# QUANTUM PHASES OF TIME-REVERSAL INVARIANT BOSE-EINSTEIN CONDENSATES 

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This dissertation is dedicated to my family.

# QUANTUM PHASES OF TIME-REVERSAL INVARIANT BOSE-EINSTEIN CONDENSATES 

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# QUANTUM PHASES OF TIME-REVERSAL INVARIANT BOSE-EINSTEIN CONDENSATES 

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Recent experimental realization of spin-orbit coupling (SOC) for ultracold atomic gases with the use of synthetic gauge fields provides a powerful platform for the study of novel quantum phenomena and the simulation of exotic condensed matter phases. However, in conventional schemes of SOC in ultracold bosonic gases, time-reversal symmetry, which plays a critical role in topologically nontrivial states, is broken by an effective transverse Zeeman field. We study the quantum phases of SOC Bose-Einstein condensates (BECs) with the use of a Hermite-Gaussian (HG) beam to induce Raman transitions. This treatment allows for SOC in bilayer BECs with inter-layer tunneling where time-reversal symmetry is preserved. New ground-state phases are introduced that are not seen in conventional SOC BECs. We propose a experimentally feasible setup and discuss the physical parameters under which time-reversal symmetry can be preserved.

The Hamiltonians for SOC BECs are often nonlinear and the methods used for calculating the ground-state wavefunctions are computationally expensive. The wavefunctions need to be calculated on an individual basis to study the ground-state quantum phases on a granular level. We propose the use of convolutional-neural-networks (CNN) to train SOC BEC systems and reduce the computational cost of these ground-state calculations. We show the overall network setup and discuss the ranges over which the model is realizable.

The proposed CNN uses a reverse-flow algorithm that allows for complex phases of the wavefunction and thus permits for a broader study of SOC BEC systems.

In summary, this dissertation details how time-reversal symmetry can be preserved in SOC BECs and how predictive analytics can be used to further understand the ground-state properties of these systems.

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## CHAPTER 1

## INTRODUCTION

### 1.1 Overview

Bose-Einstein Condensates (BECs) were first theorized in 1924 [1]. However, It was not until 1995 that the first BECs would be realized experimentally [2, 3. Since this realization, a large field of research has been opened in both theoretical and experimental ultracold atomic gases [4]. Current research focuses on both simulating more complex novel systems as well as unique nontrivial systems [5]. In this dissertation, we will focus on the analysis of producing spin-orbit coupling (SOC) in BECs via artificial gauge fields. This will be expanded into the importance of time-reversal invariance and how we propose a realistic setup to preserve this symmetry in a spin-orbit coupled BEC [6]. We then shift the focus on how the use of neural networks can be utilized to enhance the computational performance of ground-state calculations in SOC BECs.

### 1.2 Bose-Einstein Condensation

Below a critical temperature, $T_{c}$, a bosonic gas will condense into a low energy ground state. The critical temperature is defined as,

$$
\begin{equation*}
T_{c} \propto \frac{\hbar^{2} n^{2 / 3}}{m k_{B}} \tag{1.1}
\end{equation*}
$$

where $n$ is the particle density, $m$ is the boson atomic mass, and $k_{b}$ is the Boltzmann constant.
The BEC will have interatomic collisions where the strength of the interactions is given by,

$$
\begin{equation*}
g=\frac{4 \pi \hbar^{2} a_{s}}{m} \tag{1.2}
\end{equation*}
$$

where $a_{s}$ is the s-wave scattering length, which is positive for repulsive interactions and negative for attractive interactions.

If we consider the temperature of the gas to be low enough so that all atoms are in the condensed state, and taking the gas to be dilute, the ground state of the BEC can be obtained from the time-independent Gross-Pitaevskii equation (GPE),

$$
\begin{equation*}
\left(-\frac{\hbar^{2}}{2 m} \frac{\partial^{2}}{\partial \mathbf{r}^{2}}+V_{\mathrm{ext}}(\mathbf{r})+g|\psi(\mathbf{r})|^{2}\right) \psi(\mathbf{r})=\mu \psi(\mathbf{r}) \tag{1.3}
\end{equation*}
$$

where $V_{\text {ext }}(\mathbf{r})$ can be any external potential applied to the system, such as a typical harmonic trap. The GPE is a mean field theory approach to the solution of BECs systems. The nonlinearity in the interaction term makes exact solutions of the GPE a rarity. Therefore, approximation methods are often applied when using the GPE to solve a physical system.

### 1.3 Spin-Orbit Coupling

Spin-orbit coupling (SOC) is the interaction of a particles spin with its orbital angular momentum. In a simple hydrogen atom, this effect is seen by the relativistic motion of a spin- $1 / 2$ electron around a single proton, creating an interaction between the spin of the electron and the magnetic field caused by the relative motion of the proton. However, creating SOC in BECs can prove to be difficult as BECs are charge neutral.

The use of artificial gauge fields has allowed for the study of SOC in BECs. Popular methods of generating artificial gauge fields include rotation of a trapping potential, rapid or resonant modulation of a lattices, and atom-light interactions [7]. This dissertation will be focusing on and building off of the hallmark case of atom-light interactions in ${ }^{87} \mathrm{Rb}$ [8]. First, a bias magnetic field is applied to energetically separate the hyperfine levels in the $F=1$ manifold. Artificial gauge fields are then created by the use of counter-propagating Raman lasers allowing coupling between the states in this manifold. Through the process of adiabatic elimination [9], one can select just two of the hyperfine states $\left|F=1, m_{F}=-1\right\rangle$ and $\left|F=1, m_{f}=0\right\rangle$. This creates a 2-component BEC whose hyperfine states can be referred to as psuedospins; i.e. $|\uparrow\rangle=\left|m_{f}=0\right\rangle$ and $|\downarrow\rangle=\left|m_{f}=-1\right\rangle$.


Figure 1.1. (a) Lambda diagram illustrating the transition of ${ }^{87} \mathrm{Rb}$ hyperfine states using two counter-propagating lasers. (b) Shows a scheme for a common orientation of the Raman lasers with a bias magnetic field to generate spin-orbit coupling in a Bose-Einstein condensate.

First, we consider the single particle picture of a simulated spin- $1 / 2$ system, where the basis can be recognized as $|\psi\rangle=\left(\psi_{\uparrow}, \psi_{\downarrow}\right)^{T}$ as seen in Fig. 1.1. After using the rotating wave approximation to rid the Hamiltonian of the fast oscillating terms [10], the 1-D single particle two component Hamiltonian can be seen as,

$$
H=\left(\begin{array}{cc}
\frac{p_{x}^{2}}{2 m}+\frac{\Delta E}{2} & \frac{\hbar \Omega}{2} e^{i\left(2 k_{r} x-\Delta \omega t\right)}  \tag{1.4}\\
\frac{\hbar \Omega}{2} e^{-i\left(2 k_{r} x-\Delta \omega t\right)} & \frac{p_{x}^{2}}{2 m}-\frac{\Delta E}{2}
\end{array}\right),
$$

where $k_{r}$ is the wave vector along the x-axis, $\Delta E$ is the energy difference between the coupled states, and $\Delta \omega$ is the frequency difference between the two lasers. Then, by using a unitary transformation to the rotating reference frame,

$$
U_{R}=\left(\begin{array}{cc}
e^{i\left(k_{r} x-\frac{1}{2} \Delta \omega t\right)} & 0  \tag{1.5}\\
0 & e^{-i\left(k_{r} x-\frac{1}{2} \Delta \omega t\right)}
\end{array}\right)
$$



