Spin-Orbit Coupled Spinor Bose-Einstein Condensates

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An effective spin-orbit coupling can be generated in a cold atom system by engineering atom-light interactions. In this Letter we study spin-1/2 and spin-1 Bose-Einstein condensates with Rashba spin-orbit coupling, and find that the condensate wave function will develop nontrivial structures. From numerical simulation we have identified two different phases. In one phase the ground state is a single plane wave, and often we find the system splits into domains and an array of vortices plays the role of a domain wall. In this phase, time-reversal symmetry is broken. In the other phase the condensate wave function is a standing wave, and it forms a spin stripe. The transition between them is driven by interactions between bosons. We also provide an analytical understanding of these results and determine the transition point between the two phases.

The interaction between a matter field and gauge field is of central importance in quantum physics. Although atoms are neutral and do not possess gauge coupling to a real electromagnetic field, it has been proposed that a synthetic gauge field originating from the Berry phase effect can be coupled to atoms by engineering the interactions between atoms and a spatially varying laser field [1]. Very recently, this scheme has been successfully implemented in a Rb^{87} Bose-Einstein condensate (BEC) [2]. A straightforward generalization of this scheme can also create a non-Abelian gauge field to cold atoms [3–5]. This opens up a new avenue in cold atom physics, that is to study how a coherent matter wave responds to external gauge fields, in particular, the non-Abelian gauge fields.

There are already various proposals to achieve a non-Abelian gauge field. For instance, one can start with an N-pod system, where N atomic internal states are coupled to one common state by N different laser fields. It results in $N-1$ dark states which play a role as internal pseudospin degrees of freedom [3–6]. Tripod ($N = 3$) and tetrapod ($N = 4$) setup correspond to spin-1/2 and spin-1 case, respectively. Among all possibly achieved configurations of non-Abelian gauge fields $\mathbf{A}$, one of the most simplest cases with $A_x = \sigma_x$ and $A_y = \sigma_y$ is equivalent to a Rashba type spin-orbit (SO) coupling [4,5]. Very recently, BEC with SO coupling has been first realized by the NIST group using a similar scheme described in Refs. [2,6].

During the last few years, it has been extensively studied that SO coupling in an electronic system can lead to a novel state of matter of topological insulator which has many exotic physical properties [7]. Nevertheless, so far only a few papers have studied the SO effect in a boson condensate [8,9]. This Letter is devoted to study the properties of spin-1/2 and spin-1 condensate in the presence of a pure Rashba SO coupling. The model under consideration is $\hat{H} = \hat{H}_0 + \hat{H}_{\text{int}}$,

$$\hat{H}_0 = \int d^2\mathbf{r}\Psi^\dagger \frac{1}{2m}(\mathbf{k}^2 + 2\kappa\mathbf{k}\cdot\vec{\sigma})\Psi, \qquad (1)$$

