

**Loop-structure stability of a double-well-lattice Bose-Einstein condensate**Hoi-Yin Hui,<sup>1,2</sup> Ryan Barnett,<sup>1,2</sup> J. V. Porto,<sup>1</sup> and S. Das Sarma<sup>1,2</sup><sup>1</sup>*Joint Quantum Institute, University of Maryland, College Park, Maryland 20742-4111, USA*<sup>2</sup>*Condensed Matter Theory Center, Department of Physics, University of Maryland, College Park, Maryland 20742-4111, USA*

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In this work, we consider excited many-body mean-field states of bosons in a double-well optical lattice by investigating stationary Bloch solutions to the nonlinear equations of motion. We show that, for any positive interaction strength, a loop structure emerges at the edge of the band structure whose existence is entirely due to interactions. This can be contrasted to the case of a conventional optical (Bravais) lattice where a loop appears only above a critical repulsive interaction strength. Motivated by the possibility of realizing such nonlinear Bloch states experimentally, we analyze the collective excitations about these nonlinear stationary states and thereby establish conditions for the system's energetic and dynamical stability. We find that there are regimes that are dynamically stable and thus apt to be realized experimentally.

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**I. INTRODUCTION**

A wealth of nontrivial quantum states has been realized with Bose-Einstein condensates (BECs) in optical lattices [1,2]. Conventionally, these states occupy the lowest energy configuration of the parent Hamiltonian of the system. On the other hand, motivated by the low levels of dissipation in ultracold atomic gases, considerable recent effort has shifted to the possibility of realizing interesting quantum states not as the ground state, but as long-lived excited states [3]. In particular, recent experiments have realized condensates in excited bands [4–8]. Such efforts open the door to achieving, for instance, states having Néel order, which is notoriously difficult to realize as the ground state of a system of bosons [9,10], and novel fermionic states [11,12] that have no parallels in solid-state physics. Unconventional excited states realized with ultracold atoms have been considered theoretically in Refs. [13–18].

In the presence of interactions, the nonlinear Bloch band of a BEC can develop interesting features. Although its ground state is fairly conventional, at the Brillouin zone boundary, the band can develop a cusp and subsequently form a loop as interaction is increased [19–22]. However, for Bravais lattices (with one lattice site per unit cell) such a loop appears only above a critical interaction strength, which can be large. For all realistic situations, the loop is also small and hence difficult to detect. This limits the proposed experimental detection of the loops to only indirect signals such as the nonlinear Landau-Zener effect [19,23,24].

Similar looped band structures also appear for BEC on a double-well optical lattice [22,25]. Unlike the conventional looped structure described above, however, we find that a significantly large loop is induced for any interaction strength, and a large energy separation from the excited band is possible by suitably tuning the lattice depth and the lattice staggering. With the recent experimental realization of double-well optical lattices [5,26,27] and the concomitant theoretical investigations of the many-body phenomena in them [28–35], it is now an appropriate moment to consider the possibility of detecting the looped band on a double-well lattice.

Previously, the interaction-induced loop structure in a double-well optical lattice was considered theoretically for

some specific cases. In Ref. [22], a one-dimensional (1D) Kronig-Penney potential was used to demonstrate period doubling in a double-well lattice in one dimension. The special form of the potential allowed analytic solutions to be obtained. A tight-binding model of a one-dimensional double-well system was analyzed in Ref. [25]. Reference [36] found an analytical solution at the band edge for a specific interaction energy by employing the Thomas-Fermi approximation. However, the computation of the Bogoliubov spectrum, and hence the stability, around the states of a two-dimensional (2D) loop structure is lacking in the literature.

In this work, we compute the interacting Bloch solutions of the Gross-Pitaevskii equation for two-dimensional double-well lattices using realistic lattice potentials. This allows us to elucidate the behavior of the loop structure at the band edge as a function of the lattice potential. Essential to the experimental realization of the loop states is their stability. By analyzing the behavior of the collective modes about the mean-field solutions, we find that a range of states in the excited band are dynamically stable, which are in experimentally accessible parameter regimes.

