2^g)^T$ given by (2.1) has one-to-one correspondence with the ground state $\tilde{\Phi}_g = (\tilde{\phi}_1^g, \tilde{\phi}_2^g)^T$ given by (2.5) through the relation

$$(2.6) \quad \Phi_g = (\phi_1^g, \phi_2^g)^T = (e^{ik_0x}\tilde{\phi}_1^g, e^{-ik_0x}\tilde{\phi}_2^g)^T \iff \tilde{\Phi}_g = (\tilde{\phi}_1^g, \tilde{\phi}_2^g)^T = (e^{-ik_0x}\phi_1^g, e^{ik_0x}\phi_2^g)^T.$$

In what follows, the $\tilde{\cdot}$ acting on $\Phi = (\phi_1, \phi_2)^T$ always means that

$$(2.7) \quad \tilde{\Phi} = (\tilde{\phi}_1, \tilde{\phi}_2)^T = (e^{-ik_0x}\phi_1, e^{ik_0x}\phi_2)^T \iff \Phi = (\phi_1, \phi_2)^T = (e^{ik_0x}\tilde{\phi}_1, e^{-ik_0x}\tilde{\phi}_2)^T,$$

and the following equality holds:

$$(2.8) \quad E(\Phi) = \tilde{E}(\tilde{\Phi}) - \frac{k_0^2}{2}\|\Phi\|^2 = \tilde{E}(\tilde{\Phi}) - \frac{k_0^2}{2}\|\tilde{\Phi}\|^2.$$

In particular, $E(\Phi) = \tilde{E}(\tilde{\Phi}) - \frac{k_0^2}{2}$ for $\Phi \in S$.

When $k_0 = 0$, the existence and uniqueness, as well as nonexistence results of the ground state of the problem (2.1), have been studied in [5]. Hereafter, we assume $k_0 \neq 0$.

2.1. Existence and uniqueness. In 2D, i.e., $d = 2$, let C_b be the best constant in the inequality [31]

$$(2.9) \quad C_b := \inf_{0 \neq f \in H^1(\mathbb{R}^2)} \frac{\|\nabla f\|_{L^2(\mathbb{R}^2)}^2 \|f\|_{L^2(\mathbb{R}^2)}^2}{\|f\|_{L^4(\mathbb{R}^2)}^4} = \frac{1}{\pi \cdot (1.86225\dots)}.$$

Define the function $I(\mathbf{x})$ as

$$(2.10) \quad I(\mathbf{x}) = (V_1(\mathbf{x}) - V_2(\mathbf{x}) + \delta)^2 + (\beta_{11} - \beta_{12})^2 + (\beta_{12} - \beta_{22})^2,$$

where $I(\mathbf{x}) \equiv 0$ means that the SO-coupled BEC with $k_0 = \Omega = 0$ is essentially one component; denote the interaction coefficient matrix as

$$(2.11) \quad A = \begin{pmatrix} \beta_{11} & \beta_{12} \\ \beta_{21} & \beta_{22} \end{pmatrix} = A^T,$$

where A is nonnegative if $\beta_{jl} \geq 0$ ($j, l = 1, 2$).

Introduce the function space

$$X = \left\{ (\phi_1, \phi_2)^T \in H^1(\mathbb{R}^d) \times H^1(\mathbb{R}^d) \mid \int_{\mathbb{R}^d} (V_1(\mathbf{x})|\phi_1(\mathbf{x})|^2 + V_2(\mathbf{x})|\phi_2(\mathbf{x})|^2) d\mathbf{x} < \infty \right\};$$

then the following embedding results hold [5].

LEMMA 2.1. *Under the assumption that $V_j(\mathbf{x}) \geq 0$ ($j = 1, 2$) for $\mathbf{x} \in \mathbb{R}^d$ are confining potentials, i.e., $\lim_{|\mathbf{x}| \rightarrow \infty} V_j(\mathbf{x}) = \infty$ ($j = 1, 2$), we have that the embedding $X \hookrightarrow L^{p_1}(\mathbb{R}^d) \times L^{p_2}(\mathbb{R}^d)$ is compact provided that exponents p_1 and p_2 satisfy that (i) $p_1, p_2 \in [2, 6)$ when $d = 3$, (ii) $p_1, p_2 \in [2, \infty)$ when $d = 2$, and (iii) $p_1, p_2 \in [2, \infty)$ when $d = 1$.*

Then for the existence and uniqueness of the problem (2.1) or (2.5), we have the following.

THEOREM 2.2 (existence and uniqueness). *Suppose $V_j(\mathbf{x}) \geq 0$ ($j = 1, 2$) satisfying $\lim_{|\mathbf{x}| \rightarrow \infty} V_j(\mathbf{x}) = \infty$; then there exists a minimizer $\Phi_g = (\phi_1^g, \phi_2^g)^T \in S$ of (2.1) if one of the following conditions holds:*

- (i) $d = 3$ and the matrix A is either semipositive definite or nonnegative.
- (ii) $d = 2$, $\beta_{11} > -C_b$, $\beta_{22} > -C_b$, and $\beta_{12} \geq -C_b - \sqrt{(C_b + \beta_{11})(C_b + \beta_{22})}$.
- (iii) $d = 1$.

In addition, $e^{i\theta_0} \Phi_g$ is also a ground state of (2.1) for any $\theta_0 \in [0, 2\pi)$. In particular, when $\Omega = 0$, the ground state is unique up to a constant phase factor if the matrix A is semipositive definite and $I(\mathbf{x}) \not\equiv 0$ (2.10). In contrast, there exists no ground state of (2.1) if one of the following holds:

- (i) $d = 3$ $\beta_{11} < 0$ or $\beta_{22} < 0$ or $\beta_{12} < 0$ with $\beta_{12}^2 > \beta_{11}\beta_{22}$.
- (ii) $d = 2$, $\beta_{11} < -C_b$ or $\beta_{22} < -C_b$ or $\beta_{12} < -C_b - \sqrt{(C_b + \beta_{11})(C_b + \beta_{22})}$.

Proof. The proof is similar to that for the case when $k_0 = 0$ in [5] via the formulation (2.5), and the details are omitted here for brevity. \square

2.2. Properties in different limiting parameter regimes. From now on, we assume that the conditions for the existence of ground states in Theorem 2.2 hold.

Introducing an auxiliary energy functional $\tilde{E}_0(\tilde{\Phi})$ for $\tilde{\Phi} = (\tilde{\phi}_1, \tilde{\phi}_2)^T$,

$$\begin{aligned} \tilde{E}_0(\tilde{\Phi}) = \int_{\mathbb{R}^d} & \left[\sum_{j=1}^2 \left(\frac{1}{2} |\nabla \tilde{\phi}_j|^2 + V_j(\mathbf{x}) |\tilde{\phi}_j|^2 \right) + \frac{\delta}{2} (|\tilde{\phi}_1|^2 - |\tilde{\phi}_2|^2) + \frac{\beta_{11}}{2} |\tilde{\phi}_1|^4 + \frac{\beta_{22}}{2} |\tilde{\phi}_2|^4 \right. \\ (2.12) \quad & \left. + \beta_{12} |\tilde{\phi}_1|^2 |\tilde{\phi}_2|^2 \right] d\mathbf{x} = \tilde{E}(\tilde{\Phi}) - \Omega \int_{\mathbb{R}^d} \operatorname{Re}(e^{i2k_0 x} \tilde{\phi}_1 \overline{\tilde{\phi}_2}) d\mathbf{x}, \end{aligned}$$

we know that the nonconvex minimization problem

$$(2.13) \quad \tilde{E}_g^{(0)} := \tilde{E}_0(\tilde{\Phi}_g^{(0)}) = \min_{\tilde{\Phi} \in S} \tilde{E}_0(\tilde{\Phi})$$

admits a unique positive minimizer $\tilde{\Phi}_g^{(0)} = (\tilde{\phi}_1^{g,0}, \tilde{\phi}_2^{g,0})^T \in S$ if the matrix A is semipositive definite and $I(\mathbf{x}) \not\equiv 0$ (2.10) [5]. For a given $k_0 \in \mathbb{R}$, let $\tilde{\Phi}^{k_0} = (\tilde{\phi}_1^{k_0}, \tilde{\phi}_2^{k_0})^T \in S$ be a ground state of (2.5) when all other parameters are fixed; then we have the following.

THEOREM 2.3 (large k_0 limit). *Suppose the matrix A is semipositive definite and $I(\mathbf{x}) \not\equiv 0$ (2.10). When $k_0 \rightarrow \infty$, we have that the ground state $\tilde{\Phi}^{k_0} = (\tilde{\phi}_1^{k_0}, \tilde{\phi}_2^{k_0})^T$ of (2.5) converges to a ground state of (2.13) in $L^{p_1} \times L^{p_2}$ sense with p_1, p_2 given in Lemma 2.1; i.e., there exist constants $\theta_{k_0} \in [0, 2\pi)$ such that $e^{i\theta_{k_0}} (\tilde{\phi}_1^{k_0}, \tilde{\phi}_2^{k_0})^T$ converge to the unique positive ground state $\tilde{\Phi}_g^{(0)}$ of (2.13). In other words, large k_0 in the CGPEs (1.14) will remove the effect of Raman coupling Ω ; i.e., large k_0 limit is effectively letting $\Omega \rightarrow 0$.*

Proof. Let $\tilde{\Phi}^{k_0} = (\tilde{\phi}_1^{k_0}, \tilde{\phi}_2^{k_0})^T \in S$ be a ground state of (2.5); then we have

$$(2.14) \quad \tilde{E}(\tilde{\Phi}^{k_0}) \leq \tilde{E}_g^{(0)} = \min_{\tilde{\Phi} \in S} \tilde{E}_0(\tilde{\Phi}),$$

where $\tilde{E}_g^{(0)}$ is attained at the unique positive ground state of $\tilde{E}_0(\cdot)$ in (2.13).

Under the condition of the theorem, we know that $(\tilde{\phi}_1^{k_0}, \tilde{\phi}_2^{k_0})^T \in S$ is a bounded sequence in X . Hence, for any-sequence $\{k_0^m\}_{m=1}^\infty$ with $k_0^m \rightarrow \infty$, there exists a subsequence $(\tilde{\phi}_1^{k_0^m}, \tilde{\phi}_2^{k_0^m})^T$ (denoted as the original sequence for simplicity) such that

$$(2.15) \quad (\tilde{\phi}_1^{k_0^m}, \tilde{\phi}_2^{k_0^m})^T \rightharpoonup (\tilde{\phi}_1^\infty, \tilde{\phi}_2^\infty)^T \in X \text{ weakly.}$$

Lemma 2.1 ensures that such convergence is strong in $L^{p_1} \times L^{p_2}$. In particular, we get

$$(2.16) \quad \tilde{E}_0(\tilde{\phi}_1^\infty, \tilde{\phi}_2^\infty) \leq \liminf_{k_0^m \rightarrow \infty} \tilde{E}_0(\tilde{\phi}_1^{k_0^m}, \tilde{\phi}_2^{k_0^m})$$

and $(\tilde{\phi}_1^\infty, \tilde{\phi}_2^\infty)^T \in S$. Recalling that

$$\begin{aligned} \Omega \int_{\mathbb{R}^d} \operatorname{Re} \left(e^{2k_0^m ix} \tilde{\phi}_1^{k_0^m} \overline{\tilde{\phi}_2^{k_0^m}} \right) d\mathbf{x} &= \Omega \int_{\mathbb{R}^d} \operatorname{Re} \left(e^{2k_0^m ix} \left(\tilde{\phi}_1^{k_0^m} - \tilde{\phi}_1^\infty \right) \overline{\tilde{\phi}_2^{k_0^m}} \right) d\mathbf{x} \\ &+ \Omega \int_{\mathbb{R}^d} \operatorname{Re} \left(e^{2k_0^m ix} \tilde{\phi}_1^\infty \left(\overline{\tilde{\phi}_2^{k_0^m}} - \overline{\tilde{\phi}_2^\infty} \right) \right) d\mathbf{x} + \Omega \int_{\mathbb{R}^d} \operatorname{Re} \left(e^{2k_0^m ix} \tilde{\phi}_1^\infty \overline{\tilde{\phi}_2^\infty} \right) d\mathbf{x}, \end{aligned}$$

using the $L^{p_1} \times L^{p_2}$ convergence of $(\tilde{\phi}_1^{k_0^m}, \tilde{\phi}_2^{k_0^m})^T$ and the Riemann–Lebesgue lemma, we deduce that

$$(2.17) \quad \lim_{k_0^m \rightarrow \infty} \Omega \int_{\mathbb{R}^d} \operatorname{Re} \left(e^{2k_0^m ix} \tilde{\phi}_1^{k_0^m} \overline{\tilde{\phi}_2^{k_0^m}} \right) d\mathbf{x} = 0.$$

Hence,

$$(2.18) \quad \tilde{E}_0(\tilde{\phi}_1^\infty, \tilde{\phi}_2^\infty) \leq \liminf_{k_0^m \rightarrow \infty} \tilde{E}_0(\phi_1^{k_0^m}, \phi_2^{k_0^m}) \leq \liminf_{k_0^m \rightarrow \infty} \tilde{E}(\phi_1^{k_0^m}, \phi_2^{k_0^m}) \leq E_g^{(0)}.$$

This means $(\phi_1^\infty, \phi_2^\infty)^T \in S$ is also a minimizer of the energy (2.12) in the nonconvex set S . The rest then follows from the fact that the ground state of (2.12) is unique up to a constant phase factor. \square

Remark 2.4. Under the assumption of Theorem 2.3 and $\Omega = o(|k_0|)$ as $k_0 \rightarrow \infty$, the conclusion of Theorem 2.3 still holds (see details in Theorem 2.10). In fact, Theorem 2.3 holds when the matrix A is nonnegative, but the limiting profile is nonunique since there is no uniqueness for the positive ground state $\Phi_g^{(0)}$ of (2.13) [5].