where $\Psi = (\Psi_\uparrow, \Psi_\downarrow)$ for the spin-1/2 case and $\Psi = (\Psi_1, \Psi_0, \Psi_{-1})$ for the spin-1 case. Here, we consider a quasi-two-dimensional situation and in-plane SO coupling where $\mathbf{k} = \{k_x, k_y\}$ and $\vec{\sigma} = \{\sigma_x, \sigma_y\}$, where $\sigma_{x,y}$ are the spin-1/2 or spin-1 representation of Pauli matrices. For the interaction term, we note that different pseudospin components are in fact a superposition of atomic hyperfine states, and therefore the interactions between them could have a quite complicated form. However, as an initial effort to understand this rich system, in this work we try to simplify the situation by considering a simplified interaction form borrowed from conventional spinor BEC, namely, for spin-1/2, $H_{\text{int}} = \int d^2\mathbf{r}(g_1\hat{n}_\uparrow^2 + g_2\hat{n}_\downarrow^2 + 2g_{12}\hat{n}_\uparrow\hat{n}_\downarrow)$. We shall also focus on the case with $g_1 = g_2 > 0$ and then the interaction can also be rewritten as $H_{\text{int}} = \int d^2\mathbf{r}\left(\frac{c_0}{2}\hat{n}^2 + \frac{c_2}{2}\hat{S}_z^2\right)$, where $\hat{n} = \hat{n}_\uparrow + \hat{n}_\downarrow$, $\hat{S}_z = \hat{n}_\uparrow - \hat{n}_\downarrow$, and $c_0 = g_1 + g_{12}$ and $c_2 = g_1 - g_{12}$. The c_0 term is $SU(2)$ spin rotational invariant while the c_2 term breaks spin rotation symmetry. For the spin-1 case, we shall consider the standard interaction form [10] $H_{\text{int}} = \int d^2\mathbf{r}\left(\frac{c_0}{2}\hat{n}^2 + \frac{c_2}{2}\hat{\mathbf{S}}^2\right)$, where $\hat{n} = \hat{n}_1 + \hat{n}_0 + \hat{n}_{-1}$ and $\hat{\mathbf{S}} = \Psi_\alpha^\dagger \vec{\sigma}_{\alpha\beta}\Psi_\beta$. In both cases, $c_0 > 0$ and $\gamma = c_2/c_0$ can be either positive or negative.

The main results of this Letter include the following: (i) A boson condensation in the $\mathbf{k} = 0$ single-particle state is always unstable in the presence of SO coupling. (ii) The ground state has two possible phases: one is named the "plane wave phase" (PW), where the ground state is found to be a single plane wave; the other is named the "standing wave phase" (SW), where the spatial wave function of each spin component forms an oscillating standing wave,

as presented in Figs. 2 and 3. (iii) The transition between the PW phase and the SW phase depends on the interactions between bosons. For the spin-1/2 case, it is the PW phase if $\gamma > 0$ and the SW phase otherwise; while for the spin-1 case, it is the PW phase if $\gamma < 0$ and the SW phase otherwise. (iv) We often find the long-lived metastable state in which the system splits into two domains. In the parameter regime of the PW phase, it is locally a plane wave state with opposite wave vector in each domain, and an equally spaced array of vortices plays the role as the domain wall. We note, unlike BEC in a synthetic magnetic field [2], the Hamiltonian for the non-Abelian gauge field considered here preserves both time-reversal and translation symmetry, however, the "PW" phase spontaneously breaks time-reversal symmetry, which is unconventional in a bosonic system. Moreover, both phases spontaneously break space-spin rotation symmetry. This behavior is fundamentally different from the effect of SO coupling in

electronic systems. We have also verified that other terms not considered here, such as linear and quadratic Zeeman field, the difference between g_1 and g_2, will only shift the phase boundary between these two phases, and will not affect the essence of the two phases, as long as their strength is relatively not too strong.

Instability of a condensation on the $\mathbf{k} = 0$ *state.*— Without SO coupling, the ground state of bosons is a condensation in the $\mathbf{k} = 0$ state. Hence, the question arises whether the SO coupling $\mathbf{k} \cdot \vec{\sigma}$ will have any significant effect on a BEC, in particular, if the SO coupling is weak. Here let us take the spin-1/2 case as an example, and first expand the boson field operator $\Psi_\sigma^\dagger(\mathbf{r}) = \sum_{\mathbf{k}} e^{i\mathbf{k}\mathbf{r}} b_{\mathbf{k}\sigma}^\dagger / \sqrt{V}$ (V is the volume). If we still assume a boson condensation in the $\mathbf{k} = 0$ state, i.e. $\langle b_{\sigma,\mathbf{k}=0} \rangle = \phi_\sigma$, the Bogoliubov Hamiltonian can be written as $\hat{H}_{\text{Bg}} = \sum_{\mathbf{k}} B_{\mathbf{k}}^\dagger H_{\mathbf{k}} B_{\mathbf{k}}$, where $B_{\mathbf{k}}^\dagger = (\hat{b}_{\uparrow\mathbf{k}}^\dagger, \hat{b}_{\uparrow-\mathbf{k}}, \hat{b}_{\downarrow\mathbf{k}}^\dagger, \hat{b}_{\downarrow-\mathbf{k}})$ and