The paper is organized as follows. In Sec. II, we set up the problem and indicate the specific lattice used in our analysis. We then describe the method of obtaining nonlinear Bloch solutions to the mean-field equations of motion, and present the loop band structure in Sec. III. In Sec. IV, we compute the collective excitations about the nonlinear Bloch solutions. These are used to establish the energetic and dynamical stability of the system prepared in these states. In Sec. V, we present a tight-binding model that captures some, but not all, of the salient features of the more accurate continuum results. We conclude in Sec. VI.

**II. THE DOUBLE-WELL OPTICAL LATTICE**

In a recent experiment [26], a two-dimensional double-well lattice was realized by superimposing standing waves in the  $x$  and  $y$  directions. To ensure phase stability, a single light source was used and the lattice is formed in a folded-retroreflected geometry. We consider a lattice potential that is realizable with

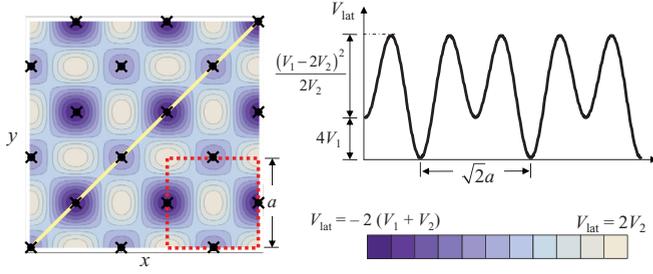


FIG. 1. (Color online) (Left) The double-well-lattice potential used in this work. The unit cell (dotted red square) and lattice constant  $a$  are shown. Each black cross corresponds to a site of a bosonic annihilation operator in Eq. (8). The minima are colored deep-blue (gray), in accordance with the scale in the lower-right. (Upper-right) A slice of the lattice potential along the diagonal line in the left panel.

this geometry, given by

$$V_{\text{lat}}(x, y) = V_1[\cos(2k_L x) - \cos(2k_L y)] + 2V_2 \cos(2k_L x) \cos(2k_L y), \quad (1)$$

where  $k_L = \pi/a$  and  $a = \lambda/\sqrt{2}$  is the lattice constant (shown in Fig. 1). By adjusting the path-length differences of the lattice beams, a more general lattice can be generated. We further restrict ourselves to the case where  $2V_2 > V_1 > 0$ , which gives double-well lattices with degenerate maxima and staggered local minima (see Fig. 1).

With this lattice potential, the full Hamiltonian of the system is given by

$$\mathcal{H} = \int d^3\mathbf{r} \left\{ \hat{\psi}^\dagger(\mathbf{r}) \left[ \frac{-\hbar^2}{2m} \nabla^2 + V_{\text{lat}}(\mathbf{r}) \right] \hat{\psi}(\mathbf{r}) + \frac{g}{2} \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}(\mathbf{r}) \hat{\psi}(\mathbf{r}) \right\}, \quad (2)$$

where  $g = \frac{4\pi\hbar^2 a_s}{m}$ ,  $\hat{\psi}(\mathbf{r})$  describes the destruction of a boson at position  $\mathbf{r}$ ,  $m$  is the mass of the constituent bosons, and  $a_s > 0$  is the  $s$ -wave scattering length.

For the mass and scattering length, we use parameters for  $^{87}\text{Rb}$ . We consider spatially averaged densities  $\bar{\rho}$  below  $1 \times 10^{14} \text{ cm}^{-3}$ , since for larger densities three-body losses become important. In the following analysis we restrict our attention to the case where  $V_1$  and  $V_2$  are  $< 10E_R$ , and set the recoil energy to be  $E_R = \frac{\hbar^2 k_L^2}{2m} = h \times 1.75 \text{ kHz}$ , given by the experimental parameters. For such parameters the tight-binding approximation is not necessarily valid. For this range of  $V_1$  and  $V_2$ , the ground state is in the superfluid phase, well away from the Mott insulating transition.