Thus, we conclude the following for the ground state of CGPEs (1.8) given by the minimization problem (2.1) when $k_0 \rightarrow \infty$.

THEOREM 2.5 (large k_0 limit). *Suppose the matrix A is semipositive definite and $I(\mathbf{x}) \not\equiv 0$ (2.10). When $k_0 \rightarrow \infty$, the ground state $\Phi_g^{k_0} = (\phi_1^g, \phi_2^g)^T$ of (2.1) corresponds to a ground state $\tilde{\Phi}_g^{k_0} = (e^{ik_0x} \tilde{\phi}_1^{g,0}, e^{-ik_0x} \tilde{\phi}_2^{g,0})^T$ of (2.5) (see (2.7)), where $\tilde{\Phi}_g^{k_0}$ converges to a ground state of (2.13); i.e., for some $\theta_{k_0} \in [0, 2\pi)$, $e^{i\theta_{k_0}}(e^{-ik_0x} \phi_1^g, e^{ik_0x} \phi_2^g)^T$ converge to the positive ground state $\tilde{\Phi}_g^{(0)}$ of (2.13) in $L^{p_1} \times L^{p_2}$ sense, where p_1, p_2 are given in Lemma 2.1. In other words, large k_0 will remove the effect of Raman coupling Ω in the CGPEs (1.8).*

Analogous to the case of the two-component BEC without SO coupling [5], i.e., $k_0 = 0$, we have the following results.

THEOREM 2.6 (large Ω limit). *Suppose the matrix A is either semipositive definite or nonnegative. When $|\Omega| \rightarrow \infty$, the ground state Φ_g of (2.1) converges to a state $(\phi_g, \text{sgn}(-\Omega)\phi_g)^T$ in $L^{p_1} \times L^{p_2}$ sense, where p_1, p_2 are given in Lemma 2.1; i.e., large Ω will remove the effect of k_0 in the CGPEs (1.8). Here ϕ_g minimizes the following energy under the constraint $\|\phi_g\|^2 := \int_{\mathbb{R}^d} |\phi_g(\mathbf{x})|^2 d\mathbf{x} = 1/2$:*

$$(2.19) \quad E_s(\phi) = \int_{\mathbb{R}^d} \left[\frac{1}{2} |\nabla \phi|^2 + \frac{V_1(\mathbf{x}) + V_2(\mathbf{x})}{2} |\phi|^2 + \frac{\beta_{11} + \beta_{22} + 2\beta_{12}}{4} |\phi|^4 \right] d\mathbf{x},$$

where ϕ_g is unique up to a constant phase shift and can be chosen as strictly positive.

THEOREM 2.7 (large δ limit). *Assume the matrix A is either semipositive definite or nonnegative. When $\delta \rightarrow +\infty$, the ground state Φ_g of (2.1) converges to a state $(0, \phi_g)^T$ in $L^{p_1} \times L^{p_2}$ sense, where p_1, p_2 are given in Lemma 2.1. Here ϕ_g minimizes the following energy under the constraint $\|\phi_g\| = 1$:*

$$E_1(\phi) = \int_{\mathbb{R}^d} \left[\frac{1}{2} |\nabla \phi|^2 + V_2(\mathbf{x}) |\phi|^2 - ik_0 \bar{\phi} \partial_x \phi + \frac{\beta_{22}}{2} |\phi|^4 \right] d\mathbf{x},$$

and such a ϕ_g is unique up to a constant phase shift. When $\delta \rightarrow -\infty$, the ground state Φ_g of (2.1) converges to a state $(\varphi_g, 0)^T$, where φ_g minimizes the following energy under the constraint $\|\varphi_g\| = 1$:

$$E_2(\varphi) = \int_{\mathbb{R}^d} \left[\frac{1}{2} |\nabla \varphi|^2 + V_1(\mathbf{x}) |\varphi|^2 + ik_0 \bar{\varphi} \partial_x \varphi + \frac{\beta_{11}}{2} |\varphi|^4 \right] d\mathbf{x},$$

and such a φ_g is unique up to a constant phase shift.

2.3. Convergence rate. From the discussion in the previous section, we find that the appearance of SO coupling term k_0 causes a new transition in the ground states of the CGPEs (1.8) [5]. When $k_0 = 0$, i.e., there is no SO coupling, the ground state $\Phi_g = (\phi_1^g, \phi_2^g)^T$ of (2.1) can be chosen as real functions $\phi_1^g = |\phi_1^g|$ and $\phi_2^g = -\text{sgn}(\Omega)|\phi_2^g|$ [5]. When $k_0 \rightarrow \infty$, $\tilde{\Phi}_g = (e^{-ik_0x}\phi_1^g, e^{ik_0x}\phi_2^g)$ of (2.7) will converge to the ground state of (2.13) (see Theorem 2.5); i.e., it is equivalent to letting $\Omega = 0$ in the large k_0 limit. Here, we are going to characterize the convergence rates of the ground state Φ_g of (2.1) in the above two cases, i.e., $k_0 \rightarrow 0$ and $k_0 \rightarrow \infty$.

For small k_0 , it is convenient to rewrite the energy (1.11) for $\Phi = (\phi_1, \phi_2)^T$ as

$$(2.20) \quad E(\Phi) = \int_{\mathbb{R}^d} \left[\sum_{j=1}^2 \left(\frac{1}{2} |(\nabla + i(3-2j)k_0\mathbf{e}_x)\phi_j|^2 + V_j(\mathbf{x})|\phi_j|^2 \right) + \frac{\delta}{2} (|\phi_1|^2 - |\phi_2|^2) + \frac{\beta_{11}}{2} |\phi_1|^4 + \frac{\beta_{22}}{2} |\phi_2|^4 + \beta_{12} |\phi_1|^2 |\phi_2|^2 + \Omega \cdot \text{Re}(\phi_1 \bar{\phi}_2) \right] d\mathbf{x} - \frac{k_0^2}{2} \|\Phi\|^2,$$

where \mathbf{e}_x is the unite vector of the x axis, and we denote

$$E_0(\Phi) = E(\Phi) - \int_{\mathbb{R}^d} (ik_0\bar{\phi}_1\partial_x\phi_1 - ik_0\bar{\phi}_2\partial_x\phi_2) d\mathbf{x},$$

with $E_0(\cdot)$ being the energy of the CGPEs (1.8) when $k_0 = 0$.

Without loss of generality, we assume $\Omega < 0$.

THEOREM 2.8. *Suppose $\Omega < 0$, $\lim_{|\mathbf{x}| \rightarrow \infty} V_j(\mathbf{x}) = \infty$ ($j = 1, 2$), and the matrix A is semipositive definite. Denoting $\hat{\Phi}_g = (\varphi_1^g, \varphi_2^g)^T \in S$ as the unique nonnegative ground state of $E_0(\Phi)$ in S [5], there exists a constant $C > 0$ independent of k_0 such that the ground state $\Phi_g = (\phi_1^g, \phi_2^g)^T \in S$ of (2.1) satisfies*

$$(2.21) \quad \|\phi_1^g - \varphi_1^g\| + \|\phi_2^g - \varphi_2^g\| \leq C|k_0|.$$

Proof. First, recalling (2.12) and (2.20), we have the lower bound of $E_g = E(\phi_1^g, \phi_2^g)$ as [5, 22]

$$(2.22) \quad E(\phi_1^g, \phi_2^g) \geq \tilde{E}_0(|\phi_1^g|, |\phi_2^g|) - |\Omega| \int_{\mathbb{R}^d} |\phi_1^g| |\phi_2^g| d\mathbf{x} - \frac{k_0^2}{2} = E_0(|\phi_1^g|, |\phi_2^g|) - \frac{k_0^2}{2},$$

and the upper bound

$$(2.23) \quad E(\phi_1^g, \phi_2^g) \leq E(\varphi_1^g, \varphi_2^g) = E_0(\varphi_1^g, \varphi_2^g).$$

Hence, $E_0(|\phi_1^g|, |\phi_2^g|) - E_0(\varphi_1^g, \varphi_2^g) \leq \frac{k_0^2}{2}$. In addition, $(\varphi_1^g, \varphi_2^g)^T \in S$ satisfies the nonlinear eigenvalue problem

$$(2.24) \quad \begin{aligned} \mu_1 \varphi_1^g &= \left[-\frac{1}{2} \nabla^2 + V_1(\mathbf{x}) + \frac{\delta}{2} + (\beta_{11} |\varphi_1^g|^2 + \beta_{12} |\varphi_2^g|^2) \right] \varphi_1^g + \frac{\Omega}{2} \varphi_2^g, \\ \mu_1 \varphi_2^g &= \left[-\frac{1}{2} \nabla^2 + V_2(\mathbf{x}) - \frac{\delta}{2} + (\beta_{12} |\varphi_1^g|^2 + \beta_{22} |\varphi_2^g|^2) \right] \varphi_2^g + \frac{\Omega}{2} \varphi_1^g, \end{aligned}$$

where μ_1 is the corresponding eigenvalue (or chemical potential). For this nonlinear eigenvalue problem, we denote the linearized operator L acting on $\Phi = (\phi_1, \phi_2)^T$ as

$$(2.25) \quad L\Phi = \begin{pmatrix} L_1 & \frac{\Omega}{2} \\ \frac{\Omega}{2} & L_2 \end{pmatrix} \Phi, \quad L_j = -\frac{1}{2} \nabla^2 + V_j(\mathbf{x}) + \frac{\delta}{2} (3-2j) + \sum_{l=1}^2 \beta_{jl} |\varphi_l^g|^2, \quad j = 1, 2.$$

It is clear that $(\varphi_1^g, \varphi_2^g)^T$ is an eigenfunction of L with eigenvalue μ_1 , and by the nonnegativity of $(\varphi_1^g, \varphi_2^g)^T$, μ_1 is the smallest eigenvalue. In fact, the eigenfunctions $(\varphi_1^k, \varphi_2^k)^T \in S$ ($k = 1, 2, \dots$) of L correspond to eigenvalue μ_k , which can be arranged in nondecreasing order, i.e., μ_k is nondecreasing. The eigenfunctions form an orthonormal basis of $L^2(\mathbb{R}^d) \times L^2(\mathbb{R}^d)$ and $\mu_1 < \mu_2$ with $(\varphi_1^g, \varphi_2^g)^T = (\varphi_1^1, \varphi_2^1)$ (nonnegative ground state is unique).

Denoting $\Phi_e = (\phi_1^e, \phi_2^e)^T := (|\phi_1^g| - \varphi_1^g, |\phi_2^g| - \varphi_2^g)$ and using the Euler–Lagrange equation for $(\varphi_1^g, \varphi_2^g)^T \in S$, we find

$$E_0(|\phi_1^g|, |\phi_2^g|) = \int_{\mathbb{R}^d} \left(\sum_{j=1}^2 \frac{\beta_{jj}}{2} (|\phi_j^g|^2 - |\varphi_j^g|^2)^2 + \beta_{12} (|\phi_1^g|^2 - |\varphi_1^g|^2) (|\phi_2^g|^2 - |\varphi_2^g|^2) \right) d\mathbf{x} \\ + E_0(\varphi_1^g, \varphi_2^g) + \int_{\mathbb{R}^d} \Phi_e^T L \Phi_e d\mathbf{x} - \mu_1 \|\Phi_e\|^2.$$

Using the fact that $L + c$ ($c \geq 0$ sufficiently large) induces an equivalent norm in X , we can take expansion $(\phi_1^e, \phi_2^e)^T = \sum_{k=1}^\infty c_k (\varphi_1^k, \varphi_2^k)^T$ with $\sum_{k=1}^\infty c_k^2 = \|\Phi_e\|^2$ and estimate

$$\int_{\mathbb{R}^d} \Phi_e^T L \Phi_e d\mathbf{x} = \sum_{k=1}^\infty \mu_k c_k^2 \geq \mu_1 c_1^2 + \mu_2 (\|\Phi_e\|^2 - c_1^2),$$

with $c_1 = \frac{1}{2} \|\Phi_e\|^2 = \frac{1}{2} (\| |\phi_1^g| - \varphi_1^g \|^2 + \| |\phi_2^g| - \varphi_2^g \|^2) < 1$. Hence, we obtain

$$E_0(|\phi_1^g|, |\phi_2^g|) - E_0(\varphi_1^g, \varphi_2^g) \geq (\mu_2 - \mu_1)(2c_1 - c_1^2) \geq (\mu_2 - \mu_1)c_1.$$

Since the gap $\mu_2 - \mu_1$ is independent of k_0 , we draw the conclusion from (2.21). \square

For large k_0 , we have similar results.

