\( \mathbb{Z}_2 \) topological insulator of ultra cold atoms in bichromatic optical lattices

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We investigate the effect of a strong bichromatic deformation to the \( \mathbb{Z}_2 \) topological insulator in ultracold atomic system proposed by B. Béri and N. R. Cooper, Phys. Rev. Lett. 107, 145301 (2011). Large insulating gap of this system allows for examination of strong perturbations. We conclude that the \( \mathbb{Z}_2 \) topological character of the system is robust against a large global perturbation which breaks the inversion symmetry but preserves the time-reversal symmetry.

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I. INTRODUCTION

Topological insulators are bulk insulators that have metallic states at their boundaries\[1, 2\]. Robustness of these states against disorder and perturbations makes them promising for applications such as spintronics\[3\] and topological quantum computation \[4\]. Topological invariants of the bulk material are essential for the robust boundary modes. This urged consideration of topological insulators on different lattice geometries\[3, 4\]. Testing these systems against strong disorder and perturbations is challenging both experimentally and theoretically. Detailed numerical investigations reveal that topological protection is safe only for surface disorder smaller than the bulk band gap\[10\].

Two and three dimensional topological insulators with band gaps in the order of the recoil energy have recently been proposed in ultracold atomic gases\[11\]. This large gap systems are described in the nearly free electron limit, which is a different perspective to examine topological insulators compared to earlier studies\[12, 14\]. The proposal utilizes interactions which preserves time reversal symmetry (TRS), analogous to synthesized spin-orbit coupling\[12\], so that the insulators are classified by the so called \( \mathbb{Z}_2 \) topological invariant\[6\].

Our aim in this Brief Report is to examine robustness of two dimensional \( \mathbb{Z}_2 \) topological insulators\[11\] against large global perturbations that breaks inversion symmetry but preserves TRS. Motivated by their recent use in quantum simulations of relativistic field theories\[15, 16\] and disorder induced localization\[17–19\], we specifically consider here bichromatic optical lattice perturbations. Similar studies of \( \mathbb{Z}_2 \) topological insulators in bichromatic potentials, but for a one-dimensional optical lattice in tight-binding limit, reveals that topological properties of the system can be probed by density measurements\[20, 21\].

This report is organized as follows. In Sec. II we briefly review the proposal of \( \mathbb{Z}_2 \) topological insulator in ultracold atomic gases\[11\], and introduce the bichromatic deformation of the lattice potential terms. In Sec. III we describe the method of calculation of the \( \mathbb{Z}_2 \) invariant in the case of absence of inversion symmetry\[22, 23\] and present the corresponding results. We conclude in Sec. IV.

II. MODEL SYSTEM

The Hamiltonian of an atom with \( N \) internal states with position \( \mathbf{r} \) and momentum \( \mathbf{p} \) can be written as,

\[
H = \frac{\mathbf{p}^2}{2 m} + \hat{V}(\mathbf{r}),
\]

here \( \hat{V}(\mathbf{r}) \) is a position dependent potential which is a \( N \times N \) matrix acting on the internal states of the atom. A \( \mathbb{Z}_2 \) topological insulator is invariant under the action of time-reversal operator \( \Theta = i \sigma_y \hat{K} \), where \( \sigma_{x,y,z} \) are Pauli matrices acting on electronic spin and \( \hat{K} \) is complex conjugation operator. This requires \( N \) to be even. The smallest potential matrix has \( N = 4 \) and can be written as,

\[
\hat{V}(\mathbf{r}) = \begin{pmatrix}
(A + B) \mathbb{I}_2 & C \mathbb{I}_2 - i \sigma \cdot \mathbf{D}
\end{pmatrix},
\]

where \( A, B \) and \( C \) are real numbers, \( \mathbf{D} \) is a 3-vector with real components and \( \mathbb{I}_2 \) is 2 \( \times \) 2 identity matrix. This Hamiltonian can be realized using an atom with four internal states as proposed by \[11\]. Ytterbium\[17\]Yb, which has nuclear spin \( I = 2 \), is a good candidate for this purpose. It has a 2–fold degenerate ground state \( (1S_0 = g) \) and a long-lived 2–fold degenerate excited state \( (3P_0 = e) \); furthermore there exists a state dependent scalar potential for a specific wavelength \( \lambda_{\text{magic}} \), in which the potential changes sign and becomes \( \pm V_{\text{am}}(\mathbf{r}) \) for the ground and excited states.