### III. MEAN-FIELD ANALYSIS OF THE INTERACTING BAND STRUCTURE

In this section we describe the numerical method used to obtain periodic mean-field stationary states of Eq. (2). These solutions are shown to exhibit extra “looped” states which are then further analyzed. We concentrate on the semiclassical regime of  $\mathcal{H}$  and approximate  $\hat{\psi}$  with  $\psi \equiv \langle \hat{\psi} \rangle$ . Thus, we seek solutions of the Gross-Pitaevskii equation (GPE)

$$\mu\psi(\mathbf{r}) = \frac{-\hbar^2}{2m} \nabla^2 \psi(\mathbf{r}) + V_{\text{lat}}(\mathbf{r})\psi(\mathbf{r}) + g|\psi(\mathbf{r})|^2\psi(\mathbf{r}). \quad (3)$$

Here we consider only a 2D system. Qualitatively similar structures should be expected in other dimensions, but we shall focus on 2D for experimental relevance. Among the solutions of this nonlinear differential equation, we are interested in the solutions of the Bloch form:

$$\psi_{n\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} u_{n\mathbf{k}}(\mathbf{r}), \quad (4)$$

where  $n$  is the band index,  $\mathbf{k}$  is the crystal momentum, and  $u_{n\mathbf{k}}(\mathbf{r})$  has the periodicity of the underlying lattice. The corresponding mean-field energy per unit cell is then

$$E_{n\mathbf{k}} = x \int_{\text{cell}} d\mathbf{r} \left( -\frac{\hbar^2}{2m} \psi_{n\mathbf{k}}^* \nabla^2 \psi_{n\mathbf{k}} + V_{\text{lat}}(\mathbf{r}) |\psi_{n\mathbf{k}}|^2 + \frac{g}{2} |\psi_{n\mathbf{k}}|^4 \right). \quad (5)$$

Throughout the paper, we choose the zero of energy such that the ground-state energy is zero.

We numerically compute the nonlinear Bloch band by expanding  $u_{n\mathbf{k}}(\mathbf{x})$  as  $u_{n\mathbf{k}}(\mathbf{x}) = \sum_{\mathbf{K}} c_{n\mathbf{K}} e^{i\mathbf{K}\cdot\mathbf{r}}$  where  $\mathbf{K}$  are reciprocal lattice vectors and the summation includes a sufficient number of harmonics to ensure accuracy. This is then substituted to Eq. (3) and a set of coupled equations is obtained by equating coefficients of equal harmonics. Together with the normalization condition,  $\{c_{n\mathbf{K}}\}$  and  $\mu$  are then solved for numerically. We start with an initial solution  $\{c_{n\mathbf{K}}\}$  at  $\mathbf{k} = \mathbf{0}$ , found with imaginary-time propagation. Then  $\mathbf{k}$  is changed stepwise and  $\{c_{n\mathbf{K}}\}$  is computed through numerical root finding at each step. The nonlinear band structures for several sets of parameters are shown in Fig. 2.

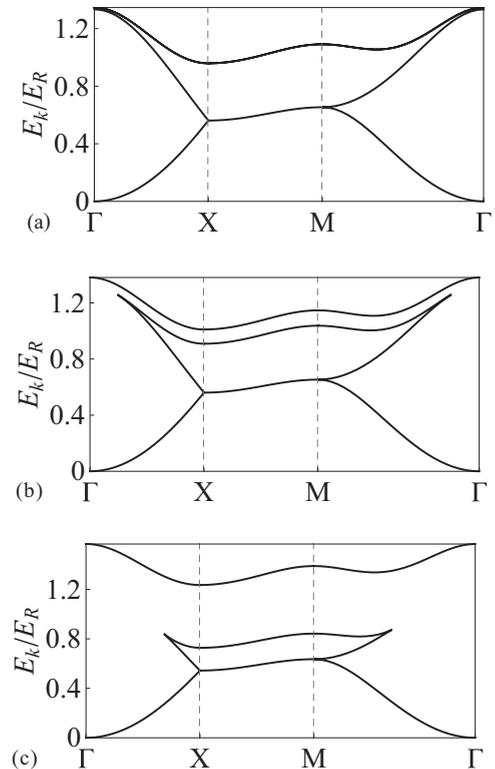


FIG. 2. The lowest two bands computed with  $g\bar{\rho} = 0.4E_R$  and  $V_2 = 4.8E_R$ , while  $V_1$  are (a) 0 (i.e., no staggering), (b)  $0.04E_R$ , and (c)  $0.2E_R$ . The labeling of the crystal momenta  $\mathbf{k}$  follows the convention where  $\Gamma = (0,0)$ ,  $X = (\pi/a, 0)$ , and  $M = (\pi/a, \pi/a)$ .