THEOREM 2.9. *Suppose $\Omega < 0$, $\lim_{|\mathbf{x}| \rightarrow \infty} V_j(\mathbf{x}) = \infty$ ($j = 1, 2$), the matrix A is semipositive definite, and $I(\mathbf{x}) \not\equiv 0$. Denoting $\tilde{\Phi}_g^{(0)} = (\tilde{\phi}_1^{g,0}, \tilde{\phi}_2^{g,0})^T \in S$ as the unique nonnegative ground state of (2.13) (minimizer of $\tilde{E}_0(\cdot)$ of (2.12) in S), there exists a constant $C > 0$ independent of k_0 such that the ground state $\Phi_g = (\phi_1^g, \phi_2^g)^T \in S$ of (2.1) satisfies*

$$(2.26) \quad \| |\phi_1^g| - \tilde{\phi}_1^{g,0} \| + \| |\phi_2^g| - \tilde{\phi}_2^{g,0} \| \leq C/\sqrt{k_0}.$$

Proof. From (2.7), we know $\tilde{\Phi}_g = (\tilde{\phi}_1^g, \tilde{\phi}_2^g)^T = (e^{-ik_0x} \phi_1^g, e^{ik_0x} \phi_2^g)^T$ minimizes the energy \tilde{E} in (2.5). Noticing

$$\Omega \int_{\mathbb{R}^d} \operatorname{Re}(e^{i2k_0x} \tilde{\phi}_1^g \overline{\tilde{\phi}_2^g}) d\mathbf{x} = \frac{-\Omega}{2k_0} \int_{\mathbb{R}^d} \operatorname{Re} \left(ie^{i2k_0x} \partial_x \tilde{\phi}_1^g \overline{\tilde{\phi}_2^g} + ie^{i2k_0x} \tilde{\phi}_1^g \partial_x \overline{\tilde{\phi}_2^g} \right) d\mathbf{x} \\ \geq -\varepsilon (\|\partial_x \tilde{\phi}_1^g\|^2 + \|\partial_x \tilde{\phi}_2^g\|^2) - \frac{\Omega^2}{4\varepsilon k_0^2} (\|\tilde{\phi}_1^g\|^2 + \|\tilde{\phi}_2^g\|^2), \quad \varepsilon > 0,$$

we find

$$\tilde{E}(\tilde{\phi}_1^g, \tilde{\phi}_2^g) \geq \tilde{E}_0(\tilde{\phi}_1^g, \tilde{\phi}_2^g) - \frac{1}{4} (\|\partial_x \tilde{\phi}_1^g\|^2 + \|\partial_x \tilde{\phi}_2^g\|^2) - \frac{\Omega^2}{k_0^2}.$$

On the other hand, we have

$$\tilde{E}(\tilde{\phi}_1^g, \tilde{\phi}_2^g) \leq \tilde{E}(\tilde{\phi}_1^{g,0}, \tilde{\phi}_2^{g,0}) \leq \tilde{E}_0(\tilde{\phi}_1^{g,0}, \tilde{\phi}_2^{g,0}) + \frac{C_1|\Omega|}{k_0},$$

where $C_1 > 0$ is a constant. Thus, we know

$$\|\tilde{\Phi}^g\|_X^2 \leq C(1 + \Omega^2/k_0^2),$$

and it follows that for large k_0 ,

$$\tilde{E}(\tilde{\phi}_1^g, \tilde{\phi}_2^g) \geq \tilde{E}_0(\tilde{\phi}_1^g, \tilde{\phi}_2^g) - C_2 \frac{|\Omega|}{|k_0|} \|\tilde{\Phi}^g\|_X \geq \tilde{E}_0(\tilde{\phi}_1^g, \tilde{\phi}_2^g) - C_3 \frac{|\Omega|}{|k_0|},$$

where C_2 and C_3 are two positive constant. We then conclude that

$$\tilde{E}_0(|\tilde{\phi}_1^g|, |\tilde{\phi}_2^g|) \leq \tilde{E}_0(\tilde{\phi}_1^g, \tilde{\phi}_2^g) \leq \tilde{E}(\tilde{\phi}_1^g, \tilde{\phi}_2^g) + \frac{C_3|\Omega|}{|k_0|} \leq \tilde{E}_0(\tilde{\phi}_1^{g,0}, \tilde{\phi}_2^{g,0}) + \frac{C|\Omega|}{|k_0|}.$$

The rest of the proof is similar to that in Theorem 2.8 and is omitted here. \square

2.4. Competition between Ω and k_0 . In the previous subsection, we found that large Raman coupling Ω will remove the effect of SO coupling k_0 in the asymptotic profile of the ground states of (2.1), and the reverse is true; i.e., there is competition between these two parameters. Here, we are going to study how the relation between k_0 and Ω affects the ground state profile of (2.1). The results are summarized as follows.

THEOREM 2.10. *Suppose $\lim_{|\mathbf{x}| \rightarrow \infty} V_j(\mathbf{x}) = \infty$ ($j = 1, 2$) and the matrix A is either semipositive definite or nonnegative; then we have the following:*

(i) *If $|\Omega|/|k_0|^2 \gg 1$, $|\Omega| \rightarrow \infty$, the ground state $\Phi_g = (\phi_1^g, \phi_2^g)^T$ of (2.1) for the CGPEs (1.8) converges to a state $(\phi_g, \text{sgn}(-\Omega)\phi_g)^T$, where ϕ_g minimizes the energy (2.19) under the constraint $\|\phi_g\| = 1/\sqrt{2}$; i.e., the conclusion of Theorem 2.6 holds.*

(ii) *If $|\Omega|/|k_0| \ll 1$, $|k_0| \rightarrow \infty$, the ground state $\Phi_g = (\phi_1^g, \phi_2^g)^T$ of (2.1) for the CGPEs (1.8) converges to a state $(e^{-ik_0x}\tilde{\phi}_1^{g,0}, e^{ik_0x}\tilde{\phi}_2^{g,0})^T$, where $\tilde{\Phi}_g^{(0)} = (\tilde{\phi}_1^{g,0}, \tilde{\phi}_2^{g,0})^T$ is a ground state of (2.13) for the energy $E_s(\cdot)$ in (2.12); i.e., the conclusion of Theorem 2.5 holds.*

(iii) *If $|k_0| \ll |\Omega| \ll |k_0|^2$ and $|k_0| \rightarrow \infty$, the leading order of the ground state energy $E_g := E(\Phi_g)$ of (2.1) for the CGPEs (1.8) is given by $E_g = -\frac{k_0^2}{2} - C_0 \frac{|\Omega|^2}{|k_0|^2} + o(\frac{|\Omega|^2}{|k_0|^2})$, where $C_0 > 0$ is a generic constant.*

Proof. Without loss of generality, we assume $\Omega < 0$.

(i) It is obvious that Φ_g also minimizes the following energy for $\Phi = (\phi_1, \phi_2)^T \in S$:

$$E(\Phi) = -\frac{|\Omega|}{2} + \int_{\mathbb{R}^d} \left[\sum_{j=1}^2 \left(\frac{1}{2} |\nabla \phi_j|^2 + V_j(\mathbf{x}) |\phi_j|^2 \right) + \frac{\delta}{2} (|\phi_1|^2 - |\phi_2|^2) + ik_0 \bar{\phi}_1 \partial_x \phi_1 - ik_0 \bar{\phi}_2 \partial_x \phi_2 + \frac{\beta_{11}}{2} |\phi_1|^4 + \frac{\beta_{22}}{2} |\phi_2|^4 + \beta_{12} |\phi_1|^2 |\phi_2|^2 + \frac{|\Omega|}{2} |\phi_1 - \phi_2|^2 \right] d\mathbf{x}.$$

A simple choice of testing state $(\phi_g, \phi_g)^T \in S$ shows that $E(\cdot) + \frac{|\Omega|}{2}$ is uniformly bounded from above, i.e.,

$$(2.27) \quad E_g + \frac{|\Omega|}{2} = E(\Phi_g) + \frac{|\Omega|}{2} \leq E(\phi_g, \phi_g) + \frac{|\Omega|}{2} = 2E_s(\phi_g) := 2E_s^g.$$

To get a lower bound for E_g , using Cauchy inequality, we have for any $\varepsilon > 0$,

$$\begin{aligned} \int_{\mathbb{R}^d} ik_0 (\bar{\phi}_1 \partial_x \phi_1 - \bar{\phi}_2 \partial_x \phi_2) d\mathbf{x} &= \int_{\mathbb{R}^d} ik_0 [(\bar{\phi}_1 - \bar{\phi}_2) \partial_x \phi_1 - (\phi_1 - \phi_2) \partial_x \bar{\phi}_2] d\mathbf{x} \\ &\geq -\frac{\varepsilon}{2} (\|\partial_x \phi_1\|^2 + \|\partial_x \phi_2\|^2) - \frac{k_0^2}{2\varepsilon} \|\phi_1 - \phi_2\|^2. \end{aligned}$$

Hence, by setting $\varepsilon = 1$ in the above inequality and recalling $\|\phi_1 - \phi_2\| \leq \sqrt{2}$ for $\Phi = (\phi_1, \phi_2)^T \in S$, we bound E_g from below by

$$(2.28) \quad E_g + \frac{|\Omega|}{2} \geq -\frac{|\delta|}{2} - \frac{k_0^2}{2} + \frac{|\Omega|}{2} \|\phi_1^g - \phi_2^g\|^2.$$

Combining the upper and lower bounds of $E_g + \frac{|\Omega|}{2}$, we get

$$(2.29) \quad \|\phi_1^g - \phi_2^g\| \leq \frac{4E_g + |\delta|}{|\Omega|} + \frac{k_0^2}{|\Omega|}.$$

If $k_0^2/|\Omega| = o(1)$ and $|\Omega| \rightarrow \infty$, we see $\phi_1^g - \phi_2^g \rightarrow 0$ in L^2 , and the ground state sequence $\Phi_g = (\phi_1^g, \phi_2^g)^T$ is bounded in X . Analogous to the proof of Theorem 2.5 and that in [5], we can draw the conclusion, and the details are omitted.

(ii) It is equivalent to prove that, in this case, the ground state $\tilde{\Phi}_g = (\tilde{\phi}_1^g, \tilde{\phi}_2^g)^T = (e^{-ik_0x}\phi_1^g, e^{ik_0x}\phi_2^g)^T$ of (2.5) converges to the ground state of (2.13). Using integration by parts and Cauchy inequality, we get

$$(2.30) \quad \begin{aligned} \Omega \int_{\mathbb{R}^d} \operatorname{Re}(e^{i2k_0x} \tilde{\phi}_1^g \overline{\tilde{\phi}_2^g}) \, d\mathbf{x} &= \frac{\Omega}{2k_0} \int_{\mathbb{R}^d} \operatorname{Re} \left(ie^{i2k_0x} \left(\partial_x \tilde{\phi}_1^g \overline{\tilde{\phi}_2^g} + \tilde{\phi}_1^g \partial_x \overline{\tilde{\phi}_2^g} \right) \right) \, d\mathbf{x} \\ &\geq -\frac{|\Omega|}{2|k_0|} (\|\partial_x \tilde{\phi}_1^g\| \|\tilde{\phi}_2^g\| + \|\partial_x \tilde{\phi}_2^g\| \|\tilde{\phi}_1^g\|). \end{aligned}$$

Having this in hand, we can proceed as in the proof of Theorem 2.5.

(iii) Similarly to case (ii), we need only consider the ground state $\tilde{\Phi}_g = (\tilde{\phi}_1^g, \tilde{\phi}_2^g)^T \in S$ of (2.5). Applying the Cauchy inequality in (2.30), we have

$$(2.31) \quad \Omega \int_{\mathbb{R}^d} \operatorname{Re}(e^{2k_0ix} \tilde{\phi}_1^g \overline{\tilde{\phi}_2^g}) \, d\mathbf{x} \geq -\frac{1}{4} \|\partial_x \tilde{\phi}_1^g\| - \frac{1}{4} \|\partial_x \tilde{\phi}_2^g\| - \frac{2|\Omega|^2}{|k_0|^2}.$$

By choosing sufficiently smooth (e.g., $H^3 \cap X$) test states for $\tilde{E}(\cdot)$ and using integration by parts as in (2.30), it is straightforward to get the upper bound

$$(2.32) \quad \tilde{E}(\tilde{\phi}_1^g, \tilde{\phi}_2^g) \leq C + \frac{|\Omega|}{|k_0|^3}.$$

Combining (2.31) and (2.32), we find that

$$(2.33) \quad \tilde{E}(\tilde{\phi}_1^g, \tilde{\phi}_2^g) \geq C - \frac{2|\Omega|^2}{|k_0|^2}, \quad \|\tilde{\Phi}_g\|_X^2 \leq C + \frac{2|\Omega|^2}{|k_0|^2} + \frac{|\Omega|}{|k_0|^3} \leq C \frac{|\Omega|^2}{|k_0|^2}.$$

Then it follows from (2.30) that

$$(2.34) \quad \left| \Omega \int_{\mathbb{R}^d} \operatorname{Re}(e^{2k_0ix} \tilde{\phi}_1^g \overline{\tilde{\phi}_2^g}) \, d\mathbf{x} \right| \leq \frac{|\Omega|}{|k_0|} \|\tilde{\Phi}_g\|_X = O\left(\frac{|\Omega|^2}{|k_0|^2}\right).$$