Figure 1.2. Single particle band dispersion Eq. (1.7). Parameters are chosen to be $k_{0}=1$ and $\delta=0$ for varying $\Omega$. The largest value $\Omega=2.4$ (yellow) shows a single minimum in the lower band leading to a zero-momentum phase.
we end up with the transformed Hamiltonian as,

$$
\begin{align*}
H_{k} & =U_{R}^{\dagger} H U_{R}-i \hbar U_{R}^{\dagger} \frac{\partial U_{R}}{\partial t} \\
& =\left(\begin{array}{cc}
\frac{\left(p_{x}+\hbar k_{0}\right)^{2}}{2 m}+\frac{\delta}{2} & \frac{\Omega}{2} \\
\frac{\Omega}{2} & \frac{\left(p_{x}-\hbar k_{0}\right)^{2}}{2 m}-\frac{\delta}{2}
\end{array}\right) . \tag{1.6}
\end{align*}
$$

where $\delta=\Delta E-\hbar \Delta \omega$. The wavefunction thus transforms as $|\psi\rangle=U_{R}^{\dagger}|\psi\rangle$.
The energy eigenvalues of this Hamiltonian are easily solvable giving the energy dispersion,

$$
\begin{equation*}
E_{ \pm}(k)=\frac{k_{x}^{2}}{2} \pm \sqrt{\left(k_{0} k_{x}-\frac{\delta}{2}\right)^{2}+\left(\frac{\Omega}{2}\right)^{2}} . \tag{1.7}
\end{equation*}
$$

This spectrum can be seen in Fig. 1.2 for varying $\Omega$, with $m=\hbar=1$ for simplicity.

Now consider the effect of many body interactions on the ground state of this system. For this 2-component system the Hamiltonian Eq. (1.6) is modified by a spin-dependent nonlinear interaction term which can be expressed as

$$
H_{i n t}=\left(\begin{array}{cc}
g_{\uparrow \uparrow}\left|\psi_{\uparrow}\right|^{2}+g_{\uparrow \downarrow}\left|\psi_{\downarrow}\right|^{2} & 0  \tag{1.8}\\
0 & g_{\downarrow \uparrow}\left|\psi_{\uparrow}\right|^{2}+g_{\downarrow \downarrow}\left|\psi_{\downarrow}\right|^{2}
\end{array}\right)
$$

We take symmetrical intraspecies interactions $g=g_{\uparrow \uparrow}=g_{\downarrow \downarrow}$ and $\delta=0$ throughout the remainder of this section. To solve Eq. (1.3) and achieve a rich phase diagram, we take use of the variational method with an associated energy functional,

$$
\begin{equation*}
\varepsilon=\int d x\left[\psi^{\dagger} H_{k} \psi+\frac{g}{2}\left|\psi_{\uparrow}\right|^{4}+\frac{g}{2}\left|\psi_{\downarrow}\right|^{4}+\left.\left.g_{\uparrow \downarrow} \psi_{\uparrow}\right|^{2} \psi_{\downarrow}\right|^{2}\right] . \tag{1.9}
\end{equation*}
$$

We take as our ansatz

$$
\begin{equation*}
\Psi=\sqrt{\rho}\left[\left|C_{1}\right|\binom{\cos \theta}{-\sin \theta} e^{i k_{1} x}+\left|C_{2}\right|\binom{\sin \theta}{-\cos \theta} e^{-i k_{1} x}\right] \tag{1.10}
\end{equation*}
$$

where $\rho$ is the number particle density and $k_{1}$ is the momentum of the BEC [11]. Inserting Eq. (1.10) into Eq. (1.9) and minimizing with respect to the four variational parameters $\rho$, $k_{1}, C_{1}$, and $C_{2}$ with normalization condition $\left|C_{1}\right|^{2}+\left|C_{2}\right|^{2}=1$ leads to the ground state wavefunction.

For a given set of the non-variational parameters of Eq. 1.9, the interacting ground state exhibits three quantum phases: (I) stripe phase having $k_{1} \neq 0,\left|C_{1}\right|=\left|C_{2}\right|=\frac{1}{\sqrt{2}}$, and $\left\langle\sigma_{z}\right\rangle=\left\langle\sigma_{x}\right\rangle=0$; (II) plane-wave phase having $k_{1} \neq 0,\left|C_{1} C_{2}\right|=0$ and $\left|\left\langle\sigma_{z}\right\rangle\right|>0$; (III) zero-momentum phase having $k_{1}=\left|\left\langle\sigma_{z}\right\rangle\right|=0$.

### 1.4 Traditional Methods for Ground-State Calculations

One method for ground-state calculations is known as imaginary time propagation (ITP) [12]. Generally, one can evolve any initial wavefunction $|\psi(0)\rangle$ in time in a given system by use of
unitary time evolution operator $U=e^{-i H t / \hbar}$,

$$
\begin{equation*}
|\psi(t)\rangle=e^{-i H t / \hbar}|\psi(0)\rangle . \tag{1.11}
\end{equation*}
$$

This operation can be modified by use of a Wick rotation $\tau=-i t$ to find an approximation to the lowest energy eigenstate of $H$. Under this rotation, the time evolution operator becomes $U=e^{-H \tau / \hbar}$. If then an appropriate guess of the initial wave function $|\psi(0)\rangle$ is taken (i.e. a Gaussian distribution for the ground state of a 1-D simple harmonic oscillator), one can asymptotically approach the true ground state of $H$,

$$
\begin{equation*}
|\psi\rangle_{g}=e^{-H \tau / \hbar}|\psi(0)\rangle . \tag{1.12}
\end{equation*}
$$

In practice, ITP is an iterative process done on sufficiently small time steps. More details on of this procedure can be seen in Appendix A.

Another common method is the well-known variational method where one takes a trial wavefunction of the given system, known as an ansatz, with varying parameters. In general, this can be an iterative process to obtain multiple lower level eigenstates. For the purposes of the research presented in this dissertation, only the ground state is needed with this method. To obtain the ground-state wavefunction for a given Hamiltonian $H$, with $|\phi\rangle$ defined as the predetermined ansatz, the energy functional is defined as,

$$
\begin{equation*}
\varepsilon=\frac{\langle\phi| H|\phi\rangle}{\langle\phi \mid \phi\rangle} . \tag{1.13}
\end{equation*}
$$

This functional has the property $\varepsilon \geq E_{0}$, where $E_{0}$ is the ground state energy of $H$. The functional is then minimized across all variational parameters, defined in the ansatz, to achieve the ground-state wavefunction and corresponding energy.

These two methods are frequently used in current research on ultracold atomic systems. Both are invaluable tools used for the research discussed in the subsequent portions of this dissertation. More detailed analysis for each of these methods is given when the need for each method is presented.

### 1.5 Machine Learning in Quantum Systems

Predictive analytics, in the most basic form, have been around for centuries. For instance, least squares, a minimization method used in the prediction of regression models, has been used since the early $19^{\text {th }}$ century [13]. However, it was not until the recent advance of computer processing power, along with the even more recent progress of graphical-processing units (GPUs), that algorithms could be taught to learn patterns and perform predictive analysis without the need to use explicit programming. This process of learning by example is now known globally as machine learning [14]. Currently, machine learning is used across various industrial applications and in many academic settings.

There are a ever growing number of algorithms encompassed in the broad field of study known as machine learning. Each of these algorithms exceeding in specific subcategories of problems. For instance, XGBoost [15], a popular (eXtreme) gradient-tree boosting algorithm has had a lot of recent success in classification problems. However, for teaching a computer to play video games at a competitive level, deep reinforcement neural networks are a better choice [16].

Of particular interest to this study is the use of convolutional neural networks (CNNs) [17]. These neural networks make use of multiple convolutional layers to filter inputs before propagating throughout the rest of the network. In this way, the convolutional layers can be thought of as pattern-recognition layers. This is a powerful tool that is of great use to research done in imagine classification and modern computer vision. This includes the invaluable use of CNNs in current condensed matter research to detect and classify crystal structures from diffraction patterns [18].