The most prominent feature is the emergence of a looped band structure when a lattice staggering  $V_1 \neq 0$  is introduced. Similar phenomena were also discovered in interacting BECs on regular 1D [19–21,37,38] and 2D [39,40] lattices. However, a substantial looped band on a regular (unstaggered) lattice requires the interaction energy to be much larger than the lattice depth, which is experimentally a stringent condition. In contrast, a substantial looped band on a staggered lattice only requires the interaction energy to be greater than the staggering, which is achievable as a staggering of  $<1\%$  can be realized.

For a qualitative understanding of the emergence of the looped band on a double-well lattice, we consider the band structures for different staggering in Fig. 2. First consider the case of  $V_1 = 0$  [Fig. 2(a)], in which case our unit cell is twice the lattice's natural unit cell. It is known that an extra solution exists at the band edge [22] and a staggering splits the upper and lower bands and hence a loop is induced [Fig. 2(b)]. Further increasing the staggering enlarges the energy gap between the excited band and the loop [Fig. 2(c)]. The importance of using a double-well lattice is apparent in Fig. 2(c), where we see a substantial loop well separated from the excited band.

Note that sharp edges are formed in the lowest band, which can lead to interesting nonlinear Landau-Zener effects. This was proposed to detect the loop band structure experimentally in a 1D system [19,23,24]. In our current system, we expect a similar effect to appear as one traverses the band edge from the  $\Gamma$  point to the  $X$  point.

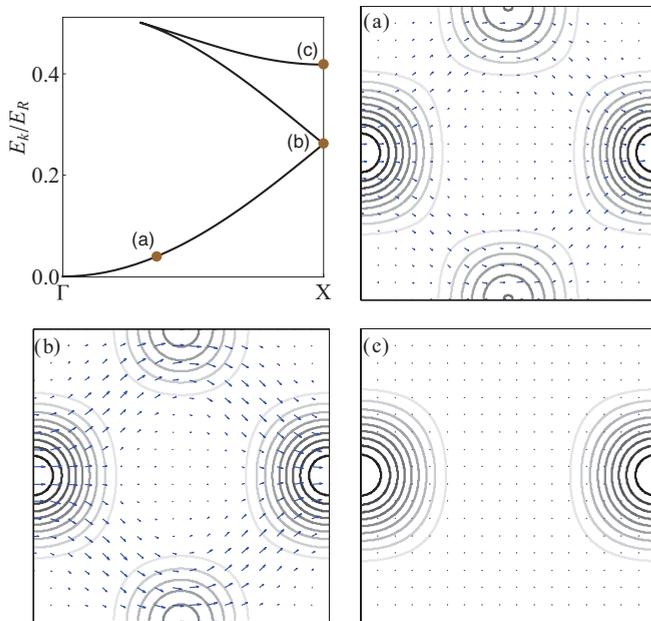


FIG. 3. (Color online) The wave function and current flow in a unit cell (shown in Fig. 1) for three eigenstates where (a)  $\mathbf{k}a = (0.18\pi, 0)$  and [(b), (c)]  $\mathbf{k}a = (\pi, 0)$ . The corresponding points on the energy band are shown in the upper-left panel. [The other degenerate solution at point (b) of the band is given by the horizontal reflection of figure (b)]. The other panels show the contours of  $|\psi(\mathbf{x})|$  and the field of  $\mathbf{j}$ . The parameters are  $g\bar{\rho} = 0.4E_R$ ,  $V_1 = 0.4E_R$ , and  $V_2 = 8E_R$ .