On the other hand, we can choose test states as follows. In 1D, let $\rho(x)$ be a C_0^∞ even real-valued function with $\|\rho\| = \sqrt{2}/2$ and choose

$$(2.35) \quad \tilde{\phi}_1(x) = N_\varepsilon \rho(x)[1 - \varepsilon \cos(2k_0x)], \quad \tilde{\phi}_2(x) = N_\varepsilon \rho(x),$$

where N_ε is a normalization constant to ensure that $(\tilde{\phi}_1, \tilde{\phi}_2)^T \in S$. We will choose $\varepsilon = O(|\Omega|/|k_0|^2)$ (see below). Using integration by parts, it is not difficult to see that $N_\varepsilon = 1 + O(\varepsilon^2)$ for large k_0 . Recalling $\tilde{E}_0(\cdot)$ in (2.12), we can calculate

$$(2.36) \quad \tilde{E}_0(\tilde{\phi}_1, \tilde{\phi}_2) = C_1 + C_2 \varepsilon^2 |k_0|^2 + o(\varepsilon^2 |k_0|^2), \quad C_2 > 0,$$

and

$$\begin{aligned} \frac{\Omega}{N_\varepsilon} \int_{\mathbb{R}} \operatorname{Re}(e^{2k_0ix} \tilde{\phi}_1 \bar{\phi}_2) dx &= \Omega \int_{\mathbb{R}} \operatorname{Re}(e^{2k_0ix} \rho^2(x)) dx + \varepsilon \Omega \int_{\mathbb{R}} \cos^2(2k_0x) \rho^2(x) dx \\ &= \frac{\varepsilon \Omega}{2} \int_{\mathbb{R}} \rho^2(x) dx + \frac{\Omega}{2} \int_{\mathbb{R}} [2 \cos(2k_0x) + \cos(4k_0x)] \rho^2(x) dx, \end{aligned}$$

where the second integral on the right-hand side is of arbitrary order at $O(|\Omega|/|k_0|^m)$ ($m \geq 0$) by using integration by parts and the property of $\rho(x)$. Hence, we find for large k_0

$$(2.37) \quad \Omega \int_{\mathbb{R}} \operatorname{Re}(e^{2k_0ix} \tilde{\phi}_1 \bar{\phi}_2) dx = -\frac{|\Omega|\varepsilon}{4} + O\left(|\Omega|\varepsilon^3 + \frac{|\Omega|}{|k_0|^4}\right).$$

Now, we get from (2.12), (2.36), and (2.37) that

$$(2.38) \quad \tilde{E}(\tilde{\phi}_1, \tilde{\phi}_2) = C_1 + C_2 \varepsilon^2 |k_0|^2 - |\Omega|\varepsilon/4 + O\left(|\Omega|\varepsilon^3 + \frac{|\Omega|}{|k_0|^4}\right).$$

Since $|\Omega| \ll |k_0|^2$, we can choose $\varepsilon = \gamma|\Omega|/|k_0|^2$ and $0 < \gamma \leq \frac{1}{8C_2}$ such that the term $C_2 \varepsilon^2 |k_0|^2 = C_2 \gamma |\Omega| \varepsilon \leq \frac{|\Omega|\varepsilon}{8}$. So, we arrive at

$$(2.39) \quad \tilde{E}(\tilde{\phi}_1^g, \tilde{\phi}_2^g) \leq \tilde{E}(\tilde{\phi}_1, \tilde{\phi}_2) \leq C - \frac{|\Omega|^2 \gamma}{8|k_0|^2} + o\left(\frac{|\Omega|^2}{|k_0|^2}\right).$$

In 2D and 3D, similar constructions will show the same estimates. Thus the conclusion is an immediate consequence of (2.8), (2.33), and (2.39). \square

Remark 2.11. For $|k_0| \ll |\Omega| \ll |k_0|^2$, the ground state of (2.1) is very complicated. The ground state energy expansion indicates that $-k_0^2/2$ is the leading order term and is much larger than the next order term. In such a situation, the above theorem shows that the ground state $\Phi_g \approx (e^{ik_0x} |\phi_1^g|, e^{-ik_0x} |\phi_2^g|)^T$, and oscillation of ground state densities $|\phi_j^g|^2$ ($j = 1, 2$) may occur at the order of $O(|\Omega|/|k_0|^2)$ in amplitude and k_0 in frequency. Such density oscillation is predicted in the physics literature [20, 21] and is known as the density modulation. It is of great interest to identify the constant C_0 in the conclusion (iii).

3. Numerical methods and results. In this section, we present efficient and accurate numerical methods for computing the ground states based on (2.1) (or (2.5)) and dynamics based on the CGPEs (1.8) (or (1.14)) for the SO-coupled BEC.

3.1. Computing ground states. Let $t_n = n\tau$ ($n = 0, 1, 2, \dots$) be the time steps with $\tau > 0$ as the time step. In order to compute the ground state $\Phi_g = (\phi_1^g, \phi_2^g)^T$ of (2.1) for an SO-coupled BEC, we propose the following gradient flow with discrete normalization (GFDN), which is widely used in computing the ground states of BEC [4, 5, 6, 8] and is also known as the imaginary time method in the physics literature. In detail, we evolve an initial state $\Phi_0 := (\phi_1^{(0)}, \phi_2^{(0)})^T$ through the following GFDN:

$$(3.1) \quad \begin{aligned} \partial_t \phi_1 &= \left[\frac{1}{2} \nabla^2 - V_1(\mathbf{x}) - ik_0 \partial_x - \frac{\delta}{2} - \sum_{l=1}^2 \beta_{1l} |\phi_l|^2 \right] \phi_1 - \frac{\Omega}{2} \phi_2, \quad t \in [t_n, t_{n+1}), \\ \partial_t \phi_2 &= \left[\frac{1}{2} \nabla^2 - V_2(\mathbf{x}) + ik_0 \partial_x + \frac{\delta}{2} - \sum_{l=1}^2 \beta_{2l} |\phi_l|^2 \right] \phi_2 - \frac{\Omega}{2} \phi_1, \quad t \in [t_n, t_{n+1}), \\ \phi_1(\mathbf{x}, t_{n+1}) &= \frac{\phi_1(\mathbf{x}, t_{n+1}^-)}{\|\Phi(\cdot, t_{n+1}^-)\|}, \quad \phi_2(\mathbf{x}, t_{n+1}) = \frac{\phi_2(\mathbf{x}, t_{n+1}^-)}{\|\Phi(\cdot, t_{n+1}^-)\|}, \quad \mathbf{x} \in \mathbb{R}^d, \\ \phi_1(\mathbf{x}, 0) &= \phi_1^{(0)}(\mathbf{x}), \quad \phi_2(\mathbf{x}, 0) = \phi_2^{(0)}(\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^d. \end{aligned}$$

Due to the confining potentials $V_1(\mathbf{x})$ and $V_2(\mathbf{x})$, the ground state $\Phi_g(\mathbf{x})$ decays exponentially fast when $|\mathbf{x}| \rightarrow \infty$, and thus in practical computations, the above GFDN (3.1) is first truncated on a bounded large computational domain U , e.g., an interval $[a, b]$ in 1D, a rectangle $[a, b] \times [c, d]$ in 2D, and a box $[a, b] \times [c, d] \times [e, f]$ in 3D, with periodic boundary conditions. Then the GFDN on U can be further discretized in space via the pseudospectral method with the Fourier basis or second-order central finite difference method and in time via the backward Euler scheme [6, 7, 8]. For details, we refer the reader to [5, 6, 7, 8] and references therein.

Remark 3.1. If the box potential

$$(3.2) \quad V_{\text{box}}(\mathbf{x}) = \begin{cases} 0, & \mathbf{x} \in U, \\ +\infty & \text{otherwise} \end{cases}$$

is used in the CGPEs (1.8) instead of the harmonic potentials (1.9), due to the appearance of the SO coupling, in order to compute the ground state, it is better to construct the GFDN based on (2.5) and then discretize it via the backward Euler sine pseudospectral (BESP) method due to the fact that the homogeneous Dirichlet boundary condition on ∂U must be used in this case. Again, for details, we refer the reader to [5, 6, 7, 8] and references therein.

To test the efficiency and accuracy of the above numerical method for computing the ground state of SO-coupled BECs, we take $d = 2$, $\delta = 0$, $\beta_{11} : \beta_{12} : \beta_{22} = 1 : 0.9 : 0.9$ with $\beta_{11} = 10$ in (1.8). The potential $V_j(\mathbf{x})$ ($j = 1, 2$) is taken as the box potential given in (3.2) with $U = [-1, 1] \times [-1, 1]$. We compute the ground state via the above BESP method with mesh size $h = \frac{1}{128}$ and time step $\tau = 0.01$ ($\tau = 0.001$ for large Ω). For the chosen parameters, it is easy to find that when $\Omega = 0$, the ground state Φ_g satisfies $\phi_1^g = 0$ [4, 5]. Figure 1 shows the ground state $\tilde{\Phi}_g = (\tilde{\phi}_1^g, \tilde{\phi}_2^g)$ of (2.5) with $\Omega = 50$ for different k_0 , which clearly demonstrates that as $k_0 \rightarrow \infty$ the effect of Ω disappears. This is consistent with Theorem 2.3. Figure 2 depicts the ground state Φ_g with $k_0 = 10$ for different Ω , from which we can observe that ϕ_1^g and ϕ_2^g tend to have the same density profile with opposite phase. This confirms Theorem 2.6.

3.2. Computing dynamics. In order to compute the dynamics of an SO-coupled BEC based on the CGPEs (1.8), we usually truncate it onto a bounded computational domain U , e.g., an interval $[a, b]$ in 1D, a rectangle $[a, b] \times [c, d]$ in 2D, and a box $[a, b] \times [c, d] \times [e, f]$ in 3D, equipped with periodic boundary conditions. Then the CGPEs (1.8) can be solved via a time-splitting technique to decouple the nonlinearity [9, 4, 6, 2]. From t_n to t_{n+1} , one first solves for $\mathbf{x} \in U$

$$(3.3) \quad i\partial_t \psi_1 = \left(-\frac{1}{2}\Delta + ik_0\partial_x + \frac{\delta}{2} \right) \psi_1 + \frac{\Omega}{2}\psi_2, \quad i\partial_t \psi_2 = -\left(\frac{1}{2}\Delta + ik_0\partial_x + \frac{\delta}{2} \right) \psi_2 + \frac{\Omega}{2}\psi_1$$

for time τ , followed by solving

$$(3.4) \quad i\partial_t \psi_j = (V_j(\mathbf{x}) + \beta_{j1}|\psi_1|^2 + \beta_{j2}|\psi_2|^2) \psi_j, \quad j = 1, 2, \quad \mathbf{x} \in U,$$

for another time τ . Equation (3.3) with periodic boundary conditions can be discretized by the Fourier spectral method in space and then integrated in time *exactly* [9, 4, 6, 2]. Equation (3.4) leaves the densities $|\psi_1|$ and $|\psi_2|$ unchanged and it can be integrated in time *exactly* [9, 4, 6, 2]. Then a full discretization scheme can be con-

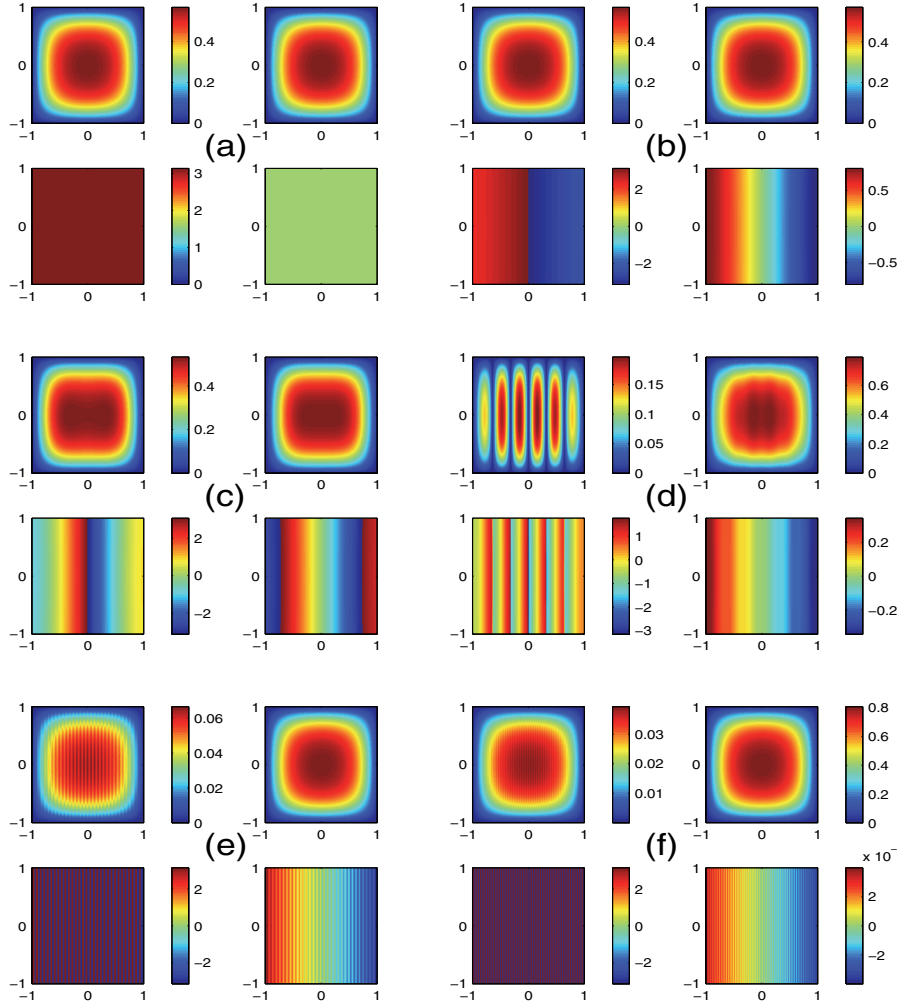


FIG. 1. Ground states $\tilde{\Phi}_g = (\tilde{\phi}_1^g, \tilde{\phi}_2^g)^T$ for an SO-coupled BEC in 2D with $\Omega = 50$, $\delta = 0$, $\beta_{11} = 10$, $\beta_{12} = \beta_{21} = \beta_{22} = 9$ for (a) $k_0 = 0$, (b) $k_0 = 1$, (c) $k_0 = 5$, (d) $k_0 = 10$, (e) $k_0 = 50$, and (f) $k_0 = 100$. In each subplot, the top panels show densities and the bottom panels show phases of the ground state $\tilde{\phi}_1^g$ (left column) and $\tilde{\phi}_2^g$ (right column).

structed via a combination of the splitting steps (3.3) and (3.4) with a second-order or higher-order time-splitting methods [9, 4, 6, 2].