$$H_{\mathbf{k}} = \begin{pmatrix} \epsilon_{\mathbf{k}\uparrow} & 2g_1\phi_\uparrow^2 & \frac{\hbar\kappa}{m}(k_x - ik_y) + 2g_{12}\phi_\uparrow^*\phi_\downarrow & 2g_{12}\phi_\uparrow\phi_\downarrow \\ 2g_1\phi_\uparrow^{*2} & \epsilon_{\mathbf{k}\uparrow} & 2g_{12}\phi_\uparrow^*\phi_\downarrow^* & \frac{\hbar\kappa}{m}(-k_x - ik_y) + 2g_{12}\phi_\uparrow^*\phi_\downarrow \\ \frac{\hbar\kappa}{m}(k_x + ik_y) + 2g_{12}\phi_\uparrow\phi_\downarrow^* & 2g_{12}\phi_\uparrow\phi_\downarrow & \epsilon_{\mathbf{k}\downarrow} & 2g_2\phi_\downarrow^2 \\ 2g_{12}\phi_\uparrow^*\phi_\downarrow^* & \frac{\hbar\kappa}{m}(-k_x + ik_y) + 2g_{12}\phi_\uparrow\phi_\downarrow^* & 2g_2\phi_\downarrow^{*2} & \epsilon_{\mathbf{k}\downarrow} \end{pmatrix},$$

where $\epsilon_{\mathbf{k}\sigma} = \mathbf{k}^2/(2m) + 2g_1|\phi_\sigma|^2$. We then introduce a generalized Bogoliubov transformation $B_{\mathbf{k}} = \Omega_{\mathbf{k}} \tilde{B}_{\mathbf{k}}$, where $\tilde{B}_{\mathbf{k}}^\dagger = (\hat{\beta}_{\uparrow\mathbf{k}}^\dagger, \hat{\beta}_{\uparrow-\mathbf{k}}, \hat{\beta}_{\downarrow\mathbf{k}}^\dagger, \hat{\beta}_{\downarrow-\mathbf{k}})$, where $\Omega_{\mathbf{k}}$ is a 4×4 matrix. To satisfy the commutation relation $[\beta_{\sigma\mathbf{k}}, \beta_{\sigma'\mathbf{k}'}^\dagger] = \delta_{\sigma\sigma'}\delta_{\mathbf{k}\mathbf{k}'}$ and $[\beta_{\sigma\mathbf{k}}, \beta_{\sigma'\mathbf{k}'}] = 0$, $\Omega_{\mathbf{k}}$ has to satisfy the relation $\Omega_{\mathbf{k}}^\dagger A \Omega_{\mathbf{k}} = A$, where A is a 4×4 matrix

$$\begin{pmatrix} \sigma_z & 0 \\ 0 & \sigma_z \end{pmatrix}.$$

Suppose $H_{\mathbf{k}}$ can be diagonalized by a $\Omega_{\mathbf{k}}$, and the diagonal values of $\Omega_{\mathbf{k}}^\dagger H_{\mathbf{k}} \Omega_{\mathbf{k}}$ are denoted by λ_i. λ_i satisfies the equation $\text{Det}[H_{\mathbf{k}} - \lambda_i A] = 0$, which gives two solutions denoted by $\lambda_{\uparrow\mathbf{k}}$ and $\lambda_{\downarrow\mathbf{k}}$. The Bogoliubov Hamiltonian becomes $\hat{H}_{\text{Bg}} = \sum_{\mathbf{k},\sigma} \lambda_{\sigma\mathbf{k}} \beta_{\sigma\mathbf{k}}^\dagger \beta_{\sigma\mathbf{k}}$. We find that one excitation branch always has a positive imaginary part in a large regime in momentum space, even for infinitesimal small SO coupling. Therefore, suppose a BEC is initially prepared in the $\mathbf{k} = 0$ state, as SO coupling is turned on, some modes will exponentially grow. Therefore, a conventional BEC on the $\mathbf{k} = 0$ mode is unstable with SO coupling, raising the question of what is the actual ground state of a spinor BEC with SO coupling.