All the \( e - g \) transitions, shown in Fig. 13 have the same frequency \( \omega_0 = (E_e - E_g)/\hbar \). We take the electric field of the lasers interacting with the atom to be \( \mathbf{E} = e e^{-i \omega t} + e^* e^{i \omega t} \). The potential in the rotating wave approximation then can be expressed as\[26\],

\[
\hat{V} = \begin{pmatrix}
\frac{h}{2} \Delta + V_{\text{am}} & i \sigma. e_d
\end{pmatrix},
\]
where $\Delta = \omega - \omega_0$ and $d_r$ is the reduced dipole moment of the atom [27].

For the two-dimensional triangular lattice, following forms are assumed for the elements of the potential matrix,

$$d_r \epsilon = [V\delta, V \cos( r \cdot k_1), V \cos( r \cdot k_2)],$$

with $k_1 = k(1,0,0)$ and $k_2 = k(\cos(\theta), \sin(\theta), 0)$. Since $\omega \approx \omega_0$, we have $k \approx 2\pi/\lambda_0$ with $\lambda_0 = 578$ nm the wavelength of the $e-g$ transition. The spatial dependence of $V_{am}$ is set by a standing wave at the antimagic wavelength $\lambda_{am}$ which creates a state-dependent potential with $|k_1 + k_2| = 4\pi/\lambda_{am}$ that leads to $\theta = 2 \arccos(2\pi/3)$. For simplicity, in all the following discussions we fix $\theta = 2\pi/3$ and define $a \equiv 4\pi/\sqrt{3k}$. Therefore the optical potential has the symmetry of a triangular lattice with lattice vectors $a_1 = (\sqrt{3}/2, -1/2)a$ and $a_2 = (0, 1)a$.

In order to examine the robustness of the $Z_2$ topological insulator to strong perturbations that breaks the inversion symmetry in the lattice, we introduce bichromatic deformations. For simplicity, we do not change the angular orientation of the lattice so that the angular variable $\theta$ is not affected by the deformation. This can be accomplished by not deforming the element introduced in Eq. 4. In addition, we do not deform the first component in the element Eq. 4. The $\delta$ dependent component plays the role of the spin orbit coupling to hybridize the lower bands of the two optical flux lattices. We choose not to perturb this essential process that mixes these bands with the non-trivial Chern numbers.

The bichromatic deformation is introduced in the remaining two terms such that

$$d_r \epsilon = [V\delta, V \cos( r \cdot k_1) + V' \cos(2r \cdot k_1 + \phi),$$

Here we examine the simple case where $V' = V''$ and $\phi = \phi' = 0$. This model is unitarily equivalent to the superposition of two bichromatic optical flux lattices that is coupled with a spin-orbit type interaction [11]. Such a configuration is illustrated in the Fig. 1(b) which is the cross section view of the potential along the $k_1$ direction. The small bumps at the potential minima is a global perturbation which is as strong as the insulating gap (see Fig. 3). We explore its effect on the topological character of the insulator in the next section.

### III. RESULTS

We determine the topological character of the insulator directly using the band structure to calculate the $Z_2$ invariant. The Hamiltonian in Eq. 1 can be numerically diagonalized using plane-wave method. In Fig. 2 the band structure is shown. In the case of inversion symmetric materials, finding the $Z_2$ can be done using the Fu and Kane method [22]. Since the parity and time-reversal operators commute, we only need to check the parity eigenvalues in four time-reversal points in $k$-space for all bands under the gap. The result for the system, without bichromatic deformation, turns out to be non-trivial so that it is either a $Z_2$ insulator or a quantum spin Hall insulator, depending on the presence or absence of $\delta$ coupling, respectively [11].

We can not use here the parity based calculation of $Z_2$ invariant given in Ref. [11] due to lack of inversion symmetry in our case of bichromatic optical lattice. A general set of expressions of the $Z_2$ invariants are developed in Ref. [22]. Equivalent expression based upon the Berry phase and the Berry curvature is constructed in Ref. [23]. This allows for a calculus recipe to determine the $Z_2$ invariant for a two-dimensional noncentrosymmetric material using the bulk band structure. We closely follow the notation and description given in Ref. [24] to apply the method of Ref. [23] to our case.

Time reversal constraint on the Bloch functions, associated with the Kramer’s degeneracy, allows for their determination using only the half of the Brillouin zone; as the other half is fixed by the constraint. In addition the constraint leads to a nonzero $Z_2$ invariant as an obstruction to smoothly defining the Bloch functions over the half Brillouin zone. Ref. [22] introduced the integral
form of the $Z_2$ invariant as,

$$D = \frac{1}{2\pi} \int_{\partial \mathcal{B}^+} d\mathbf{k} \cdot \mathbf{A} - \int_{\mathcal{B}^+} d^2k F(\mathbf{k}) \mod 2,$$

where $\mathcal{B}^+$ is half of the Brillouin zone, and $A(\mathbf{k}) = i \sum_n \langle u_n(\mathbf{k}) | \nabla_{\mathbf{k}} u_n(\mathbf{k}) \rangle$ is the Berry connection and $F = \nabla_{\mathbf{k}} \times \mathbf{A}$ is the Berry curvature. The sum is over the occupied bands which is $n = 1, 2, 4$ for our case, where the lowest two bands are two-fold degenerate. The obstruction of the Bloch wave function over the Brillouin zone gives the $Z_2 = 1$ for topological insulator, and $Z_2 = 0$ normal insulator.