For the convenience of the reader, here we present the method in 1D for simplicity of notation. Extensions to 2D and 3D are straightforward. In 1D, let $h = \Delta x = (b - a)/N$ (N an even positive integer) and $x_j = a + jh$ ($j = 0, \dots, N$), let $\Psi_j^n = (\psi_{1,j}^n, \psi_{2,j}^n)^T$ be the numerical approximation of $\Psi(x_j, t_n) = (\psi_1(x_j, t_n), \psi_2(x_j, t_n))^T$, and, for each fixed $l = 1, 2$, denote ψ_l^n as the vector consisting of $\psi_{l,j}^n$ for $j = 0, 1, \dots, N - 1$. From time $t = t_n$ to $t = t_{n+1}$, a second-order time-splitting Fourier

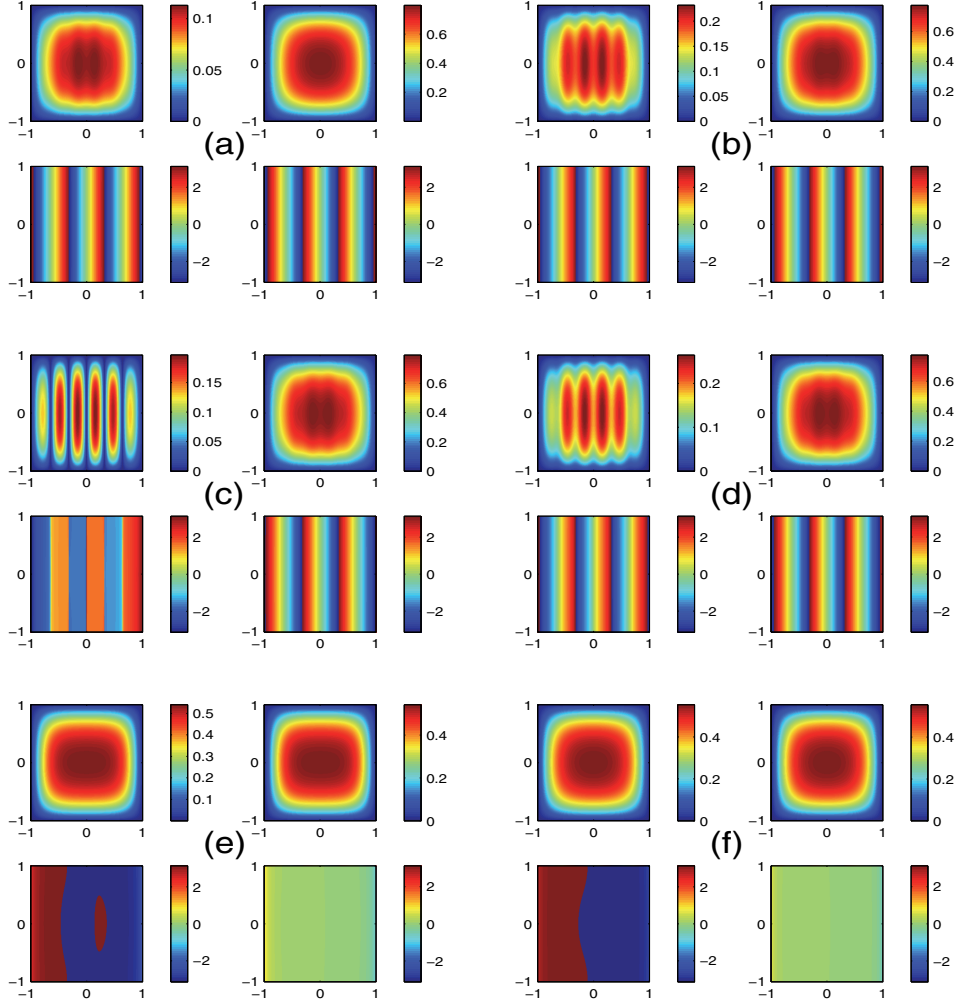


FIG. 2. Ground states $\Phi_g = (\phi_1^g, \phi_2^g)^T$ for an SO -coupled BEC in 2D with $k_0 = 10$, $\delta = 0$, $\beta_{11} = 10$, $\beta_{12} = \beta_{21} = \beta_{22} = 9$ for (a) $\Omega = 1$, (b) $\Omega = 10$, (c) $\Omega = 50$, (d) $\Omega = 200$, (e) $\Omega = 300$, and (f) $\Omega = 500$. In each subplot, top panels show densities and bottom panels show phases of the ground state ϕ_1^g (left column) and ϕ_2^g (right column).

pseudospectral (TSFP) method for the CGPEs (1.8) in 1D reads [9, 6, 2]

$$\begin{aligned}
 \Psi_j^{(1)} &= \frac{1}{N} \sum_{k=-N/2}^{N/2-1} e^{i\mu_k(x_j-a)} Q_k^T e^{-\frac{i\tau}{4}U_k} Q_k(\widetilde{\Psi}^n)_k, \\
 \Psi_j^{(2)} &= e^{-i\tau P_j^{(1)}} \Psi_j^{(1)}, \quad j = 0, 1, \dots, N-1, \\
 \Psi_j^{n+1} &= \frac{1}{N} \sum_{k=-N/2}^{N/2-1} e^{i\mu_k(x_j-a)} Q_k^T e^{-\frac{i\tau}{4}U_k} Q_k(\widetilde{\Psi}^{(2)})_k,
 \end{aligned}
 \tag{3.5}$$

where for each fixed $k = -\frac{N}{2}, -\frac{N}{2} + 1, \dots, \frac{N}{2} - 1$, $\mu_k = \frac{2k\pi}{b-a}$, and $(\tilde{\Psi}^n)_k = ((\tilde{\psi}_1^n)_k, (\tilde{\psi}_2^n)_k)^T$ with $(\tilde{\psi}_l^n)_k$ being the discrete Fourier transform coefficients of ψ_l^n ($l = 1, 2$), $U_k = \text{diag}(\mu_k^2 + 2\lambda_k, \mu_k^2 - 2\lambda_k)$ is a diagonal matrix, and

$$Q_k = \begin{pmatrix} \frac{\sqrt{\lambda_k - \chi_k}}{\sqrt{2\lambda_k}} & \frac{\frac{\Omega}{2}}{\sqrt{2\lambda_k(\lambda_k - \chi_k)}} \\ -\frac{\sqrt{\lambda_k + \chi_k}}{\sqrt{2\lambda_k}} & \frac{\frac{\Omega}{2}}{\sqrt{2\lambda_k(\lambda_k + \chi_k)}} \end{pmatrix} \quad \text{with} \quad \chi_k = k_0\mu_k - \frac{\delta}{2}, \quad \lambda_k = \frac{1}{2}\sqrt{4\chi_k^2 + \Omega^2},$$

and

$$P_j^{(1)} = \text{diag} \left(V_1(x_j) + \sum_{l=1}^2 \beta_{1l} |\psi_{l,j}^{(1)}|^2, V_2(x_j) + \sum_{l=1}^2 \beta_{2l} |\psi_{l,j}^{(1)}|^2 \right)$$

for $j = 0, 1, \dots, N-1$.

3.3. Box potential case. In some recent experiments of SO-coupled BECs, the box potential (3.2) is used. In this situation, due to the fact that the homogeneous Dirichlet boundary condition on ∂U must be used for the CGPEs (1.8), similarly to the computation of the ground states, it is better to adopt the CGPEs (1.14) for computing the dynamics. From $t = t_n$ to t_{n+1} , the CGPEs (1.14) will be split into the following three steps due to the appearance of the SO coupling. One first solves

$$(3.6) \quad i\partial_t \tilde{\psi}_1 = \left(-\frac{1}{2}\Delta + \frac{\delta}{2} \right) \tilde{\psi}_1, \quad i\partial_t \tilde{\psi}_2 = \left(-\frac{1}{2}\Delta - \frac{\delta}{2} \right) \tilde{\psi}_2, \quad \mathbf{x} \in U,$$

for time step τ , then solves

$$(3.7) \quad i\partial_t \tilde{\psi}_j = \left(V_j(\mathbf{x}) + \beta_{j1} |\tilde{\psi}_1|^2 + \beta_{j2} |\tilde{\psi}_2|^2 \right) \tilde{\psi}_j, \quad j = 1, 2, \quad \mathbf{x} \in U,$$

for time step τ , followed by solving

$$(3.8) \quad i\partial_t \tilde{\psi}_1 = \frac{\Omega}{2} e^{-i2k_0 x} \tilde{\psi}_2, \quad i\partial_t \tilde{\psi}_2 = \frac{\Omega}{2} e^{i2k_0 x} \tilde{\psi}_1, \quad \mathbf{x} \in U,$$

for time step τ . Again, (3.6) with homogeneous Dirichlet boundary conditions can be discretized by the sine spectral method in space and then integrated in time *exactly* [9, 4, 6, 2]. Equation (3.7) leaves the densities $|\tilde{\psi}_1|$ and $|\tilde{\psi}_2|$ unchanged and it can be integrated in time *exactly* [9, 4, 6, 2]. In addition, (3.8) is a linear ODE and can be integrated in time *exactly* as

$$(3.9) \quad \tilde{\Psi}(\mathbf{x}, t_{n+1}) = T(x)^* e^{-i\tau\Omega J} T(x) \tilde{\Psi}(\mathbf{x}, t_n) \quad \text{with} \quad T(x) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & e^{-i2k_0 x} \\ -1 & e^{-i2k_0 x} \end{pmatrix},$$

where $J = \text{diag}(1, -1)$ and $T(x)^* = \overline{T(x)}^T$ is the adjoint matrix of $T(x)$. Then a full discretization scheme can be constructed via a combination of the splitting steps (3.6)–(3.8) with a second-order method [9, 4, 6, 2]. The details are omitted here for brevity.

4. Dynamics of center-of-mass. In this section, we study the dynamics of the center-of-mass of an SO-coupled BEC by using the CGPEs (1.8).

4.1. General initial data. Let $\Psi = (\psi_1, \psi_2)^T$ be the wave function describing the SO-coupled BEC, which is governed by the CGPEs (1.8). Define the center-of-mass of the BEC as

$$(4.1) \quad \mathbf{x}_c(t) = \int_{\mathbb{R}^d} \mathbf{x} \sum_{j=1}^2 |\psi_j(\mathbf{x}, t)|^2 d\mathbf{x}, \quad t \geq 0,$$

and the momentum as

$$(4.2) \quad \mathbf{P}(t) = \int_{\mathbb{R}^d} \sum_{j=1}^2 \text{Im} \left(\overline{\psi_j(\mathbf{x}, t)} \nabla \psi_j(\mathbf{x}, t) \right) d\mathbf{x}, \quad t \geq 0,$$

where $\text{Im}(f)$ denotes the imaginary part of the function f . In addition, we introduce the difference between the masses $N_1(t)$ and $N_2(t)$ in (1.12) of the two components in the SO-coupled BEC as

$$(4.3) \quad \delta_N(t) := N_1(t) - N_2(t) = \int_{\mathbb{R}^d} [|\psi_1(\mathbf{x}, t)|^2 - |\psi_2(\mathbf{x}, t)|^2] d\mathbf{x}, \quad t \geq 0.$$

Then the following lemma holds.

LEMMA 4.1. *Let $V_1(\mathbf{x}) = V_2(\mathbf{x})$ be the d -dimensional ($d = 1, 2, 3$) harmonic potentials given in (1.9); then the motion of the center-of-mass $\mathbf{x}_c(t)$ for the CGPEs (1.8) is governed by*

$$(4.4) \quad \ddot{\mathbf{x}}_c(t) = -\Lambda \mathbf{x}_c(t) - 2k_0\Omega \text{Im} \left(\int_{\mathbb{R}^d} \overline{\psi_1(\mathbf{x}, t)} \psi_2(\mathbf{x}, t) d\mathbf{x} \right) \mathbf{e}_x, \quad t > 0,$$

where Λ is a $d \times d$ diagonal matrix with $\Lambda = \gamma_x^2$ in 1D ($d = 1$), $\Lambda = \text{diag}(\gamma_x^2, \gamma_y^2)$ in 2D ($d = 2$), and $\Lambda = \text{diag}(\gamma_x^2, \gamma_y^2, \gamma_z^2)$ in 3D ($d = 3$), and \mathbf{e}_x is the unit vector for the x axis. The initial conditions for (4.4) are given as

$$\mathbf{x}_c(0) = \int_{\mathbb{R}^d} \mathbf{x} \sum_{j=1}^2 |\psi_j(\mathbf{x}, 0)|^2 d\mathbf{x}, \quad \dot{\mathbf{x}}_c(0) = \mathbf{P}(0) - k_0\delta_N(0) \mathbf{e}_x.$$

In particular, (4.4) implies that the center-of-mass $\mathbf{x}_c(t)$ is periodic in the y -component with frequency γ_y when $d = 2, 3$, and in the z -component with frequency γ_z when $d = 3$. If $k_0\Omega = 0$, $\mathbf{x}_c(t)$ is also periodic in the x -component with frequency γ_x .