The superfluid current density is obtained from the Bloch solution  $\psi_{n\mathbf{k}}(\mathbf{x})$  as

$$\begin{aligned} \mathbf{j}_{n\mathbf{k}} &= \frac{\hbar}{m} \text{Im}(\psi_{n\mathbf{k}}^* \nabla \psi_{n\mathbf{k}}) \\ &= \frac{\hbar}{m} \sum_{\mathbf{K}\mathbf{K}'} (\mathbf{K} + \mathbf{k}) c_{n\mathbf{K}}^* c_{n\mathbf{K}} \cos(\mathbf{K}' \cdot \mathbf{r} - \mathbf{K} \cdot \mathbf{r}). \end{aligned} \quad (6)$$

In Fig. 3 we plot the wave function and current density of several indicated states. A currentless state is found at the band edge of the interaction-induced state [Fig. 3(c)]. For a noninteracting system, it is well known that the cell-averaged current satisfies  $\bar{\mathbf{j}}_{n\mathbf{k}} = \frac{1}{\hbar} \nabla_{\mathbf{k}} E_{n\mathbf{k}}$ . This relation, in fact, can also be shown to hold for the nonlinear system in Eq. (3). Therefore currentless solutions can only appear at the  $\Gamma$  point or the (c) point in Fig. 3, where the energy band attains its local extrema. The state at (c), however, has identically zero current everywhere instead of just an average zero current. This is because the period doubled state can be taken to be real everywhere, and hence currentless by virtue of Eq. (6). It is easy to see that a real solution is possible only at the  $\Gamma$ ,  $X$ , or  $M$  points of the Brillouin zone. Because  $\psi(\mathbf{r}) = \sum_{\mathbf{K}} c_{\mathbf{K}} e^{i(\mathbf{K}+\mathbf{k})\cdot\mathbf{r}}$ , the reality of  $\psi$  requires  $2\mathbf{k}$  be equal to a reciprocal lattice vector and that  $c_{\mathbf{K}} = c_{-\mathbf{K}-2\mathbf{k}}$ . This is satisfied by the states of the loop at the  $X$  and  $M$  points.

#### IV. STABILITY

A crucial factor determining the realizability of the states on the loop is their stability. In general, there are two qualitatively different types of instabilities that could potentially occur for interacting BEC: energetic instability and dynamical instability. Energetic instability occurs if the system is not at a local minimum of the mean-field energy. This, however, is often unimportant in experiments since the time scales for energy dissipation are long. In contrast, when the system has collective fluctuations with complex frequencies, small perturbations will grow exponentially fast: a dynamical instability. This type of instability does not require energy dissipation, and it will cause rapid depletion and fragmentation of the condensate [41,42]. Thus realizing a dynamically unstable state is difficult if the instability time scale is much shorter than the experimental time scale.

To analyze the stability of states [19], it is therefore necessary to consider the fluctuation modes of the metastable excited states (every point on the nonlinear Bloch band). We follow the standard procedure for computing the Bogoliubov spectrum. That is, we expand the Hamiltonian to quadratic order in the field:  $\hat{\psi} \rightarrow \psi_{n\mathbf{k}} + e^{i\mathbf{k}\cdot\mathbf{r}} \hat{\phi}(\mathbf{x})$  where  $\psi_{n\mathbf{k}}$  is the stationary nonlinear Bloch solution. Hence the term linear in  $\hat{\phi}$  vanishes and the term of second order in  $\hat{\phi}$  is

$$\begin{aligned} \delta^2 \mathcal{H} &= \sum_{\mathbf{K}\mathbf{q}} \left[ \frac{(\mathbf{k} + \mathbf{K} + \mathbf{q})^2}{2m} \hat{\phi}_{\mathbf{q}+\mathbf{K}}^\dagger \hat{\phi}_{\mathbf{q}+\mathbf{K}} \right. \\ &\quad + V_{\mathbf{K}-\mathbf{K}'} \hat{\phi}_{\mathbf{q}+\mathbf{K}}^\dagger \hat{\phi}_{\mathbf{q}+\mathbf{K}'} + 2g\rho_{\mathbf{K}-\mathbf{K}'} \hat{\phi}_{\mathbf{q}+\mathbf{K}}^\dagger \hat{\phi}_{\mathbf{q}+\mathbf{K}'} \\ &\quad \left. + g(\tilde{\rho}_{\mathbf{K}-\mathbf{K}'}^* \hat{\phi}_{\mathbf{q}+\mathbf{K}} \hat{\phi}_{-\mathbf{q}-\mathbf{K}'}^\dagger + \tilde{\rho}_{\mathbf{K}-\mathbf{K}'} \hat{\phi}_{\mathbf{q}+\mathbf{K}}^\dagger \hat{\phi}_{-\mathbf{q}-\mathbf{K}'}^\dagger) \right], \end{aligned} \quad (7)$$