In addition, we note that the spectrum shown in Fig. 1 breaks spatial rotation symmetry. This is also an effect of SO coupling. Since the Hamiltonian of Eq. (1) only possesses a symmetry of simultaneous rotation of both spin and space, namely $k_x + ik_y \rightarrow e^{i\theta}(k_x + ik_y)$ and $\sigma_x \pm i\sigma_y \rightarrow e^{\pm i\theta}(\sigma_x \pm i\sigma_y)$. However, the Bose condensation locks the relative phase between different spin components

and therefore breaks spin rotation symmetry. Consequently, this symmetry breaking manifests itself in real space.

Numerical simulation for the spin-1/2 case.—We implement the mean-field approximation and numerically look for the condensate wave function that can minimize Gross-Pitaevskii energy using the imaginary time evolution method. For the spin-1/2 case the Gross-Pitaevskii energy is written as

$$\mathcal{E} = \int d^2\mathbf{r} \left\{ \sum_{\sigma=\uparrow,\downarrow} \varphi_\sigma^* \left(-\frac{\hbar^2}{2m}\nabla^2 + \frac{1}{2}m\omega^2 r^2 \right) \varphi_\sigma \right.$$
$$+ \frac{\hbar\kappa}{m}[\varphi_\uparrow^*(-i\partial_x - \partial_y)\varphi_\downarrow + \varphi_\downarrow^*(-i\partial_x + \partial_y)\varphi_\uparrow]$$
$$\left. + \frac{c_0}{2}(|\varphi_\uparrow|^2 + |\varphi_\downarrow|^2)^2 + \frac{c_2}{2}(|\varphi_\uparrow|^2 - |\varphi_\downarrow|^2)^2 \right\}. \quad (2)$$
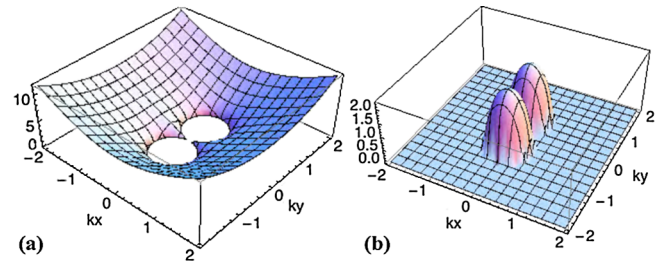

FIG. 1 (color online). An example of real (a) and imaginary (b) part of unstable branch of excitation spectrum with SO coupling.

What we find are shown in Fig. 2. For $\gamma = c_2/c_0 > 0$, the densities of both component have no particular structure, while the phase of both components behave as a plane wave, as shown in Figs. 2(a1) and 2(a2) and named as the PW phase. Time-reversal symmetry is broken in this phase. For $\gamma < 0$, the wave functions of both components behave as standing waves and lead to periodic density modulation of both components, as shown in Figs. 2(b1) and 2(b2) and named as the SW phase. Time-reversal symmetry is preserved. Moreover, the higher density regime of the spin-up component coincides with the lower density regime of the spin-down component, which represents a microscopic phase separation, and also represents a spin stripe state.