Proof. For $j = 1, 2$, differentiating $\mathbf{x}_j(t) = \int_{\mathbb{R}^d} \mathbf{x} |\psi_j(\mathbf{x}, t)|^2 d\mathbf{x}$, using the CGPEs (1.8) and integral by parts, we find

$$\dot{\mathbf{x}}_j(t) = \mathbf{P}_j(t) - k_0(3 - 2j)N_j(t) \mathbf{e}_x - \frac{i\Omega}{2} \int_{\mathbb{R}^d} \mathbf{x} (\overline{\psi_j} \psi_{3-j} - \psi_j \overline{\psi_{3-j}}) d\mathbf{x},$$

where $\mathbf{P}_j(t) := \int_{\mathbb{R}^d} \text{Im}(\overline{\psi_j(\mathbf{x}, t)} \nabla \psi_j(\mathbf{x}, t)) d\mathbf{x}$. Summing the above equation for $j = 1, 2$ and noticing (4.1) and (4.2), we get

$$(4.5) \quad \dot{\mathbf{x}}_c(t) = \mathbf{P}(t) - k_0\delta_N(t) \mathbf{e}_x, \quad t \geq 0.$$

Differentiating (4.5) once more, we get

$$(4.6) \quad \ddot{\mathbf{x}}_c(t) = \dot{\mathbf{P}}(t) - k_0\dot{\delta}_N(t) \mathbf{e}_x.$$

We now compute the right-hand side of (4.6). First, for $j = 1, 2$, differentiating $\mathbf{P}_j(t)$, making use of the CGPEs (1.8) and integral by parts, we get

$$\dot{\mathbf{P}}_j(t) = \int_{\mathbb{R}^d} [-|\psi_j|^2 \nabla V_j(\mathbf{x}) - \beta_{12} |\psi_{3-j}|^2 \nabla |\psi_j|^2 + \Omega \operatorname{Re}(\overline{\psi_{3-j}} \nabla \psi_j)] \, d\mathbf{x},$$

which immediately gives

$$(4.7) \quad \dot{\mathbf{P}}(t) = - \int_{\mathbb{R}^d} \Lambda \mathbf{x} \sum_{j=1}^2 |\psi_j|^2 \, d\mathbf{x} = -\Lambda \mathbf{x}_c(t),$$

with Λ being the diagonal matrix described in the lemma. Second, for $j = 1, 2$, differentiating $N_j(t)$, making use of the CGPEs (1.8) and integral by parts, we obtain

$$\dot{N}_j(t) = -\frac{i\Omega}{2} \int_{\mathbb{R}^d} (\overline{\psi_j} \psi_{3-j} - \overline{\psi_{3-j}} \psi_j) \, d\mathbf{x},$$

which again immediately implies

$$(4.8) \quad \dot{\delta}_N(t) = 2\Omega \operatorname{Im} \int_{\mathbb{R}^d} \overline{\psi_1(\mathbf{x}, t)} \psi_2(\mathbf{x}, t) \, d\mathbf{x}.$$

Combining (4.8), (4.7), and (4.6), we draw the conclusion from (4.4). \square

From Lemma 4.1, the effect of SO coupling on the motion of the center-of-mass $\mathbf{x}_c(t)$ appears in the x -component. Denote the x -component of $\mathbf{x}_c(t)$ as $x_c(t)$ and the x -component of $\mathbf{P}(t)$ as $P^x(t)$. Then we have the following results.

THEOREM 4.2. *Let $V_1(\mathbf{x}) = V_2(\mathbf{x})$ be the harmonic potential as (1.9) in d -dimensions ($d = 1, 2, 3$) and $k_0\Omega \neq 0$. For the x -component $x_c(t)$ of the center-of-mass $\mathbf{x}_c(t)$ of the CGPEs (1.8) with any initial data $\Psi(\mathbf{x}, 0) := \Psi_0(\mathbf{x})$ satisfying $\|\Psi_0\| = 1$, we have*

$$(4.9) \quad x_c(t) = x_0 \cos(\gamma_x t) + \frac{P_0^x}{\gamma_x} \sin(\gamma_x t) - k_0 \int_0^t \cos(\gamma_x(t-s)) \delta_N(s) \, ds, \quad t \geq 0,$$

where $x_0 = \int_{\mathbb{R}^d} x \sum_{j=1}^2 |\psi_j(\mathbf{x}, 0)|^2 \, d\mathbf{x}$ and $P_0^x = \int_{\mathbb{R}^d} \sum_{j=1}^2 \operatorname{Im}(\overline{\psi_j(\mathbf{x}, 0)} \partial_x \psi_j(\mathbf{x}, 0)) \, d\mathbf{x}$. In addition, if $\delta \approx 0$, $|k_0|$ is small, $\beta_{11} \approx \beta$, $\beta_{12} = \beta_{21} \approx \beta$, and $\beta_{22} \approx \beta$ with β a fixed constant, we can approximate the solution $x_c(t)$ as follows:

(i) If $|\Omega| = \gamma_x$, we can get

$$(4.10) \quad x_c(t) \approx \left(x_0 - \frac{k_0}{2} \delta_N(0) t \right) \cos(\gamma_x t) + \frac{1}{\gamma_x} \left(P_0^x - \frac{k_0}{2} \delta_N(0) - \operatorname{sgn}(\Omega) \frac{\gamma_x k_0 C_0}{2} t \right) \sin(\gamma_x t),$$

where $C_0 = 2 \operatorname{Im} \int_{\mathbb{R}^d} \overline{\psi_1(\mathbf{x}, 0)} \psi_2(\mathbf{x}, 0) \, d\mathbf{x}$.

(ii) If $|\Omega| \neq \gamma_x$, we can get

$$(4.11) \quad \begin{aligned} x_c(t) \approx & \left(x_0 + \frac{k_0 C_0}{\gamma_x^2 - \Omega^2} \right) \cos(\gamma_x t) + \frac{1}{\gamma_x} \left(P_0^x - \frac{\gamma_x^2 k_0 \delta_N(0)}{\gamma_x^2 - \Omega^2} \right) \sin(\gamma_x t) \\ & - \frac{k_0 C_0}{\gamma_x^2 - \Omega^2} \cos(\Omega t) + \frac{k_0 \delta_N(0) \Omega}{\gamma_x^2 - \Omega^2} \sin(\Omega t). \end{aligned}$$

Based on the above approximation, if $|\Omega| = \gamma_x$ or $\frac{\Omega}{\gamma_x}$ is an irrational number, $x_c(t)$ is not periodic, and if $\frac{\Omega}{\gamma_x}$ is a rational number, $x_c(t)$ is a periodic function, but its frequency is different from the trapping frequency γ_x .

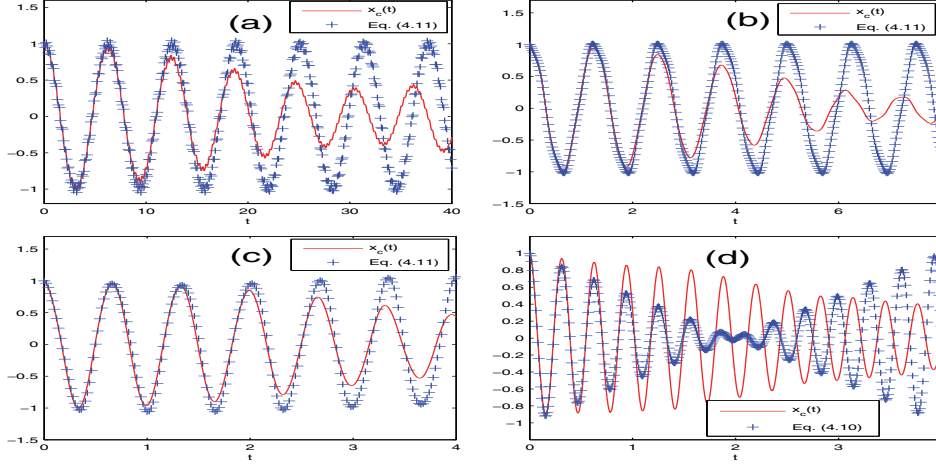


FIG. 3. Time evolution of the center-of-mass $x_c(t)$ for the CGPEs (1.8) obtained numerically from its numerical solution (i.e., labeled “ $x_c(t)$ ” with solid lines) and asymptotically as (4.10) and (4.11) in Theorem 4.2 (i.e., labeled by “Eq.” with “+ + +”) with $\Omega = 20$ and $k_0 = 1$ for different γ_x : (a) $\gamma_x = 1$, (b) $\gamma_x = 5$, (c) $\gamma_x = 3\pi$, and (d) $\gamma_x = 20$.

Proof. Solving (4.4) by the variation-of-constant formula and using (4.8), we have

$$x_c(t) = x_c(0) \cos(\gamma_x t) + \frac{P^x(0) - k_0 \delta_N(0)}{\gamma_x} \sin(\gamma_x t) - \frac{k_0}{\gamma_x} \int_0^t \cos(\gamma_x(t-s)) \dot{\delta}_N(s) ds,$$

and (4.9) follows by applying integration by parts.

In order to obtain the prescribed approximation, we first find the equation for $\delta_N(t)$. Differentiating (4.8) and using (1.8), we get

$$\begin{aligned} \ddot{\delta}_N(t) = & -\Omega^2 \delta_N(t) + 2\Omega \operatorname{Re} \int_{\mathbb{R}^d} [(V_1(\mathbf{x}) - V_2(\mathbf{x}) + \delta + (\beta_{11} - \beta_{21})|\psi_1|^2 \\ & + (\beta_{12} - \beta_{22})|\psi_2|^2) \overline{\psi_1} \psi_2 + ik_0 (\overline{\psi_1} \partial_x \psi_2 - \overline{\partial_x \psi_1} \psi_2)] d\mathbf{x}. \end{aligned}$$

Thus, if $|k_0|$ is small, $\delta \approx 0$, $\beta_{11} \approx \beta$, $\beta_{12} = \beta_{21} \approx \beta$, and $\beta_{22} \approx \beta$, the above equation is approximated by

$$(4.12) \quad \ddot{\delta}_N(t) \approx -\Omega^2 \delta_N(t),$$

and the initial condition $\dot{\delta}_N(0)$ can be obtained via (4.8) with $t = 0$. Solving the above ODE, we find

$$(4.13) \quad \delta_N(t) \approx \delta_N(0) \cos(\Omega t) + \frac{\dot{\delta}_N(0)}{\Omega} \sin(\Omega t).$$

Plugging (4.13) into (4.9), we obtain the approximate solution of $x_c(t)$. \square

To verify the asymptotic (or approximate) results for $x_c(t)$ in Theorem 4.2, we numerically solve the CGPEs (1.8) with (1.9) in 2D (i.e., $d = 2$), take $\beta_{11} = \beta_{12} = \beta_{22} = 1$, $\delta = 0$, and choose the initial data as

$$(4.14) \quad \psi_1(\mathbf{x}, 0) = \pi^{-1/2} e^{-\frac{|\mathbf{x}-\mathbf{x}_0|^2}{2}}, \quad \psi_2(\mathbf{x}, 0) = 0, \quad \mathbf{x} \in \mathbb{R}^2,$$

where $\mathbf{x}_0 = (1, 1)^T$. Figure 3 depicts time evolution of $x_c(t)$ obtained numerically and asymptotically as in Theorem 4.2 with $\Omega = 20$ and $k_0 = 1$ for different γ_x . From this figure, we see that for short time t , the approximation given in Theorem 4.2 is very accurate, and when $t \gg 1$, it becomes inaccurate, which is due to the fact that the assumption on $\delta_N(t)$ obeying (4.13) becomes inaccurate.

4.2. For ground state with a shift. Now we consider a special kind of initial data, i.e., shift of the ground state $\Phi_g = (\phi_1^g, \phi_2^g)^T$ of (2.1) for the CGPEs (1.8), i.e., the initial condition for (1.8) is chosen as

$$(4.15) \quad \psi_1(\mathbf{x}, 0) = \phi_1^g(\mathbf{x} - \mathbf{x}_0), \quad \psi_2(\mathbf{x}, 0) = \phi_2^g(\mathbf{x} - \mathbf{x}_0), \quad \mathbf{x} \in \mathbb{R}^d,$$

where $\mathbf{x}_0 = x_0$ in 1D, $\mathbf{x}_0 = (x_0, y_0)^T$ in 2D, and $\mathbf{x}_0 = (x_0, y_0, z_0)^T$ in 3D. Then we have the approximate dynamical law for the center-of-mass in the x -direction $x_c(t)$.

THEOREM 4.3. *Suppose $V_1(\mathbf{x}) = V_2(\mathbf{x})$ for $\mathbf{x} \in \mathbb{R}^d$ are harmonic potentials given in (1.9), and the initial data for the CGPEs (1.8) is taken as (4.15). Then we have*

(i) *when $\frac{|k_0|^2}{|\Omega|} \gg 1$, the dynamics of the center-of-mass $x_c(t)$ can be approximated by the ODE*

$$(4.16) \quad \ddot{x}_c(t) = -\gamma_x^2 x_c(t), \quad x_c(0) = x_0, \quad \dot{x}_c(0) = 0,$$

i.e., $x_c(t) = x_0 \cos(\gamma_x t)$, which is the same as the case without SO coupling k_0 ;

(ii) *when $\frac{|k_0|^2}{|\Omega|} \ll 1$, $\beta_{11} \approx \beta$, $\beta_{12} = \beta_{21} \approx \beta$, and $\beta_{22} \approx \beta$ with β a fixed constant, the dynamics of the center-of-mass $x_c(t)$ can be approximated by the ODE*

$$(4.17) \quad \dot{x}_c(t) = P^x(t) - \frac{k_0[2k_0 P^x(t) - \delta]}{\sqrt{[2k_0 P^x(t) - \delta]^2 + \Omega^2}}, \quad \dot{P}^x(t) = -\gamma_x^2 x_c(t), \quad t \geq 0,$$

with $x_c(0) = x_0$ and $P^x(0) = k_0 \delta_N(0)$. In particular, the solution to (4.17) is periodic, and, in general, its frequency is different with the trapping frequency γ_x .