A basic example of how such image classification can be done using CNNs is seen Fig. 1.3. Here, the input image, which the computer sees as an array of pixel values, is fed into multiple convolutional layers. Each of these convolutional filters is independent of each other and serves a unique purpose. The total number, and overall types, of convolutional layers used


Figure 1.3. Setup of a typical convolutional neural network for imagine classification. The first layers (input) are images that can realized as matrices of pixel values. These matrices are fed into preprocessing (not shown) and convolutional layers (orange). The outputs from the convolutional layers then are fed into two fully-connected (also known as dense) layers (green). The final output layer is a normalized vector whose components relate to each possible predefined category.
is dependent on the given problem. The output of these convolutional layers is fed into the more traditional dense neural network layers. The final layer is an output vector consisting of the classification probabilities.

Since the input of CNNs can be thought of a tensor containing spatial information, the use of CNNs is not just limited to image classification. Recently, the ground-state solutions to the Schrodinger equation for various potentials was solved using CNNs [19]. The input for the network were the potentials chosen belonging to the classes of simple harmonic oscillators, infinite wells, double-well inverted Gaussians, and pseudo-random potential functions. The network trained in this study showed promising results with a median absolute error of 5.90 mHa across all classes. Fig. 1.4 shows a simplistic schematic of the components of this network. In direct comparison to the classification of image inputs (as in Fig 1.3), the potential energy function is simply a tensor of values relating to the magnitude of the


Figure 1.4. Illustration of how a convolutional neural network can be used to predict groundstate wavefunctions for various potentials in a quantum system. Here, the input of the network is a tensor whose components correspond to the magnitude of the potential at each point in space. The setup of the hidden layers is similar to imagine classification problems and can be tuned for robustness. The output is the ground-state wavefunction $\Psi_{g}$. This is a regression network in contrast to Fig. 1.3, which is setup to output a classification.
potential at each discrete point in space. However, in contrast to image classification, this is a regression problem and the outputs will be the normalized ground-state wavefunction for each input potential. The research presented here will be crucial to studies presented later in this dissertation.

## CHAPTER 2

# TIME-REVERSAL-INVARIANT SPIN-ORBIT-COUPLED BILAYER BOSE-EINSTEIN CONDENSATES표 

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[^0]
### 2.1 Time-Reversal Symmetry

Time-reversal invariance constitutes a fundamental symmetry in quantum physics. A halfinteger spin system always possesses two-fold degenerate quantum states, or Kramers degeneracy [20], under the time-reversal symmetry. In solid-state materials, the presence of time-reversal symmetry and spin-orbit coupling, interaction between particle spin and orbital degrees of freedom, is responsible for many exotic phenomena such as quantum spin Hall effects and topological insulators [21, 22, 23], whose key physical features-a gapless edge state - is guaranteed by Kramers degeneracy. Recently, a class of exotic quantum phases have been found in ultracold atoms through the engineering of various types of spin-orbit coupling via light-matter interaction [24, 25, 26, 27, 28, 29], including spin-linear-momentum coupling [30, 31, 32, 33, 34, 35, 36, 11, 37, 38, 39, 40, 41, 42, 43, 44, which has been widely studied in experiments [8, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55], and proposed spin-orbital-angular-momentum [56, 57, 58, 59, 60, 61] as well as spin-tensor-momentum 62] couplings. However, in these schemes, the spin-orbit interaction is generated by a laser-induced Raman transition between atomic hyperfine states, which manifests as a constant Zeeman field along a fixed direction and hence inevitably breaks the time-reversal symmetry. For further pursuit of new quantum phases with nontrivial physics due to the interplay between time-reversal symmetry and spin-orbit couplings, we look to create time-reversal invariance coexisting with spin-orbit coupling in these systems.

Recently, there has been a focus on spin-orbit coupled degenerate Fermi gases preserving time-reversal symmetry [63]. In the succeeding, I provide detailed analysis on such a scheme that generates time-reversal symmetry in ultracold atoms and investigate interacting BoseEinstein condensates (BECs) realized with it. This approach generalizes the scheme of Sec. 1.3 [8], in which two Gaussian lasers are applied to a spinor gas, by replacing one laser beam with a first-order Hermite-Gaussian (HG) beam [see Fig. 2.1(b)]. The HG beam


Figure 2.1. (a) Raman transition of ${ }^{87} \mathrm{Rb}$ hyperfine states. (b) Scheme for generating spinorbit coupled BECs preserving time-reversal symmetry. A pair of counter-propagating Gaussian (G) and Hermite-Gaussian (HG) beams induce a Raman transition that have opposite amplitudes between upper ( $y>0$, red) and lower ( $y<0$, blue) regions. Additional fardetuned HG laser beam can be used to create a bilayer structure with interlayer tunneling $t$. The modes for the beams ( $\Omega_{1,0}$ and $\Omega_{0,0}$ ) can be seen in Eq. 2.2 )
confines the bosonic gas into two coupled spatial layers, induces spin-orbit coupling, and preserves the bilayer system under time-reversal operation,

$$
\begin{equation*}
\Theta=i \sigma_{y} \tau_{x} K \tag{2.1}
\end{equation*}
$$

where $\boldsymbol{\sigma}$ and $\boldsymbol{\tau}$ are Pauli matrices in spin and layer space, respectively, and $K$ is the conjugate operator. Note that $\Theta$ exhibits the same physical properties as the regular time-reversal operator by being anti-unitary and $\Theta^{2}=-1$. This setup focuses on both the single-particle picture and interacting Bose gases to find interesting ground-state phase diagrams and other correlations that have not been found in regular spin-orbit coupled BECs. The key results of this study can be summarized as:
(i) The system's single-particle energy bands pair as time-reversal partners and are also subject to a spin-layer symmetry $\sigma_{z} \tau_{x}$. The Kramers degeneracy prevents the gap opening between the paired two bands at zero momentum, resulting in double finite-momentum band minima that always exist, i.e., the zero-momentum state can never be the single-particle ground state even at a large Raman coupling, unless the two layers completely decouple.
(ii) The interacting phase diagram of a ground-state Bose gas exhibits layer-stripe, planewave, and zero-momentum phases. The layer-stripe phase (and its Kramers partner), occurring at weak Raman coupling, exhibits spatially modulating layer polarization but no total density modulation due to the time-reversal symmetry. At large interaction and large Raman coupling, the many-body effects drive the BEC to a zero-momentum ground state (or its Kramers partner), even if the zero momentum is not the single-particle band minimum.
(iii) The Bose gas exhibits a global spin-layer correlation $\left\langle\sigma_{x} \tau_{z}\right\rangle \neq 0$, while either the spin or the layer component vanishes, $\left\langle\sigma_{x}\right\rangle=\left\langle\tau_{z}\right\rangle=0$. This is needed for experiments to measure spin and layer properties simultaneously rather separately.

### 2.2 Model and Hamiltonian

The setup begins with ultracold atoms with two hyperfine spin states $\left(\psi_{\uparrow} \psi_{\downarrow}\right)^{T}$, subject to a pair of counter-propagating lasers $E^{ \pm}$along the $x$-direction, with transverse electromagnetic modes of a general Hermite form. The laser amplitudes are given as

$$
\begin{equation*}
\Omega_{m, n}^{ \pm}=A H_{m}\left(\frac{\sqrt{2} y}{w}\right) H_{n}\left(\frac{\sqrt{2} z}{w}\right) e^{-\frac{y^{2}+z^{2}}{w^{2}} \pm i k_{R} x} \tag{2.2}
\end{equation*}
$$