Though, in the numerical simulation, we have included a very weak harmonic trap which helps to avoid artifact from a sharp boundary and also simulates the practical situation in cold atom experiment, the results can be understood from a homogeneous case. With SO coupling, the single-particle spectrum becomes $E_{\pm \mathbf{k}} = (\hbar^2 \mathbf{k}^2 \pm 2\kappa\hbar|\mathbf{k}|)/(2m)$, where $\pm$ denotes different helicity (spin parallel or anti-parallel to wave vector). The single-particle ground state is in the negative helicity branch with $|\mathbf{k}| = \kappa/\hbar$, and the wave function is given by

$$\phi_{\mathbf{k}} = \frac{1}{\sqrt{2}} e^{i\mathbf{k}\mathbf{r}} \begin{pmatrix} 1 \\ -e^{i\varphi_{\mathbf{k}}} \end{pmatrix}, \qquad (3)$$

where $\varphi_{\mathbf{k}} = \arg(k_x + ik_y)$ and $\varphi_{-\mathbf{k}} = \varphi_{\mathbf{k}} + \pi$. Let us first consider a simple case that assumes the condensate wave function is a superposition of two opposite wave vector states as

$$\varphi = \begin{pmatrix} \varphi_\uparrow \\ \varphi_\downarrow \end{pmatrix} = \frac{\alpha_1}{\sqrt{2}} e^{i\mathbf{k}\mathbf{r}} \begin{pmatrix} 1 \\ -e^{i\varphi_{\mathbf{k}}} \end{pmatrix} + \frac{\alpha_2}{\sqrt{2}} e^{-i\mathbf{k}\mathbf{r}} \begin{pmatrix} 1 \\ -e^{i\varphi_{-\mathbf{k}}} \end{pmatrix}.$$

Using this ansatz to minimize the interaction energy, it is easy to find, for $c_2 < 0$, it favors $\alpha_1 = \alpha_2 = 1/\sqrt{2}$,
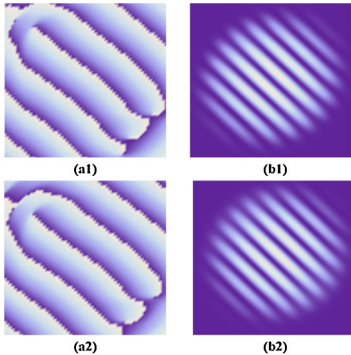

(a1)   (b1)

(a2)   (b2)

FIG. 2 (color online). Numerical results for the spin-$1/2$ case. a1 and a2 show the phase of condensate wave function of both spin-up (a1) and down (a2) component increase from $-\pi$ (grey regime) to π (dark regime) periodically in the PW regime; b1 and b2 show the density of both the spin-up (b1) and down (b2) component oscillate periodically in the SW regime. $\gamma = c_2/c_0 = 0.4$ for a1 and a2, and $\gamma = 0.1$ for b1 and b2.

therefore, $\varphi_\uparrow \sim \cos\mathbf{k}\mathbf{r}$ and $\varphi_\downarrow \sim i\sin\mathbf{k}\mathbf{r}$. While for $c_2 > 0$, it favors the case $\alpha_1 = 1$, $\alpha_2 = 0$, or $\alpha_1 = 0$, $\alpha_2 = 1$, namely, the wave function is a single plane wave.

The next question is whether there will be more than one single $\mathbf{k}$ state, or a pair of $\{\mathbf{k}, -\mathbf{k}\}$ states entering the condensate wave function φ. In general, one shall assume a superposition of all states in the degenerate circle

$$\varphi = \int d\varphi_{\mathbf{k}} \frac{\alpha_{\mathbf{k}}}{\sqrt{2}} e^{i\mathbf{k}\mathbf{r}} \begin{pmatrix} 1 \\ -e^{i\varphi_{\mathbf{k}}} \end{pmatrix}, \qquad (4)$$

where the amplitude of $\mathbf{k}$ is fixed at $\kappa/\hbar$ to minimize the single-particle energy. For instance, if $\alpha_{\mathbf{k}}$ is independent of the angle of $\mathbf{k}$, one can obtain