where  $\hat{\phi}_{\mathbf{q}}$  is the Fourier transform of  $\hat{\phi}(\mathbf{x})$ .  $\rho = |\psi_{n\mathbf{k}}|^2$  is an effective potential created by the BEC, and  $\tilde{\rho} = \psi_{n\mathbf{k}}^2$ . The

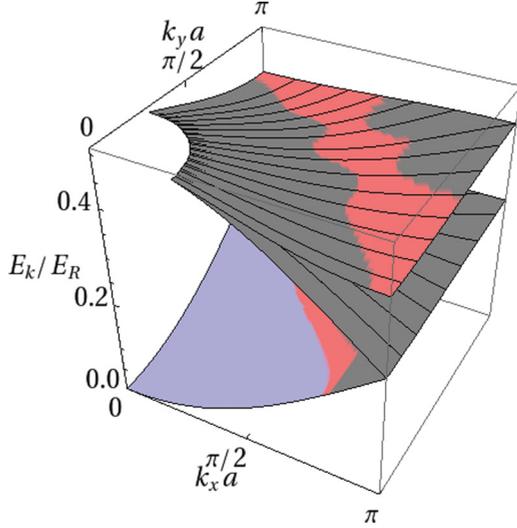


FIG. 4. (Color online) Nonlinear Bloch bands with the same parameters as Fig. 3, in the first quadrant of the Brillouin zone. States in the blue region are stable, while states in gray regions are unstable, both dynamically and energetically. Red regions are energetically unstable but dynamically stable. The excited band is separated from the ground band by  $\sim 1E_R$  and is not shown here.

Bogoliubov spectrum is then numerically found by canonical transformation of Eq. (7). For each crystal momentum  $\mathbf{k}$ , we compute the spectrum  $\omega_{\mathbf{q}}$ . The presence of any complex  $\omega_{\mathbf{q}}$  implies both dynamical and energetic instabilities, while negative  $\omega_{\mathbf{q}}$  indicates an energetic instability. The stabilities of the Bloch states are shown in Fig. 4. We find the top of the loop has a region of dynamically stable states, which trace out a roughly circular path in the Brillouin zone.

The stability phase diagram of the state at the tail at  $\mathbf{k}\mathbf{a} = (\pi, 0)$  as a function of  $V_1$  and  $V_2$  is shown in Fig. 5. It is divided into three regions: (1) when the lattice staggering is

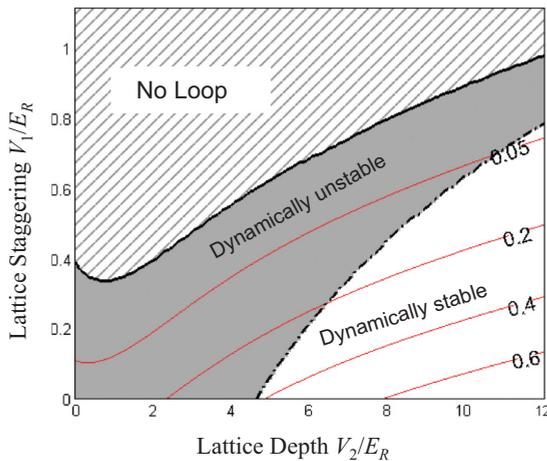


FIG. 5. (Color online) Stability of the eigenstate at  $\mathbf{k}\mathbf{a} = (\pi, 0)$  on the loop, as a function of  $V_1$  (the staggering) and  $V_2$  (the lattice depth) in Eq. (1), with  $g\bar{\rho} = 0.4E_R$  (corresponding to a density  $\bar{\rho} = 9 \times 10^{13} \text{ cm}^{-3}$ ). The hashed region has no loop. The shaded region is dynamically unstable and the white region is energetically unstable but dynamically stable. Contours show the loop size [i.e., vertical distance between (b) and (c) in Fig. 3] in units of  $E_R$ .

sufficiently large, the loop is totally suppressed; (2) as the staggering becomes smaller, a loop is formed but with all states on it dynamically unstable; (3) further reducing staggering enlarges the loop and a band of stable states is formed on it, of which Fig. 4 is an example.