where $A$ represents the overall beam strength, $H_{n}$ is the $n$th Hermite polynomials, $w$ is the beam waist, and $k_{R}$ is the wave vector. The two beams impart spin-dependent linear momentum into the atoms and also induce Raman transition $\Omega_{\mathrm{R}}(\boldsymbol{r})=\Omega^{+*} \Omega^{-} / \Delta$ between the spin states, as shown in Fig. 2.1 (a) ( $\Delta$ is a uniform detuning). If both beams are of the lowest mode $\Omega_{0,0}^{ \pm}$(two Gaussian beams), we have the traditional setup for generating the spin-linearmomentum coupling as discussed in Sec. 1.3. To generate time-reversal invariance, the focus will be on a practical generalization of the Hermite modes $\Omega_{1,0}^{+}$and $\Omega_{0,0}^{-}$, i.e., left-propagating Gaussian and right-propagating HG beams. A schematic of this setup is shown in Fig. 2.1(b). The Raman transition amplitude $\Omega_{\mathrm{R}}(\boldsymbol{r})$ now has an odd spatial parity along the $y$ direction with maximum strength at $y= \pm w / \sqrt{2}$. Along the $y$ direction, a bilayer trapping potential
can be realized using a repulsive potential at the center of a tight harmonic trap or a single far-detuning HG laser beam of the $(1,0)$ mode. Such additional far-detuning trapping lasers avoid the heating from the trapping and ensure the independent tunability of the interlayer tunneling. Performing a unitary transformation as in Eq. 1.5 and integrating out the $y$ and $z$ degrees of freedom leads to the effective single-particle Hamiltonian for upper and lower layers, respectively, as $\frac{1}{2}\left(p_{x}^{2}-2 p_{x} \sigma_{z} \pm \Omega \sigma_{x}\right)$, where $p_{x} \sigma_{z}$ is the spin-orbit coupling and $\Omega$ is the effective Raman coupling. Here we take $k_{R}$ and $\hbar^{2} k_{R}^{2} / 2 m$ as momentum and energy units, respectively ( $m$ is the atomic mass). The only difference between the two layers is the opposite sign of Raman coupling due to the HG beam. If the two layers have a slight overlap, the dominant interlayer coupling is particle tunneling between the two layers. We can treat the two layers as another two-level degrees of freedom and write down the whole Hamiltonian in spin-layer basis $\left(\begin{array}{llll}\psi_{1 \uparrow} & \psi_{1 \downarrow} & \psi_{2 \uparrow} & \psi_{2 \downarrow}\end{array}\right)^{T}$, as

$$
\begin{equation*}
H=\frac{1}{2}\left(p_{x}^{2}-2 p_{x} \sigma_{z}+\Omega \sigma_{x} \tau_{z}-t \tau_{x}\right) \tag{2.3}
\end{equation*}
$$

where $t$ is the tunneling strength. In general, the Hamiltonian can have a detuning term $\delta_{z} \sigma_{z}$. This term, however, needs to be tuned to zero for the symmetry we are interested in.

The Hamiltonian exhibits a spin-layer time-reversal symmetry,

$$
\begin{equation*}
\Theta H\left(p_{x}\right) \Theta^{-1}=H\left(-p_{x}\right), \tag{2.4}
\end{equation*}
$$

with the energy dispersion of the lower bands expressed as,

$$
\begin{equation*}
E_{0}^{ \pm}(k)=\frac{1}{2}\left(k^{2}-\sqrt{(2 k \pm t)^{2}+\Omega^{2}}\right) . \tag{2.5}
\end{equation*}
$$

These bands become time-reversal partners, i.e., $E^{+}(k)$ and $E^{-}(-k)$ form degenerate Kramers pairs, as shown in Fig. 2.2. The fact $E^{+}(0)=E^{-}(0)$ leads to a symmetry protected band crossing (or gap closing) at $k=0$. Similarly, the upper two bands,

$$
\begin{equation*}
E_{1}^{ \pm}(k)=\frac{1}{2}\left(k^{2}+\sqrt{(2 k \pm t)^{2}+\Omega^{2}}\right), \tag{2.6}
\end{equation*}
$$



Figure 2.2. Single particle band dispersion Eq. (2.5) and Eq. (2.6) in the spin-layer basis. The band crossing at $k=0$ is time-reversal symmetry protected. Each band also satisfies a spin-layer symmetry $\left\langle\sigma_{z} \tau_{x}\right\rangle= \pm 1$ (light red and dark blue, respectively). Other parameters are set to $\Omega=1$ and $t=0.5$.
are also time-reversal partners crossing at $k=0$. At $\Omega=0$, the lower band $E_{0}$ has its minimum at $k_{\text {min }}= \pm 1$. As $\Omega$ increases, the minimum shifts toward the zero momentum and approaches $k_{\text {min }}=\frac{t}{\Omega-2}+O\left(\Omega^{-3}\right)$ in the large $\Omega$ limit $(\Omega \gg 2)$. Considering the minimum of the $E_{0}^{ \pm}$bands at $\pm k_{\text {min }}$, we see that the single-particle ground states are double degenerate and always possess finite momentum $\pm k_{\text {min }} \neq 0$-the crossing point $k=0$ can never be the ground state - with the presence of interlayer coupling $t \neq 0$. If the layers are completely decoupled, or $t=0$, the lower bands $E_{0}^{ \pm}(k)$ become identical, and the ground states undergo a transition from finite to zero momentum at $\Omega_{c}=2$, the same critical value as in the conventional spin-orbit coupled system.

In addition to the time-reversal symmetry, the Hamiltonian also exhibits a spin-layer symmetry,

$$
\begin{equation*}
\left[H, \sigma_{z} \tau_{x}\right]=0 . \tag{2.7}
\end{equation*}
$$

The paired bands $E_{0}^{\mp}\left(E_{1}^{ \pm}\right)$exhibit spin-layer symmetry $\left\langle\sigma_{z} \tau_{x}\right\rangle= \pm 1$ [red and blue colors in Fig. 2.2, respectively]. By measuring this symmetry, one could distinguish a state from its Kramers partner.

### 2.3 Interacting Bose Gases

Now we consider of the effects of particle interactions Bose gas in this time-reversal-invariant setup. As outlined in Sec. 1.4 , two complementary methods are used to find the ground state wavefunction: variational analysis and Gross-Pitaeviskii equation (GPE) numerics. Details of the variational method are outlined in the following.

We adopt a variational wavefunction as a general superposition of a Kramers pair as

$$
\begin{align*}
\Psi=\sqrt{\rho} & {\left[\left|C_{1}\right|\left(\begin{array}{c}
\cos \theta \cos \gamma_{1} e^{i \delta_{1}} \\
\cos \theta \sin \gamma_{1} e^{i \delta_{2}} \\
\sin \theta \cos \gamma_{2} e^{i \delta_{3}} \\
\sin \theta \sin \gamma_{2}
\end{array}\right) e^{i k_{1} x}\right.} \\
& \left.+\left|C_{2}\right|\left(\begin{array}{c}
\sin \theta \sin \gamma_{2} \\
-\sin \theta \cos \gamma_{2} e^{-i \delta_{3}} \\
\cos \theta \sin \gamma_{1} e^{-i \delta_{2}} \\
-\cos \theta \cos \gamma_{1} e^{-i \delta_{1}}
\end{array}\right) e^{-i k_{1} x}\right] \tag{2.8}
\end{align*}
$$

with particle number density $\rho$ and normalization condition $\left|C_{1}\right|^{2}+\left|C_{2}\right|^{2}=1$. The ansatz is generalized from the conventional spin-orbit-coupled system but respects the time-reversal associated degeneracy. By setting $\theta=\pi / 4$ and $\gamma_{1}=\gamma_{2}$, the top-layer components (first two rows) of $\Psi$ reproduce the previous results without time-reversal symmetry in Ref. [11].

The BEC's energy density is expressed as

$$
\begin{equation*}
\varepsilon=\int d x\left[\Psi^{\dagger} H \Psi+\frac{g}{2}|\Psi|^{4}+g_{\uparrow \downarrow} \sum_{j=1,2}\left|\psi_{j \uparrow}\right|^{2}\left|\psi_{j \downarrow}\right|^{2}\right] \tag{2.9}
\end{equation*}
$$

where $g$ and $g_{\uparrow \downarrow}$ are interatomic interaction between same and opposite spin species, respectively. Inserting Eq. (2.8) into Eq. 2.9), leads to the energy density as a functional of 8 independent variables $k_{1},\left|C_{1}\right|, \theta, \gamma_{1,2}$, and $\delta_{1,2,3}$. The energy functional can be broken down into three terms: the single-particle $\varepsilon_{0}$, intraspin interaction $\varepsilon_{g}$, and the interspin interaction $\varepsilon_{f}$. Combining these terms gives the full energy functional $\varepsilon=\varepsilon_{0}+\varepsilon_{g}+\varepsilon_{f}$. A full overview of this energy functional and all of its terms can be seen in Appendix B.