$$\varphi = \frac{1}{\sqrt{2}} \begin{pmatrix} \pi J_0(|\mathbf{k}||\mathbf{r}|) \\ i\pi J_1(|\mathbf{k}||\mathbf{r}|) e^{i\theta} \end{pmatrix}, \qquad (5)$$

where θ is the angle of $\mathbf{r}$. This is a symmetric skyrmion solution, which has also been proposed by Ref. [9]. However, if one substitutes the ansatz Eq. (4) into the energy function Eq. (2) and minimizes the energy with respect to all $\alpha_{\mathbf{k}}$, we can find the most favorable solution is always that $\alpha_{\mathbf{k}}$ is nonzero either for a single $\mathbf{k}$ or for a pair of $\{\mathbf{k}, -\mathbf{k}\}$, and we do not find a parameter regime in which the condensate wave function contains more than two wave vector components.

Numerical simulation for the spin-1 case.—We now move to study the spin-1 case, whose energy functional is given by

$$\mathcal{E} = \int d^3\mathbf{r} \Bigg\{ \sum_{\sigma=1,0,-1} \varphi_\sigma^* \left(-\frac{\hbar^2}{2m}\nabla^2 + \frac{1}{2}m\omega^2 r^2 \right) \varphi_\sigma$$

$$+ \frac{\hbar\kappa}{m} \left[\varphi_1^*(-i\partial_x - \partial_y)\varphi_0 + \varphi_0^*(-i\partial_x - \partial_y)\varphi_{-1} \right.$$

$$+ \text{H.c.}] + \frac{c_0}{2}(|\varphi_1|^2 + |\varphi_0|^2 + |\varphi_{-1}|^2)^2 + \frac{c_2}{2}$$

$$\times [(|\varphi_1|^2 - |\varphi_{-1}|^2)^2 + 2|\varphi_1^*\varphi_0 + \varphi_0^*\varphi_{-1}|^2] \Bigg\}. \qquad (6)$$

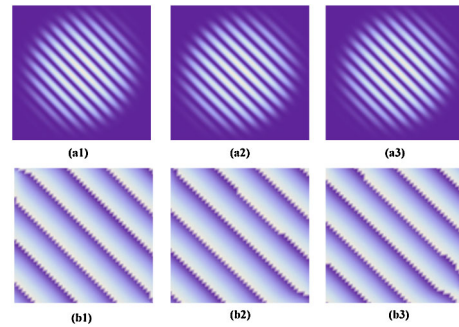(a1)   (a2)   (a3)

(b1)   (b2)   (b3)

FIG. 3 (color online). Numerical results for spin-1 case. a1–a3 are density of 1, 0, and -1 component in the SW regime; and b1–b3 are phase of and b3 are 1, 0, and -1 component in the PW regime. $\gamma = c_2/c_0 = 0.2$ for a1–a3, and $\gamma = -0.2$ for b1–b3.

The results from numerical simulation are displayed in
Fig. 3. As shown in Fig. 3, for $\gamma > 0$ it is the SW phase
and for $\gamma < 0$ it is the PW phase.

The result of spin-1 can be understood with similar
analysis above. The wave function for the single-particle
ground state is now

$$\phi_{\mathbf{k}} = \frac{1}{2} \begin{pmatrix} 1 \\ -\sqrt{2}e^{i\varphi_{\mathbf{k}}} \\ e^{i2\varphi_{\mathbf{k}}} \end{pmatrix} e^{i\mathbf{k}\mathbf{r}}. \qquad (7)$$

We shall also consider a superposition as $\alpha_1 \phi_{\mathbf{k}} + \alpha_2 \phi_{-\mathbf{k}}$.
The c_0 term is independent of $\alpha_{1,2}$, however, for $\alpha_1 = \alpha_2 = 1/\sqrt{2}$, $\langle \mathbf{S} \rangle^2 = 0$ and it is favored when $c_2 > 0$. This
state is also a special case of the so-called "polar" or
"nematic" phase in the discussion of spin-1 BEC [10];
while for $\alpha_1 = 0$, $\alpha_2 = 1$ or $\alpha_1 = 1$, $\alpha_2 = 0$, $\langle \mathbf{S} \rangle^2 = 1$ and
it is favored when $c_2 < 0$. This is also called the "ferro-
magnetic" phase.