## V. TIGHT-BINDING MODEL

In this section, we use a tight-binding model to understand some of our previous results, in the limit of large lattice potentials. The tight-binding Hamiltonian we consider is

$$\begin{aligned} \mathcal{H}_{\text{TB}} = & -t \sum_{\langle \mathbf{r}\mathbf{r}' \rangle} (\hat{b}_{\mathbf{r}}^\dagger \hat{b}_{\mathbf{r}'} + \text{H.c.}) + \Delta \sum_{\mathbf{r}} e^{i\mathbf{Q}\cdot\mathbf{r}} \hat{b}_{\mathbf{r}}^\dagger \hat{b}_{\mathbf{r}} \\ & + \frac{U}{2} \sum_{\mathbf{r}} \hat{b}_{\mathbf{r}}^\dagger \hat{b}_{\mathbf{r}}^\dagger \hat{b}_{\mathbf{r}} \hat{b}_{\mathbf{r}}, \end{aligned} \quad (8)$$

where  $\hat{b}_{\mathbf{r}}$  annihilates a boson at position  $\mathbf{r}$  on a square lattice with unit lattice constant,  $\sum_{\langle \mathbf{r}\mathbf{r}' \rangle}$  indicates summation over nearest neighbors, and  $\mathbf{Q} = (\pi, \pi)$ . The hopping amplitude is given by  $t$ ,  $\Delta > 0$  is the on-site energy staggering between sites, while  $U$  denotes the on-site interaction energy between bosons. This model describes Eq. (2) in the limit of a strong lattice potential, where we associate a bosonic annihilation operator to each local minimum of the lattice (see Fig. 1). Note that a term of staggered hopping is unnecessary because the lattice has fourfold rotational symmetry and all nearest-neighbor links are equivalent.

In the superfluid regime, the system is described by a mean-field equation  $\mu b_{\mathbf{r}} = -t \sum_{\delta} b_{\mathbf{r}+\delta} + \Delta e^{i\mathbf{Q}\cdot\mathbf{r}} b_{\mathbf{r}} + U|b_{\mathbf{r}}|^2 b_{\mathbf{r}}$ , where  $b_{\mathbf{r}} = \langle \hat{b}_{\mathbf{r}} \rangle$  and  $\delta$  denote the positions of the nearest neighbors. This is solved by

$$b_{\mathbf{r}} = \sqrt{\rho} \left( \cos \frac{\alpha_{\mathbf{k}}}{2} + e^{i\mathbf{Q}\cdot\mathbf{r}} \sin \frac{\alpha_{\mathbf{k}}}{2} \right) e^{i\mathbf{k}\cdot\mathbf{r}}, \quad (9)$$

where  $\alpha_{\mathbf{k}}$  satisfies

$$\begin{aligned} 2t(\cos k_x + \cos k_y) \sin \alpha_{\mathbf{k}} + \Delta \cos \alpha_{\mathbf{k}} \\ + U\rho \sin \alpha_{\mathbf{k}} \cos \alpha_{\mathbf{k}} = 0. \end{aligned} \quad (10)$$

This yields the nonlinear Bloch band  $E_{\mathbf{k}}/\rho = \Delta \sin \alpha_{\mathbf{k}} - 2t(\cos k_x + \cos k_y) \cos \alpha_{\mathbf{k}} - U\rho(\frac{1}{2} \cos^2 \alpha_{\mathbf{k}} - 1)$ .