Minimizing the functional with respect to the 8 variables leads to the ground state wavefunction. It is important to note that $\Theta \Psi$, the time-reversal state of $\Psi$, is always orthogonal to $\Psi$ and gives the same energy functional $\varepsilon$. This means that the ground states are always doubly degenerate and are time-reversal partners of each other. The variational ansatz also allows us to compute the associated physical properties as

$$
\begin{align*}
\left\langle\sigma_{z}\right\rangle= & \left(\cos ^{2} \theta \cos 2 \gamma_{1}+\sin ^{2} \theta \cos 2 \gamma_{2}\right)\left(\left|C_{1}\right|^{2}-\left|C_{2}\right|^{2}\right), \\
\left\langle\sigma_{x}\right\rangle= & {\left[\sin 2 \gamma_{1} \cos ^{2} \theta \cos \delta_{12}+\sin 2 \gamma_{2} \sin ^{2} \theta \cos \delta_{3}\right] } \\
& \times\left(\left|C_{1}\right|^{2}-\left|C_{2}\right|^{2}\right), \\
\left\langle\sigma_{x} \tau_{z}\right\rangle= & \cos ^{2} \theta \sin 2 \gamma_{1} \cos \delta_{12}-\sin ^{2} \theta \sin 2 \gamma_{2} \cos \delta_{3}, \\
\left\langle\sigma_{z} \tau_{x}\right\rangle= & \sin 2 \theta\left[\cos \gamma_{1} \cos \gamma_{2} \cos \delta_{13}-\sin \gamma_{1} \sin \gamma_{2} \cos \delta_{2}\right] \\
& \times\left(\left|C_{1}\right|^{2}-\left|C_{2}\right|^{2}\right), \tag{2.10}
\end{align*}
$$

where $\delta_{i j} \equiv \delta_{i}-\delta_{j}$.
The interacting ground state exhibits three phases: (I) layer-stripe phase having $k_{1} \neq 0$, $\left|C_{1}\right|=\left|C_{2}\right|=\frac{1}{\sqrt{2}}$, and $\left\langle\sigma_{z}\right\rangle=\left\langle\sigma_{x}\right\rangle=\left\langle\sigma_{z} \tau_{x}\right\rangle=0$, which results in a spatially modulated layer polarization; (II) plane-wave phase having $k_{1} \neq 0,\left|C_{1} C_{2}\right|=0,\left|\left\langle\sigma_{z}\right\rangle\right|>0$, and $\left|\left\langle\sigma_{z} \tau_{x}\right\rangle\right|=1$; (III) zero-momentum phase having $k_{1}=\left|\left\langle\sigma_{z}\right\rangle\right|=0$.

First we look at typical phase transitions for moderately interacting $\operatorname{BEC}\left(g, g_{\uparrow \downarrow}\right)=$ $(1,0.9)$ as the Raman strength $\Omega$ varies. Figure 2.3 (a) shows the momentum $k_{1}$ as a monotonically decreasing function of $\Omega$ for either coupled ( $t=0.5$, green curve) or decoupled


Figure 2.3. (a) Momentum $k_{1}$ vs Raman strength $\Omega$ for cases of decoupled layers $t=0$ (purple) and coupled layers $t=0.5$ (green). The discontinuity in both curves (enlarged in the inset) indicates the transition between layer-stripe and plane-wave phases. In the $t=0$ case, the plane-wave phase can make a transition to the zero-momentum phase ( $k_{1}$ dropping to zero), which does not occur at $t=0.5$. (b) Spin polarization $\left|\left\langle\sigma_{z}\right\rangle\right|$ (red) and spin-layer symmetry $\left|\left\langle\sigma_{z} \tau_{x}\right\rangle\right|$ (blue) vs $\Omega$ at $t=0.5$. Note that both curves are zero and hence overlap each other in the layer-stripe phase region at small $\Omega$. In both (a) and (b), the interaction is set to $\left(g, g_{\uparrow \downarrow}\right)=(1,0.9)$, and curves (symbols) represent the variational (numerical GPE) results.
( $t=0$, purple curve) layers. At small $\Omega$, the system is in the layer-stripe phase (I). As $\Omega$ increases, the $k_{1}$ curves exhibit discontinuities, at which the system undergoes a first-order phase transition to the plane-wave phase (II). With further increase in $\Omega$, the $k_{1}$ curve of decoupled layer drops to zero at a critical value, representing a second-order transition to the zero-momentum phase (III), while that of coupled layers smoothly decreases but does not drops to zero, i.e. no transition to phase (III). The disappearance of phase (III) due to the interlayer coupling agrees with the single-particle physics discussed previously.

Figure 2.3 (b) shows spin polarization $\left|\left\langle\sigma_{z}\right\rangle\right|$ and spin-layer symmetry $\left|\left\langle\sigma_{z} \tau_{x}\right\rangle\right|$ as a function of $\Omega$ for coupling strength $t=0.5$. The layer-stripe phase (I) is spin unpolarized $\left|\left\langle\sigma_{z}\right\rangle\right|=0$, while the plane-wave phase (II) is spin polarized. This implies that the large discontinuity in spin polarization could provide a measurable experimental signature for the (I)-(II) transi-


Figure 2.4. (a) Phase diagram in the $g-\Omega$ plane for $t=0.5$. In $g<40$ ( $>40$ ), the system undergoes a transition from the layer-stripe phase (I) to the plane-wave phase (II) [zeromomentum phase (III)]. (b) Phase diagram in the $t-\Omega$ plane for $g=1$. The zero-momentum phase only occurs in the case of decoupled layers $t=0$ at $\Omega>2$. The color in both (a) and (b) represents momentum $k_{1}$, as scaled in the bar graph. (c) Top (black) and bottom (blue) layer density profiles $\rho_{ \pm}(x)$ of a layer-stripe phase at $\Omega=t=0.5$ in (b), exhibiting out-of-phase modulations between maximum $\rho_{M}$ and minimum $\rho_{m}$, or spatial modulations in $\left\langle\tau_{z}\right\rangle$. (d) Modulation amplitude $\tau_{z, \text { max }}\left[\equiv\left(\rho_{M}-\rho_{m}\right) / 2\right]$ versus $t$ (orange, top axis) and $g$ (green, bottom axis). The interspin interaction is set to be $g_{\uparrow \downarrow}=0.9 \mathrm{~g}$ for all the panels.
tion. The spin-layer symmetry $\left|\left\langle\sigma_{z} \tau_{x}\right\rangle\right|=0$ in the layer-stripe phase indicates an interaction induced symmetry breaking that equally mixes two states of opposite symmetry.

We turn to explore the interacting ground-state phases in a wider parameter region. Figure 2.4(a) shows the ground-state phase diagram in the $g-\Omega$ plane for $t=0.5$ and $g_{\uparrow \downarrow}=$ $0.9 g$. The (I)-(II) phase transition is shown to be allowed for $0<g<40$, in which the layer-
stripe phase region increases with $g$. When $g>40$, the plane-wave phase (II) disappears, and the system make transitions from layer-stripe (I) to the zero-momentum (III) phase for varying $\Omega$. Since the zero-momentum state is never energetically favored by the singleparticle Hamiltonian with finite $t$, this zero-momentum phase region is fully attributed to the interaction effect. In fact, the system staying at zero-momentum state costs higher singleparticle energy but saves more ferromagnetic interaction energy $\propto\left(g-g_{\uparrow \downarrow}\right) \rho$. Experimentally, this region can be achieved by increasing the atomic two-body scattering length through the Feshbach resonance [64] as well as the atomic density.