Proof. (i) If $\frac{|k_0|^2}{|\Omega|} \gg 1$, we know from Theorem 2.10 and Remark 2.11 that the leading order of the ground state energy is given by $-k_0^2/2$ which ensures that the ground state $\Phi_g \approx (e^{ik_0x}|\phi_1^g|, e^{-ik_0x}|\phi_2^g|)^T$. As long as the energy increase due to the shift of Φ_g in (4.15) is much smaller compared to $k_0^2/2$, wave function $\Psi(\mathbf{x}, t) = (\psi_1, \psi_2)^T$ satisfying CGPEs (1.8) with initial value (4.15) preserves a similar profile. From (4.8), we see

$$(4.18) \quad \dot{\delta}_N(t) \approx \Omega \operatorname{Im} \int_{\mathbb{R}^d} e^{-i2k_0x} |\psi_1(\mathbf{x}, t)| |\psi_2(\mathbf{x}, t)| d\mathbf{x} = O(\Omega/|k_0|^m), \quad m \geq 1,$$

where m depends on the regularity of $|\psi_j(\mathbf{x}, t)|$. Noticing (4.8) and (4.4), assuming that the density $|\psi_j(\mathbf{x}, t)|$ ($j = 1, 2$) is smooth, we get $\ddot{x}_c(t) \approx -\gamma_x^2 x_c(t)$, and the initial values $x_c(0)$ and $\dot{x}_c(0)$ follow the property of ground state Φ_g .

(ii) The initial condition for the ODE (4.17) comes from the initial value (4.15) for the CGPEs (1.8). We will treat the BEC system as a uniform system $V_1(\mathbf{x}) = V_2(\mathbf{x}) = \text{constant}$ locally, i.e., a local density approximation (LDA). We begin with the uniform case. The wave function $\Psi = (\psi_1, \psi_2)^T$ is assumed to remain in the ground mode of the Hamiltonian during the evolution,

$$(4.19) \quad \mathbf{H} = \begin{pmatrix} -\frac{\nabla^2}{2} + ik_0 \partial_x + \frac{\delta}{2} + \beta |\Psi|^2 & \frac{\Omega}{2} \\ \frac{\Omega}{2} & -\frac{\nabla^2}{2} - ik_0 \partial_x - \frac{\delta}{2} + \beta |\Psi|^2 \end{pmatrix},$$

and be localized near the center-of-mass $\mathbf{x}_c(t)$ in physical space and near the momentum $\mathbf{P}(t)$ in the phase space. Thus, the wave function can be written as

$$(4.20) \quad \Psi = (\psi_1, \psi_2)^T = e^{i\xi \cdot (\mathbf{x} - \mathbf{x}_c(t))} \vec{v}, \quad \vec{v} \text{ is a vector in } \mathbb{C}^2,$$

and $\xi = (\xi_1, \dots, \xi_d)^T \in \mathbb{R}^d$ is centered around $\mathbf{P}(t)$. Plugging (4.20) into (4.19), we obtain a two-by-two matrix, and the two eigenvalues and the corresponding eigenvectors are

$$(4.21) \quad \mathcal{E}_\pm = \frac{|\xi|^2}{2} + \beta|\vec{v}|^2 \pm \tilde{\lambda}, \quad \vec{v}_\pm = \left(\frac{(\tilde{\lambda} \mp \tilde{\chi})^{1/2}}{(2\tilde{\lambda})^{1/2}}, \frac{\Omega}{2(2\tilde{\lambda}(\tilde{\lambda} \mp \tilde{\chi}))^{1/2}} \right)^T,$$

with $\tilde{\lambda} = \frac{1}{2}\sqrt{(2k_0\xi_1 - \delta)^2 + \Omega^2}$ and $\tilde{\chi} = k_0\xi_1 - \frac{\delta}{2}$. By our assumption that the evolution is in the lower eigenstate, we find $\vec{v} = |\vec{v}| \vec{v}_-$ and

$$(4.22) \quad |\psi_1|^2 : |\psi_2|^2 = 4(\tilde{\lambda} + \tilde{\chi})^2 : \Omega^2.$$

Since the phase space is assumed to be localized around $\mathbf{P}(t)$, we can approximate the above equation by letting $\xi_1 = P^x := P^x(t)$, and we get

$$(4.23) \quad \frac{|\psi_1|^2}{|\psi_2|^2} \approx \frac{4(\lambda + \chi)^2}{\Omega^2}, \quad \lambda = \frac{1}{2}\sqrt{(2k_0P^x - \delta)^2 + \Omega^2}, \quad \chi = k_0P^x - \frac{\delta}{2}.$$

For the case with harmonic potentials $V_1(\mathbf{x}) = V_2(\mathbf{x})$, using the LDA, we get the same relation between densities as (4.23) for each position \mathbf{x} which leads to

$$(4.24) \quad \delta_N(t) = [4(\lambda + \chi)^2 - \Omega^2]/[4(\lambda + \chi)^2 + \Omega^2].$$

Plugging (4.24) into (4.5), noticing (4.7), we obtain the ODE system (4.17) approximating the dynamics of $x_c(t)$. Using (4.17), it is easy to find

$$(4.25) \quad \frac{d}{dt} \left(\gamma_x^2 x_c^2(t) + (P^x(t))^2 - \sqrt{[2k_0P^x(t) - \delta]^2 + \Omega^2} \right) = 0,$$

which shows that $(x_c(t), P^x(t))^T$ is a closed curve and periodic. \square

Again, to verify the asymptotic (or approximate) results for $x_c(t)$ in Theorem 4.3, we numerically solve the CGPEs (1.8) with (1.9) in 2D (i.e., $d = 2$), take $\beta_{11} = \beta_{12} = \beta_{22} = 10$, $\gamma_x = \gamma_y = 2$, and $\delta = 0$, and choose the initial data as (4.15) with $\mathbf{x}_0 = (2, 2)^T$ and the ground state computed numerically. Figure 4 depicts time evolution of $x_c(t)$ obtained numerically and asymptotically as in Theorem 4.3 with different Ω and k_0 .

From Figure 4 and numerous tests we have done (not shown here for brevity), we find that for the very special initial data (4.15), equation (4.17) provides a very good approximation for the dynamics of the center-of-mass over a long time when $|\Omega| \gg \gamma_x$ and $|\Omega| \gg |k_0|$; when $0 < \gamma_x \ll |\Omega|$ and $|k_0|^2 \gg |\Omega|$, (4.16) fits the center-of-mass $x_c(t)$ very well; for $|\Omega|$ which is comparable to γ_x , $x_c(t)$ is damped in time and nonperiodic.

Remark 4.4. Theorem 4.3 does not contradict Theorem 4.2 because Theorem 4.2 holds for small k_0 , where the Ω frequency contribution is very small and $x_c(t)$ is almost periodic.

5. Semiclassical scaling and limits. For strong interaction $\beta_{jl} \gg 1$, we could rescale (1.8) by choosing $\mathbf{x} \rightarrow \mathbf{x}\varepsilon^{-1/2}$, $\psi_j \rightarrow \psi_j^\varepsilon \varepsilon^{d/4}$, $\varepsilon = 1/\beta^{2/(d+2)}$, $\beta = \max\{|\beta_{11}|, |\beta_{12}|, |\beta_{22}|\}$, which gives the CGPEs

$$(5.1) \quad \begin{aligned} i\varepsilon\partial_t\psi_1^\varepsilon &= \left[-\frac{\varepsilon^2}{2}\nabla^2 + V_1(\mathbf{x}) + ik_0\varepsilon^{3/2}\partial_x + \frac{\delta\varepsilon}{2} + \sum_{j=1}^2 \beta_{1j}^0 |\psi_j^\varepsilon|^2 \right] \psi_1^\varepsilon + \frac{\Omega\varepsilon}{2}\psi_2^\varepsilon, \\ i\varepsilon\partial_t\psi_2^\varepsilon &= \left[-\frac{\varepsilon^2}{2}\nabla^2 + V_2(\mathbf{x}) - ik_0\varepsilon^{3/2}\partial_x - \frac{\delta\varepsilon}{2} + \sum_{j=1}^2 \beta_{2j}^0 |\psi_j^\varepsilon|^2 \right] \psi_2^\varepsilon + \frac{\Omega\varepsilon}{2}\psi_1^\varepsilon, \end{aligned}$$

where $\beta_{j,l}^0 = \frac{\beta_{jl}}{\beta}$ and the potential functions are given in (1.9). It is of great interest to study the behavior of (5.1) when the small parameter ε tends to 0.

In the linear case, i.e., $\beta_{jl}^0 = 0$ for $j, l = 1, 2$, (5.1) collapses to

$$(5.2) \quad i\varepsilon\partial_t\Psi^\varepsilon = \begin{bmatrix} -\frac{\varepsilon^2}{2}\Delta + ik_0\varepsilon^{3/2}\partial_x + \frac{\delta\varepsilon}{2} + V_1 & \frac{\Omega\varepsilon}{2} \\ \frac{\Omega\varepsilon}{2} & -\frac{\varepsilon^2}{2}\Delta - ik_0\varepsilon^{3/2}\partial_x - \frac{\delta\varepsilon}{2} + V_2 \end{bmatrix} \Psi^\varepsilon,$$

where $\Psi^\varepsilon = (\psi_1^\varepsilon, \psi_2^\varepsilon)^T$. We now describe the limit as $\varepsilon \rightarrow 0^+$ using the Wigner transform

$$(5.3) \quad W^\varepsilon(\Psi^\varepsilon)(\mathbf{x}, \xi) = (2\pi)^{-d} \int_{\mathbb{R}^d} \Psi^\varepsilon(\mathbf{x} - \varepsilon v/2) \otimes \Psi^\varepsilon(\mathbf{x} + \varepsilon v/2) e^{iv \cdot \xi} dv,$$

where W^ε is a 2×2 matrix-valued function. The symbol corresponding to (5.2) can be written as

$$(5.4) \quad P^\varepsilon(\mathbf{x}, \xi) = \frac{i}{2}|\xi|^2 + i \begin{bmatrix} k_0\varepsilon^{1/2}\xi_1 + V_1(\mathbf{x}) + \frac{\delta\varepsilon}{2} & \frac{\Omega\varepsilon}{2} \\ \frac{\Omega\varepsilon}{2} & -k_0\varepsilon^{1/2}\xi_1 + V_2(\mathbf{x}) - \frac{\delta\varepsilon}{2} \end{bmatrix},$$

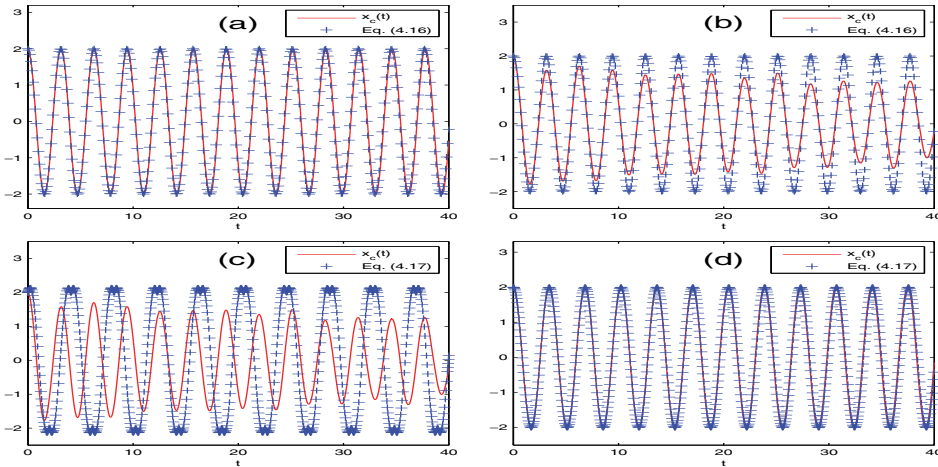


FIG. 4. Time evolution of the center-of-mass $x_c(t)$ for the CGPEs (1.8) obtained numerically from its numerical solution (i.e., labeled as $x_c(t)$ with solid lines) and asymptotically as (4.16) and (4.17) in Theorem 4.3 (i.e., labeled “Eq.” with “+ + +”) for different sets of parameters: (a) $(\Omega, k_0) = (50, 20)$, (b) and (c) $(\Omega, k_0) = (2, 2)$, and (d) $(\Omega, k_0) = (50, 2)$.

where $\xi = (\xi_1, \xi_2, \dots, \xi_d)^T$. Let us consider the principal part P of $P^\varepsilon = P + O(\varepsilon)$; i.e., we omit small term $O(\varepsilon)$, and we know that $-iP(\mathbf{x}, \xi)$ has two eigenvalues $\lambda_1(\mathbf{x}, \xi)$ and $\lambda_2(\mathbf{x}, \xi)$. Let Π_j ($j = 1, 2$) be the projection matrix from \mathbb{C}^2 to the eigenvector space associated with λ_j . If $\lambda_{1,2}$ are well separated, then $W^\varepsilon(\Psi^\varepsilon)$ converges to the Wigner measure W^0 , which can be decomposed as [15]

$$(5.5) \quad W^0 = u_1(\mathbf{x}, \xi, t)\Pi_1 + u_2(\mathbf{x}, \xi, t)\Pi_2,$$

where $u_j(\mathbf{x}, \xi, t)$ satisfies the Liouville equation

$$(5.6) \quad \partial_t u_j(\mathbf{x}, \xi, t) + \nabla_\xi \lambda_j(\mathbf{x}, \xi, t) \cdot \nabla_{\mathbf{x}} u_j(\mathbf{x}, \xi, t) - \nabla_{\mathbf{x}} \lambda_j(\mathbf{x}, \xi, t) \cdot \nabla_\xi u_j(\mathbf{x}, \xi, t) = 0.$$

It is known that such a semiclassical limit fails at regions when λ_1 and λ_2 are close.