In vanishing interaction ( $U = 0$ ), this tight-binding model generates two bands. When  $U$  is raised above a critical threshold, however, four solutions appear in some regions of  $\mathbf{k}$  near the band edge. These are the extra states of the loop. Since Eq. (10) has four solutions if  $(U\rho)^{2/3} > \Delta^{2/3} + [2t(\cos k_x + \cos k_y)]^{2/3}$ , the condition to have a loop without it filling up the entire Brillouin zone (hence forming a separate band) is therefore  $\Delta < U\rho < [\Delta^{2/3} + (4t)^{2/3}]^{3/2}$ . Further, by demanding all Bogoliubov modes to be real, we find that the condition of having the state at  $\mathbf{k} = (\pi, 0)$  on the loop dynamically stable is  $t < \frac{(U\rho - \Delta)^{3/2}}{8\sqrt{U\rho + \Delta}}$ . Since in our lattice [Eq. (1)]  $V_1$  controls the amount of staggering and  $V_2$  controls lattice depth, the phase diagram in the continuum (Fig. 5) is in qualitative agreement with the tight-binding model. The wave function at the band edge ( $\cos k_x + \cos k_y = 0$ ) can be analytically solved. When  $U\rho > \Delta$ , the state on the loop has  $\alpha = -\frac{\pi}{2}$ . Thus the state at the tail is  $b_{\mathbf{r}} = \sqrt{2\rho}$  if

$e^{i\mathbf{Q}\cdot\mathbf{r}} = -1$  and zero otherwise, i.e., has all particles on the lower wells. This too agrees with the continuum calculations in Fig. 3.

This loop structure could also be understood from the period-doubled solution [22]. It is known that this tight-binding model without staggering ( $\Delta = 0$ ) admits period- $p$  solutions, where  $p$  is any positive integer. In particular, a period-doubled solution  $\frac{E_k}{\rho} = \frac{4t^2(\cos k_x + \cos k_y)^2}{2U\rho} + U\rho$  always exists near the band edge [21]. If we introduce small staggering  $\Delta$ , the extra band splits in a manner that generates a looped band structure (Fig. 2). As the staggering gets larger, the splitting between the two bands also increases but simultaneously suppresses the loop size. As splitting becomes large,  $\Delta > U\rho$ , the whole loop structure is destroyed.

The adequacy of tight-binding models in describing our loop structure could be compared with the situations in purely interaction-induced loop structure [20,40]. In those systems, a tight-binding model can never produce the loop structure in continuum regardless of the lattice depth, and this was attributed to an inappropriate choice of Wannier functions [40]. In our system, although a loop structure can be captured with the tight-binding model, some qualitative features of the continuum calculations are missing in the tight-binding model. For instance, the tight-binding model predicts that a dynamically stable region on the loop, if present, must include the band edge. This is not consistent with our continuum calculations in Sec. III, as shown in Fig. 4.

Although the tight-binding model is simple and gives a physical picture, the continuum calculations are more relevant from an experimental viewpoint. This is because the experimentally tunable parameters are  $V_1$ ,  $V_2$ , and  $\bar{\rho}$ , and it is difficult to compute from these the suitable tight-binding parameters  $t$ ,  $\Delta$ , and  $U$  of Eq. (8) as shown in [43]. In contrast, the results we obtained for continuum Hamiltonian Eq. (2) can be directly compared with experimental results. There are also

experimentally relevant regimes considered above, where a single-orbital tight-binding approximation is not correct.

## VI. CONCLUSIONS

In this work, we have numerically computed the nonlinear Bloch band structure for an interacting BEC on a 2D double-well optical lattice. We also computed the Bogoliubov modes of all the states, and thereby mapped out the stability phase diagram as a function of lattice depth and staggering for experimentally realistic parameters. A tight-binding model was also considered and it is found to reproduce some qualitative features of the system.

We find that the interaction energy required to create a looped band is smaller on a double-well lattice, compared with a Bravais lattice. Further, we find a stable state on the loop can be realized within an experimental accessible parameter range. This raises the possibility of directly exciting a BEC onto the loop with Raman excitation and/or dynamic manipulation of the lattice structure [5,26]. Time-of-flight spectroscopy of the momentum distribution could be used to experimentally confirm the unique loop structure.

In future work, a more careful treatment of the important possibility of Mott correlations of the states on the loop will be interesting to study. When the system is in the tight-binding regime, the Gutzwiller method (which is more general than the treatment provided in Sec. V) will be suitable for this purpose. The effects of the nonlinear Bloch states on the dynamics of BECs in double-well lattices will also be of interest.

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