Additionally, we study the phase diagram in the $t$ - $\Omega$ plane for fixed $\left(g, g_{\uparrow \downarrow}\right)=(1,0.9)$ in Fig. 2.4(b). The interlayer tunneling is shown to linearly increase the layer-stripe phase region with respect to an increase in $\Omega$. In the plane-wave phase (II), the system momentum increases with $t$ at given $\Omega$. The zero-momentum phase (III) appears only at $t=0$, in which the system returns to the layer-independent conventional spin-orbit coupled BEC and hence exhibits the (II)-(III) transition at $\Omega_{c}=2$ as shown in Fig. 2.3(a) (green curve).

We further look into the detailed structure of the layer-stripe phase. Figure 2.4(c) shows the top and bottom layer density profiles, respectively, of a layer-stripe state $\Psi_{s}$ at $\Omega=t=0.5$ and $\left(g, g_{\uparrow \downarrow}\right)=(1,0.9)$. The two density profiles show out-of-phase spatial modulations. In other words, the system exhibits a layer-polarization stripe pattern $\tau_{z}(x)=\Psi_{s}^{*}(x) \tau_{z} \Psi_{s}(x)$ with wavelength $\lambda_{s}=\pi / k_{1}$. The zero total density modulation is a direct consequence of time-reversal symmetry, which makes the plane-wave states of $k$ and $-k$ in Eq. 2.8) orthogonal to each other at any spatial point. This contrasts the conventional system of Ref. 11 or a bilayer system with same-sign Raman coupling on both layers, the stripe phase exhibits total density modulations. Moreover, the layer-stripe phase is doubly degenerate. The other degenerate state is the Kramer partner $\Theta \Psi_{s}$, which has a time reversed layer-polarization modulation $-\tau_{z}(x)$. Figure $2.4(\mathrm{~d})$ shows the oscillation amplitude of $\tau_{z}(x)$, denoted by $\tau_{z, \text { max }}$, vs tunneling strength $t$ and interaction strength $g$. This quantity


Figure 2.5. (a) Spin-layer correlation $\left\langle\sigma_{x} \tau_{z}\right\rangle$ vs. Raman strength $\Omega$ in the case of decoupled layers $t=0$ (red) and coupled layers $t=0.5$ (blue). (b) Phase diagram in the $t-\Omega$ plane with color scale representing $\left\langle\sigma_{x} \tau_{z}\right\rangle$. In both (a) and (b), the interaction is set to $\left(g, g_{\uparrow \downarrow}\right)=(1,0.9)$.
decreases as either $t$ or $g$ increases. Experimentally, he layer-stripe phase can be detected by the standard time-of-fight (TOF) image, showing the co-occupation of both momentum minima. The out-of-phase stripe pattern may be probed with the Bragg diffraction, which has successfully revealed the density stripe structure of ultracold atomic gases 65].

Final analysis is done on the intrinsic spin-layer correlation $\left\langle\sigma_{x} \tau_{z}\right\rangle$ of the bilayer BEC. All three phases of the system are unpolarized in the $x$-spin direction $\left\langle\sigma_{x}\right\rangle=0$ and density balanced between the two layers $\left\langle\tau_{z}\right\rangle=0$. However, the product observable of both quantities $\left\langle\sigma_{x} \tau_{z}\right\rangle$ does exhibits non-zero expectation value. In Fig. 2.5(a) we plot $\left\langle\sigma_{x} \tau_{z}\right\rangle$ vs $\Omega$ for $t=0$ and 0.5 at $\left(g, g_{\uparrow \downarrow}\right)=(1,0.9)$. As $\Omega$ increases there is a gradual increase in the spin-layer correlation, along with a discontinuity in the curves that represents a (I)-(II) phase transition for both coupled and decoupled layers. When the system is in the zero-momentum phase it is shown that the spin-layer correlation is at it maximum value of $\left\langle\sigma_{x} \tau_{z}\right\rangle=1$, which is only the case for $t=0$ at low interaction strengths. Figure 2.5(b) shows the ground-state phase diagram in the $t-\Omega$ plane with color denoting $\left\langle\sigma_{x} \tau_{z}\right\rangle$. The layer-stripe phase has relatively
small correlations compared with the plane-wave phase. Such a spin-layer correlation is particularly useful for characterizing the phase diagram in experiments.

The experimental conditions for our time-reversal invariant system are similar to but slightly modified from the current setups. We consider a ${ }^{87} \mathrm{Rb}$ bilayer BEC created in a quasi-one-dimensional harmonic trap in the $x$ direction and a double-well shaped potential in the $y$ direction. The wavelength of HG Raman laser is 788 nm , which corresponds to the recoil energy $E_{R}=h \times 3697 \mathrm{~Hz}$. If one tunes the bilayer separation to be $0.4 \mu \mathrm{~m}$ and the double-well barrier to be $2 E_{R}$, the effective tunneling is $t=0.2 E_{R}$, with which important physics of our model can be explored. Higher tunneling is achievable by decreasing the separation or the barrier.

The layer-stripe phase can be detected by the standard time-of-fight (TOF) image, showing the co-occupation of both momentum minima. The out-of-phase stripe pattern may be probed with the Bragg diffraction, which has successfully revealed the density stripe structure of ultracold atomic gases [65]. Moreover, we suggest the use of spin-layer correlation $\left\langle\sigma_{x} \tau_{z}\right\rangle$ to experimentally determine the phase diagram and phase transitions. In experiment, such correlation must be determined by performing both spin-resolved and layer-resolved measurements. Simply measuring spin or layer components leads to trivial results.

## CHAPTER 3

## CONVOLUTIONAL NEURAL NETWORKS FOR BOSE-EINSTEIN CONDENSATES

The study presented in this chapter focuses on the building and training of a convolutional neural network (CNN) to predict the ground-state wavefunctions of a bosonic many body system. We generalize the ideas presented in Sec. 1.5 by expanding on the network and results presented in Ref. [66] by modifying the CNN structure to allow for complex phases. In general, the ground-state wavefunctions of SOC BECs are complex and therefore the ability to calculate these complex phases is crucial. We will focus on building a CNN for a two-component BEC with SOC such as that presented in Ref. [8] and detailed in Sec. 1.3 . However, the generalization of the CNN presented in the following sections allows for easy modifications to study many areas in ultracold atomic gases, including time-reversal invariant SOC BECs.

### 3.1 Network Generalization for Spin-Orbit Coupling

Exact analytical ground-state solutions of ultracold quantum many-body systems, particularly SOC BECs, are a rarity. This is due primarily to the nonlinearity of the Hamiltonian in these systems. Studies of the ground-state wavefunctions and their phases require various numerical strategies that are often computationally intensive. These traditional methods are detailed, and not limited to those shown, in Sec. 1.4. Recently, convolutional neural networks (CNNs), most commonly today used in problems involving computer vision [67], were trained to predict the solutions of a two-component BEC without SOC [66]. We propose a modified use of CNNs to allow for the prediction of the complex components in SOC BECs ground-state wavefunctions.

The procedure taken in this study can be seen in Fig. 3.1 and is as follows: First, we define the parameters to create the Hamiltonian of the two-component SOC BEC. Then, we


Figure 3.1. Flowchart showing our process from problem assessment to network evaluation. After defining the our Hamiltonian Eq. (3.1), the entire dataset is generated over the range of $\Omega$ using an iterative imaginary-time evolution process for each data point. The dataset is then broken into two subsets. The network is then trained on the larger training dataset minimizing the MSE and watching for overfitting. The network is then evaluated on the smaller test dataset. Any further network tuning is then used at this point to retrain the network and to increase its predictive performance capabilities.
create a base dataset using imaginary-time evolution on the dimensionless Gross-Pitaevskii equation [68]. The CNN is then trained on a large subset of the base dataset and further tested on the remaining hold-out validation set. Any further tuning to the network's parameters, known as hyperparameters, is then performed to optimize the defined loss-function (error metric).