Domains and domain wall.—Our numerical simulation
also finds long-lived metastable states with domains. For
instance, if we start with a random initial configuration, in
most cases the imaginary time evolution leads to a state in
which the system often splits into two domains. In the PW
phase, the system is locally a single plane wave state in
each domain, and the wave vector is opposite between two
domains. This is very similar to the situation of ferromag-
netism, where one always finds a ferromagnetic state made
up with locally magnetized domains.

In the presence of domains, we find that both up and
down components of the condensate wave function contain
an array of vortices, as shown in Fig. 4(a). We have
checked that the vorticity of all vortices are the same,
and the vortices in different components locate alternately.
The vortex array plays the role as a domain wall. Consider
an array of vortices with the same vorticity, located at $x = nl$ and $y = 0$, where n are integers, in a uniform superfluid
the gradient of the superfluid phase $\vec{\partial}\theta$ at (x, y) is given by
$\partial_x\theta = \frac{1}{l} \sum_{n=-\infty}^{+\infty} y/l/((x/l + n)^2 + (y/l)^2)$ and $\partial_y\theta = -\frac{1}{l} \sum_{n=-\infty}^{+\infty} (x/l + n)/((x/l + n)^2 + (y/l)^2)$. $\vec{\partial}\theta$ as a func-
tion of (x, y) is shown in Figs. 4(c) and 4(d). As one can
see, when $|y| > l$, $\partial_x\theta \to \pi/l$ is a constant and $\partial_y\theta \to 0$.
Hence the system is locally a plane wave state. To mini-
mize the single-particle energy, one requires $l = \pi\hbar/\kappa$;
namely, the vortex line density increases as the increase of
SO coupling.

Hence, we have established the conclusion (i–iv) sum-
marized above within a mean-field theory. In future studies
we will include quantum fluctuations. Due to the degener-
acy of the single-particle ground states, quantum fluctua-
tion, in particular, the fluctuation of rotation mode, may lead
to fragmentation. However, it is known that the fragmented
state is usually very fragile for a realistic system with a large
number of bosons and is not stable against external pertur-
bations. In this case, effects such as anisotropy of trapping
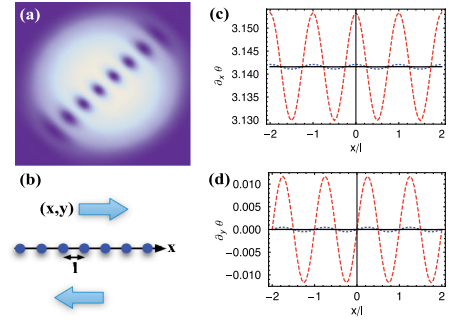potential will break the spatial rotational symmetry and pin

FIG. 4 (color online). (a) Density of the up (or down) compo-
nent with two domains in the PW phase. (b) A schematic of the
vortex array as a domain wall between two regimes with oppo-
site wave vector. (c)–(d) Consider array of vortices separated by
distance l located in x axes, $\partial_x\theta$ (c) and $\partial_y\theta$ (d) (in unit of $1/l$) at
position (x, y) as a function of x/l is shown for $|y| = l$ (red
dashed line), $|y| = 1.5l$ (blue dotted line) and $|y| = 2l$ (black
solid line). θ is the phase of condensate wave function.

the direction of plane wave or density stripe, and prevent the
fluctuation of the rotation mode from restoring the symme-
try. Mean-field results become more stable and the predic-
tions of this work can be verified experimentally very soon.

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