Specifically, when $k_0 = O(1)$, $\delta = O(1)$, and $\Omega = O(1)$, the limit of the Wigner transform $W^\varepsilon(\Psi^\varepsilon)$ only has diagonal elements, and we have

$$(5.7) \quad P = \frac{i}{2}|\xi|^2 + i \begin{bmatrix} V_1(\mathbf{x}) & 0 \\ 0 & V_2(\mathbf{x}) \end{bmatrix}, \quad \lambda_1 = \frac{1}{2}|\xi|^2 + V_1(\mathbf{x}), \quad \lambda_2 = \frac{1}{2}|\xi|^2 + V_2(\mathbf{x}).$$

In the limit of this case, W^0 in (5.5), Π_1 and Π_2 are diagonal matrices, which means that the two components of Ψ^ε in (5.2) are decoupled as $\varepsilon \rightarrow 0^+$. In addition, the Liouville equation (5.6) is valid with λ_1 and λ_2 defined in (5.7).

Similarly, when $k_0 = O(1/\varepsilon^{1/2})$, $\delta = O(1/\varepsilon)$, and $\Omega = O(1/\varepsilon)$, e.g. $k_0 = \frac{k_\infty}{\varepsilon^{1/2}}$, $\Omega = \frac{\Omega_\infty}{\varepsilon}$, and $\delta = \frac{\delta_\infty}{\varepsilon}$ with k_∞ , Ω_∞ , and δ_∞ nonzero constants, the limit of the Wigner transform $W^\varepsilon(\Psi^\varepsilon)$ has nonzero diagonal and off-diagonal elements, and we have

$$(5.8) \quad P = \frac{i}{2}|\xi|^2 + i \begin{bmatrix} k_\infty \xi_1 + V_1(\mathbf{x}) + \frac{\delta_\infty}{2} & \frac{\Omega_\infty}{2} \\ \frac{\Omega_\infty}{2} & -k_\infty \xi_1 + V_2(\mathbf{x}) - \frac{\delta_\infty}{2} \end{bmatrix}$$

and

$$(5.9) \quad \lambda_{1,2} = \frac{|\xi|^2}{2} + \frac{V_1(\mathbf{x}) + V_2(\mathbf{x})}{2} \pm \frac{\sqrt{[V_1(\mathbf{x}) - V_2(\mathbf{x}) + 2k_\infty \xi_1 + \delta_\infty]^2 + \Omega_\infty^2}}{2}.$$

In the limit of this case, W^0 in (5.5), Π_1 and Π_2 are full matrices, which means that the two components of Ψ^ε in (5.2) are coupled as $\varepsilon \rightarrow 0^+$. Again, the Liouville equation (5.6) is valid with λ_1 and λ_2 defined in (5.9).

Of course, for the nonlinear case, i.e., $\beta_{jl}^0 \neq 0$ for $j, l = 1, 2$, only the case when $\Omega = 0$ and $k_0 = 0$ has been addressed [19]. For $\Omega \neq 0$ and $k_0 \neq 0$, it is still not clear about the semiclassical limit of the CGPEs (5.1).

6. Conclusions. We have studied analytically and asymptotically, as well as numerically, ground states and dynamics of two-component spin-orbit-coupled Bose-Einstein condensates (BECs) based on the coupled Gross-Pitaevskii equations (CGPEs) with the spin-orbit (SO) and Raman couplings. For ground state properties, we established existence and uniqueness, as well as nonexistence, of the ground states in different parameter regimes and studied their limiting behavior and structure with various combination of the SO and Raman coupling strengths. Efficient and accurate numerical methods were designed for computing the ground states and dynamics of SO-coupled BECs, especially for box potentials. Numerical results for the ground states were reported under different parameter regimes, which confirmed

our analytical results on ground states. For dynamical properties, we obtained the dynamical laws governing the motion of the center-of-mass and showed that the dynamics of the center-of-mass in the SO-coupled direction is either nonperiodic or a periodic function with different frequency than the trapping frequency, which is completely different from the case without SO coupling. Numerical results were presented to confirm our asymptotical (or approximate) results on the dynamics of the center-of-mass. Finally, we described the semiclassical limit of the CGPEs in the linear case via the Wigner transform method.

Acknowledgments. Part of this work was done when the authors were visiting the Institute for Mathematical Sciences at the National University of Singapore in 2015.

REFERENCES

- [1] M. H. ANDERSON, J. R. ENSHER, M. R. MATTHEWA, C. E. WIEMAN, AND E. A. CORNELL, *Observation of Bose-Einstein condensation in a dilute atomic vapor*, Science, 269 (1995), pp. 198–201.
- [2] X. ANTOINE, W. BAO, AND C. BESSE, *Computational methods for the dynamics of the nonlinear Schrödinger/Gross-Pitaevskii equations*, Comput. Phys. Commun., 184 (2013), pp. 2621–2633.
- [3] W. BAO, *Mathematical models and numerical methods for Bose-Einstein condensation*, Proceeding of International Congress of Mathematicians, 2014, to appear (arXiv: 1403.3884).
- [4] W. BAO, *Ground states and dynamics of multicomponent Bose-Einstein condensates*, Multiscale Model. Simul., 2 (2004), pp. 210–236.
- [5] W. BAO AND Y. CAI, *Ground states of two-component Bose-Einstein condensates with an internal atomic Josephson junction*, East Asia J. Appl. Math., 1 (2010), pp. 49–81.
- [6] W. BAO AND Y. CAI, *Mathematical theory and numerical methods for Bose-Einstein condensation*, Kinet. Relat. Models, 6 (2013), pp. 1–135.
- [7] W. BAO, I-L. CHERN, AND F. Y. LIM, *Efficient and spectrally accurate numerical methods for computing ground and first excited states in Bose-Einstein condensates*, J. Comput. Phys., 219 (2006), pp. 836–854.
- [8] W. BAO AND Q. DU, *Computing the ground state solution of Bose-Einstein condensates by a normalized gradient flow*, SIAM J. Sci. Comput., 25 (2004), pp. 1674–1697.
- [9] W. BAO, D. JAKSCH, AND P. A. MARKOWICH, *Numerical solution of the Gross-Pitaevskii equation for Bose-Einstein condensation*, J. Comput. Phys., 187 (2003), pp. 318–342.
- [10] N. B. ABDALLAH, F. MÉHATS, C. SCHMEISER, AND R. M. WEISHÄUPL, *The nonlinear Schrödinger equation with a strongly anisotropic harmonic potential*, SIAM J. Math. Anal., 37 (2005), pp. 189–199.
- [11] S. M. CHANG, C. S. LIN, T. C. LIN, AND W. W. LIN, *Segregated nodal domains of two-dimensional multispecies Bose-Einstein condensates*, Phys. D, 196 (2004), pp. 341–361.
- [12] K. B. DAVIS, M. O. MEWES, M. R. ANDREWS, N. J. VAN DRUTEN, D. S. DURFEE, D. M. KURN, AND W. KETTERLE, *Bose-Einstein condensation in a gas of sodium atoms*, Phys. Rev. Lett., 75 (1995), pp. 3969–3973.
- [13] Y. DENG, J. CHENG, H. JING, C. P. SUN, AND S. YI, *Spin-orbit-coupled dipolar Bose-Einstein condensates*, Phys. Rev. Lett., 108 (2012), 125301.
- [14] V. GALITSKI AND I. B. SPIELMAN, *Spin-orbit coupling in quantum gases*, Nature, 494 (2012), pp. 49–54.
- [15] P. GÉRARD, P. A. MARKOWICH, N. J. MAUSER, AND F. POUPAUD, *Homogenization limits and Wigner transforms*, Comm. Pure Appl. Math., 50 (1997), pp. 323–379.
- [16] C. HAMNER, Y. ZHANG, M. A. KHAMEHCHI, M. J. DAVIS, AND P. ENGELS, *Spin-orbit coupled Bose-Einstein condensates in a one-dimensional optical lattice*, Phys. Rev. Lett., 114 (2015), 070401.
- [17] M. Z. HASAN AND C. L. KANE, *Colloquium: Topological insulators*, Rev. Mod. Phys., 82 (2010), pp. 3045–3067.
- [18] H. HU, B. RAMACHANDHRAN, H. PU, AND X. LIU, *Spin-orbit coupled weakly interacting Bose-Einstein condensates in harmonic traps*, Phys. Rev. Lett., 108 (2012), 010402.
- [19] C.-C. LEE AND T.-C. LIN, *Incompressible and compressible limits of two-component Gross-Pitaevskii equations with rotating fields and trap potentials*, J. Math. Phys., 49 (2008), 043517.

- [20] Y. LI, L. PITAEVSKII, AND S. STRINGARI, *Quantum tricriticality and phase transitions in spin-orbit coupled Bose-Einstein condensates*, Phys. Rev. Lett., 108 (2012), 225301.
- [21] Y. LI, G. I. MARTONE, L. PITAEVSKII, AND S. STRINGARI, *Superstripes and the excitation spectrum of a spin-orbit-coupled Bose-Einstein condensate*, Phys. Rev. Lett., 110 (2013), 235302.
- [22] E. H. LIEB AND M. LOSS, Analysis, 2nd ed., Grad. Stud. Math. 14, Amer. Math. Soc., Providence, RI, 2001.
- [23] E. H. LIEB, R. SEIRINGER, AND J. YNGVASON, *Bosons in a trap: A rigorous derivation of the Gross-Pitaevskii energy functional*, Phys. Rev. A, 61 (2000), 043602.
- [24] E. H. LIEB AND J. P. SOLOVEJ, *Ground state energy of the two-component charged Bose gas*, Comm. Math. Phys., 252 (2004), pp. 485–534.
- [25] Y. J. LIN, K. JIMÉNEZ-GARCIA, AND I. B. SPIELMAN, *Spin-orbit-coupled Bose-Einstein condensates*, Nature, 471 (2011), pp. 83–86.
- [26] C. H. LIU, Y. YU, S.-C. GOU, AND W. M. LIU, *Vortex chain in anisotropic spin-orbit-coupled spin-1 Bose-Einstein condensates*, Phys. Rev. A, 87 (2013), 063630.
- [27] C. H. LIU AND W. M. LIU, *Spin-orbit-coupling-induced half-skyrmion excitations in rotating and rapidly quenched spin-1 Bose-Einstein condensates*, Phys. Rev. A, 86 (2012), 033602.
- [28] Z. LIU, *Two-component Bose-Einstein condensates*, J. Math. Anal. Appl., 348 (2008), pp. 274–285.
- [29] L. P. PITAEVSKII AND S. STRINGARI, *Bose-Einstein Condensation*, Clarendon Press, Oxford, UK, 2003.
- [30] C. WANG, C. GAO, C. JIAN, AND H. ZHAI, *Spin-orbit coupled spinor Bose-Einstein condensates*, Phys. Rev. Lett., 105 (2010), 160403.
- [31] M. I. WEINSTEIN, *Nonlinear Schrödinger equations and sharp interpolation estimates*, Comm. Math. Phys., 87 (1983), pp. 567–576.
- [32] L. WEN, Q. SUN, H. Q. WANG, A. C. JI, AND W. M. LIU, *Ground state of spin-1 Bose-Einstein condensates with spin-orbit coupling in a Zeeman field*, Phys. Rev. A, 86 (2012), 043602.
- [33] D. XIAO, M. CHANG, AND Q. NIU, *Berry phase effects on electronic properties*, Rev. Mod. Phys., 82 (2010), pp. 1959–2007.
- [34] J. ZHANG, S. JI, Z. CHEN, L. ZHANG, Z. DU, B. YAN, G. PAN, B. ZHAO, Y. DENG, H. ZHAI, S. CHEN, AND J. PAN, *Collective dipole oscillations of a spin-orbit coupled Bose-Einstein condensate*, Phys. Rev. Lett., 109 (2012), 115301.
- [35] Y. ZHANG, W. BAO, AND H. LI, *Dynamics of rotating two-component Bose-Einstein condensates and its efficient computation*, Phys. D, 234 (2007), pp. 49–69.
- [36] Y. ZHANG, L. MAO, AND C. ZHANG, *Mean-field dynamics of spin-orbit coupled Bose-Einstein condensates*, Phys. Rev. Lett., 108 (2012), 035302.
- [37] Q. ZHU, C. ZHANG, AND B. WU, *Exotic superfluidity in spin-orbit coupled Bose-Einstein condensates*, Europhys. Lett., 100 (2012), 50003.