We now discuss the Hamiltonian and parameters chosen for this study. We consider a one-dimensional two-component SOC BEC in the presence of an external potential. The external trapping potential is weak harmonic potential $V_{\text {ext }}(x)=0.25 x^{2}$. The Hamiltonian in terms of the time-independent GPE is defined as

$$
\begin{equation*}
H=\frac{1}{2}\left(p_{x}^{2}-2 p_{x} \sigma_{z}+\Omega \sigma_{x}\right)+V_{e x t}(x)+H_{i n t} \tag{3.1}
\end{equation*}
$$

where $\sigma_{i}$ are the Pauli matrices, $\Omega$ is the Raman coupling strength, and $H_{\text {int }}$, given as Eq. (1.8), is the particle interaction term. The ground-state wavefunctions of this Hamiltonian are well known and have been studied extensively [11], where comparison to the GPE


Figure 3.2. A reverse setup of a convolutional neural network for imagine classification (Like that shown in Fig. 1.3). The main layers of the network are the same (fully-connected and convolutional layers) expect the network is now propagating in the reverse direction. The intuition is that a certain input classification, or a combination of classification inputs, could be used to generate an output tensor. Here, the output tensor would be an image. The network setup in this orientation serves as a template for a single-input to wavefunctionoutput network.
solutions can be compared against the variational minimization of the energy functional to a very high degree of accuracy.

The algorithm used in this study is a deep convolutional neural network with $\Omega$ as the true inputs and ground-state wavefunctions as the outputs. The overall setup of the network will be similar in structure to [66]. The composition of the network cleverly mimics a high dimensional input classification convolutional neural network propagating in the reverse direction, an intuitive example of which is shown in Fig. 3.2. The true input $\Omega$ is modified to an input-tensor via two sequential dense layers. The input-tensor is then fed into the first convolutional layers (seen in Fig. 3.3 in orange) where the pattern recognition takes place. The two-component ground-state wavefunctions of the Hamiltonian Eq. (3.1) will be the output. In general, each spin-component of the ground-state wavefunction is complex. For


Figure 3.3. Our convolutional neural network setup to take the Raman coupling strength $\Omega$ as an input and to output the ground-state wavefunction of a two-component spin-orbit coupled BEC. The input $\Omega$ is fed into two fully-connected layers before going into a series of convolutional layers. The output of the network will be the two components of the groundstate. Note that since, in general, the ground-state will be a complex function, the output is divided into real and imaginary pairs for both spin components, leaving us with four output vectors. Leaky ReLu activation functions are used after each convolutional layer (not shown).
that reason, the spin-component outputs $\left(\psi_{\uparrow} \psi_{\downarrow}\right)$ are further split into real and imaginary components. Therefore, the output of the neural network will be a four-component vector $\left(\psi_{\uparrow r} \psi_{\uparrow i} \psi_{\downarrow r} \quad \psi_{\downarrow i}\right)$, as can be seen in the right of Fig. 3.3. Further generalization of this CNN leads to an output of a $2 \times j$ vector, where $j$ would be the number of components (for spin, layers, etc...) of the original ground-state wavefunction.

For creating the training samples, we vary the Raman coupling strength $\Omega \in[0,3]$. We hold the particle interaction terms for the BEC static in the moderately interacting regime $\left(g, g_{\uparrow \downarrow}\right)=(1,0.9)$ for the rest of this study. The parameter space in this range will display all three ground-state phases of a traditional SOC BEC: stripe-phase, plane-wave phase, and zero-momentum phase. Further details of these ground-state phases and a discussion of the experimental setup of this scheme are outlined in Sec. 1.3. The number of points chosen for the position space is $2^{9}$ in one-dimensional space. The overall size of the dataset is 3000 GPE


Figure 3.4. Sample of two momentum space wavefunctions for stripe-phase and plane-wave phase. The left column shows the wavefunctions obtained from imaginary time evolution of the GPE with spin-up in red and spin-down in blue. The right column shows the predicted wavefunctions generated from the trained CNN model. The stripe-phase was taken at $\Omega=$ 0.25 and the plane-wave phase at $\Omega=1.7$.
generated ground-state wavefunctions uniformly distributed over the full range of $\Omega$, with 2400 used as the training dataset and 600 used as the validation dataset. Care was taken to ensure that the train-test splitting contained an equal ratio of ground states between each of the three phases. This process, generally known as stratified-splitting, is a critical step to guarantee that the network is not trained on a majority of phases belonging to one, or at most two, classes and tested on the left-over phases.

The loss-function used in the training of the deep CNN uses mean-squared-error between the predicted ground-state wavefunctions and the ones obtained from the GPE evolution $M S E=\int d x\left|\psi_{\text {pred }}-\psi_{\text {real }}\right|^{2}$, where we take real wave-function to be the GPE solution and the predicted wave-function to be the CNN generated solution for the remainder of this
study. The CNN is trained until the mean-squared-error has reached a minimum value, while watching for overfitting. Since an acceptable lower bound of $M S E$ is difficult to quantify, we compare the ground-state energy calculations of the CNNs predicted values vs GPE evolutions using the relative energy difference after training has completed. The relative energy difference is given by,

$$
\begin{align*}
\varepsilon & =\langle\phi| H|\phi\rangle \\
\varepsilon_{r d} & =\frac{\left|\varepsilon_{\text {real }}-\varepsilon_{\text {pred }}\right|}{\varepsilon_{\text {real }}}, \tag{3.2}
\end{align*}
$$

where H is given as Eq. (3.1). This error term gives a better sense of how close the CNN is to predicting the true ground-states.

We now will analyze the output of the CNN which has been trained on the full spectrum training dataset. Fig. 3.4 shows an example of two GPE generated momentum-space wavefunctions (left), one stripe-phase and one plane-wave phase, compared to the CNN output (right) for the same parameters. Fig. 3.5(a) shows the momentum $k_{1}$ as a function of $\Omega$, while Fig. 3.5 (b) shows spin polarization $\left|\left\langle\sigma_{z}\right\rangle\right|$ as a function of $\Omega$. The GPE results are shown in blue. A random subsample of the test dataset is used to predict both $k_{1}$ and $\left|\left\langle\sigma_{z}\right\rangle\right|$ (shown as red-circles). For small $\Omega$, we see the largest discrepancy between the two methods. For larger values of $\Omega$, past the range of the stripe-phase, the results of the CNN and the GPE are fairly similar. The average relative energy difference over full range of $\Omega$ for the test set is $\left\langle\varepsilon_{r d}\right\rangle=1.67 \times 10^{-2}$, with particularly poor performance near the phase transition boundaries (shown by the dotted-lines in Fig. 3.5). This performance metric can be improved with a larger training dataset over a more granular range of $\Omega$. Overall, the average computational cost decreased for the generation of one ground-state wavefunction from 100 seconds for imaginary-time evolution (over $8 \times 10^{5}$ iterations) to 1 millisecond for CNN prediction. This model was trained with a learning-rate of $10^{-2}$ on 1000 epochs.


Figure 3.5. (a) Momentum $k_{1}$ vs Raman strength $\Omega$. The plane-wave phase makes a transition to the zero-momentum phase at $\Omega=2$. (b) Spin polarization $\left|\left\langle\sigma_{z}\right\rangle\right|$ vs $\Omega$. In both (a) and (b), the interaction is set to $\left(g, g_{\uparrow \downarrow}\right)=(1,0.9)$, and dotted-blue and open-red represent the numerical GPE results and subsampled CNN results respectively. All three phases are shown: stripe, plane-wave (P-W), and zero-momentum (Z-M) phases. The discontinuity indicates the transition between stripe and plane-wave phases.

### 3.2 Stripe-Phase

Designing and building a singular CNN that allows for accurate regression across phase transitions is a formidable task. To achieve more precise results, the CNN should be segmented for each phase; i.e., one CNN for each of the three phases. We now take the generalization of Sec. 3.1 and narrow the focus to training one of the segmentations, namely the stripe-phase. The primary reasons the stripe-phase is chosen as the region of interest is two-fold: (I) the stripe-phase contains complex phases and thus is suitable to study the of the 4 -component output of the setup seen in Fig. 3.3; (II) this phase has seen a lot of recent interest in SOC BECs as the stripe-phase behaves like a superfluid [65]. The other phase segmentations would be assembled and tested in a similar manner to what follows, with a change to the appropriate range of $\Omega$.

The parameters of learning-rate, number of epochs, external potential, interaction strengths $g$, along with the completed structure of the CNN, remain the same as the previous section. $\Omega$ is limited to a smaller range to only encompass the stripe-phase. The size of the training (validation) dataset is 800 (200). Fig. 3.6 shows the relative energy difference as a function of increasing $\Omega$. The average relative energy difference over the validation set for the stripe-phase region is $\left\langle\varepsilon_{r d}\right\rangle=6.02 \times 10^{-3}$. When $\Omega$ is close to zero, the stripe-phase collapses to a wavefunction resembling a zero-momentum phase, which leads to a larger error in this region. Note the additional spike in error around the mid-region of $\Omega$ given in the figure. This model was trained with a learning-rate of $10^{-2}$ on 1000 epochs, with a similar increase in computation speed as seen in Sec. 3.1.

In summary, we realized a generalizable CNN to predict the complex ground-state wavefunctions for traditional SOC BECs. The network was first trained over a wide range of parameters to allow for predictions of three very different quantum phases. The results were then improved, in terms of relative energy difference, when the CNN became segmented. We tested the segmented model on the strip-phase. However, we should expect similar results


Figure 3.6. Relative energy difference (Eq. (3.2)) vs $\Omega$ over the range of the stripe phase. The average relative energy difference for the stripe phase is $\left\langle\varepsilon_{r d}\right\rangle=6.02 \times 10^{-3}$.
for the other two segmentations. Additional improvements to the error metric of this model would follow with a larger training dataset, further hyperparameter tuning, and modification to the hidden layers of the network. Slight modifications to the input, hidden, and output layers would allow for the CNN presented in this study to be applied to a wider range of research. This network is setup using a popular online library developed by Google called TensorFlow [69]. The minimization of the loss-function during training is done using the Adam optimizer [70].

## CHAPTER 4

## CONCLUSION

In this dissertation, we have studied the effect of spin-orbit coupling on Bose-Einstein condensates through the use of artificial gauge fields. We investigated a realistic setup to preserve time-reversal symmetry, which is typically absent in conventional experiments on spinorbit coupled ultracold gases. This was accomplished by using different modes of HermiteGaussian beams to create a bilayer system which would allow for tunneling. We further studied the ground-state phase diagram and found an interaction-induced layer-stripe phase which exhibits spatially modulated layer polarization. We also found a zero-momentum phase region which cannot be described by single-particle physics.

We then transitioned into the use of machine learning, in particular convolutional neural networks, to predict the ground-states of ultracold atomic gases. For the case of spin-orbit coupled Bose-Einstein condensates, we varied the Raman coupling strength to encompass all three ground-state phases and used a static harmonic potential trap and particle interaction strengths to predict the ground-states. We found that predicting the ground-states over this full spectrum of Raman strengths of the spin-orbit coupled gas was too complex for the current CNN structure, and a segmented model was created for the stripe-phase. Overall, the temporal computational improvement from traditional ground-state calculations to CNN predicted wavefunctions proved to be several orders of magnitude.

The results of the research presented in this dissertation show that spin-orbit coupling with artificial gauge fields in Bose-Einstein condensates, produced by the various modes of Hermite-Gaussian beams, provide for the study of new novel quantum phases. Deep learning algorithms can be trained to study the ground-states of spin-orbit coupled gases as well more traditional quantum systems. These algorithms lead to faster ground-state simulations as they are not as computationally intensive. Deep leaning is a field that has expanded quickly in recent years due to the rapid increase in both central and graphical processing units. There
are still many areas of study in the field of ultracold gases where this type of predictive power can be used for further breakthroughs.

## APPENDIX A

## IMAGINARY TIME EVOLUTION

Any general wavefunction $\Psi$ can be expressed as a summation of eigenfunctions of a Hamiltonian $H$,

$$
\begin{equation*}
\Psi(x, \tau)=\sum_{j} \psi_{j}(x) e^{-i E_{j} \tau / \hbar} \tag{A.1}
\end{equation*}
$$

Using a Wick rotation $\tau=-$ it and expanding,

$$
\begin{equation*}
\Psi(x,-i t)=e^{-E_{0} t / \hbar} \sum_{j} \psi_{j}(x) e^{-\Delta_{j 0} t / \hbar} \tag{A.2}
\end{equation*}
$$

where $\Delta_{j 0}=E_{j}-E_{0}$. As $t \rightarrow \infty$ the excited states decay and we are left with the ground state $\psi_{0}$.

## APPENDIX B

## BILAYER ENERGY FUNCTIONAL

For the single-particle,

$$
\begin{align*}
\varepsilon_{0}= & \frac{k_{0}^{2}}{2}+\frac{k_{1}^{2}}{2}-k_{1} k_{0}\left(\cos ^{2} \theta \cos 2 \gamma_{1}+\sin ^{2} \theta \cos 2 \gamma_{2}\right)  \tag{B.1}\\
& +\frac{\Omega}{2}\left(\cos ^{2} \theta \sin 2 \gamma_{1} \cos \delta_{21}-\sin ^{2} \theta \sin 2 \gamma_{2} \cos \delta_{3}\right) \\
& -\frac{t}{2} \sin 2 \theta\left(\cos \gamma_{1} \cos \gamma_{2} \cos \delta_{13}+\sin \gamma_{1} \sin \gamma_{2} \cos \delta_{2}\right)
\end{align*}
$$

For the interaction energy, the intraspin interaction is,

$$
\begin{align*}
\varepsilon_{g}= & \frac{n g}{2}\left[(1-2 \beta)\left(\cos ^{4} \theta \cos ^{4} \gamma_{1}+\cos ^{4} \theta \sin ^{4} \gamma_{1}+\frac{3 \sin ^{4} \theta}{4}+\frac{\sin ^{4} \theta \cos 4 \gamma_{2}}{4}\right)\right. \\
& \left.+2 \beta \sin ^{2} 2 \theta\left(\cos ^{2} \gamma_{2} \sin ^{2} \gamma_{1}+\cos ^{2} \gamma_{1} \sin ^{2} \gamma_{2}\right)\right] \tag{B.2}
\end{align*}
$$

where $\beta=\left|C_{1}\right|^{2}\left|C_{2}\right|^{2}$, and the interspin interaction,

$$
\begin{align*}
\varepsilon_{f}= & \frac{n g_{\uparrow \downarrow}}{4}(1-2 \beta)\left(\cos ^{4} \theta \sin ^{2} 2 \gamma_{1}+\sin ^{4} \theta \sin ^{2} 2 \gamma_{2}\right)+ \\
& n g_{\uparrow \downarrow} \beta \cos ^{2} \theta \sin ^{2} \theta\left[2 \cos ^{2} \gamma_{1} \cos ^{2} \gamma_{2} 2 \sin ^{2} \gamma_{1} \sin ^{2} \gamma_{2}\right. \\
& \left.-\sin 2 \gamma_{1} \sin 2 \gamma_{2} \cos \left(\delta_{1}-\delta_{2}-\delta_{3}\right)\right] . \tag{B.3}
\end{align*}
$$

Combining these terms gives the full energy functional $\varepsilon=\varepsilon_{0}+\varepsilon_{g}+\varepsilon_{f}$.

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