In order to implement this formula numerically, a link variable $U_n(\mathbf{k}_j) = \det \langle u_n(\mathbf{k}_j) | u_m(\mathbf{k}_j + \mu) \rangle / \mathcal{N}(\mathbf{k}_j)$ is introduced [24], where $\mathcal{N}(\mathbf{k}_j) = |\det \langle u_n(\mathbf{k}_j) | u_n(\mathbf{k}_j + \mu) \rangle|$. Here $\mu$ is the unit vector on mesh. The discrete version of Berry connection and corresponding Berry curvature are given as $A = \text{Im} \ln U_n(\mathbf{k}_j)$ and $F = \text{Im} \ln U_n(\mathbf{k}_j) U_{\nu}(\mathbf{k}_j + \mu) U_n^{-1}(\mathbf{k}_j + \nu) U_{\nu}^{-1}(\mathbf{k}_j)$ respectively, where the complex logarithm is defined within its principal branch $(-\pi, \pi]$. Since we have time-reversal symmetry in our system, Kramer’s pair at time-reversal invariant points 0, $\mathbf{k}_1/2$, $\mathbf{k}_2/2$ and $(\mathbf{k}_1 + \mathbf{k}_2)/2$ for $\varepsilon_n = \varepsilon_{n-1}$ need to obey,

$$|u_n(\mathbf{k}_j)| = \Theta |u_{n-1}(\mathbf{k}_j)|.$$

After numerically evaluating the Bloch functions at each grid point on the Brillouin zone, we use this extra gauge condition for the time-reversal constraint to determine the Bloch functions at the critical points.

The discretized version of Eq. 6 can be written as the summation over the half Brillouin zone $D = \sum_{k_j} n(k_j)$ where the integer $n(k_j)$ field is defined for each plaquette of $\mathcal{B}^+$ by

$$n(k_j) = \frac{1}{2\pi}[ (\Delta_\mu A_\nu - \Delta_\nu A_\mu) - F(k_j) ].$$

Here, $\Delta_\mu$ represents the forward differing operation. To calculate the Bloch wave functions we need to diagonalize the Hamiltonian Eq. 11 with the potential elements of Eq. 6. The band structure is shown in Fig. 2. Four-fold degeneracy of the lowest band is removed by the $\delta$ dependent spin-orbit like interaction and reduced to two-fold degeneracy except at a few points. Upper panel shows the case when there is no bichromatic deformation. In this case there are three points, (1, 1), (0, 1) and (1, 0), which are four-fold degenerate. Under the bichromatic perturbation only the point (1, 1) can retain its four-fold degeneracy as shown in the lower panel. By changing the values of $V'$ from zero to values as large as the insulating gap, we see that in special points in $k$–space the degen-
eracy is lifted eventually. The gap becomes as large as $0.1E_R$ for $V \gtrsim 0.2E_R$ and remains preserved despite the strong perturbations $V'$ as large as the gap itself. The number of occupied bands that are relevant for the $\mathbb{Z}_2$ invariant calculation is still four when the bichromatic lattice is introduced.

The points $\Gamma_{mn}$ shown in the band diagram corresponds to the upper right quadrant of the Brillouin zone depicted in Fig. 3. We determine the Bloch functions for the lowest four bands at every mesh point in the shaded region, $\mathfrak{B}^+$, of the Brillouin zone. The Bloch functions for the critical points are updated according to the time-reversal gauge constraint in Eq. 8. This final set of Bloch functions are then used to determine the Berry curvature and the Berry connection to calculate the integer field for the each plaquette of $\mathfrak{B}^+$. The sum over the half Brillouin zone $\mathfrak{B}^+$ gives the $\mathbb{Z}_2$ invariant $D$. It can be checked in Fig. 3 that the sum over the entire zone gives the first Chern number which is zero. We repeat the calculation systematically for different strengths of the perturbation potential. The results are summarized in Table I.

Table I: The $D$ parameter for different values of strength of the bichromatic optical lattice’s depth relative to the primary lattice. The 0 and 1 values of the $D$ parameter show the triviality and non-triviality of the system respectively.

| $V_1/V$ | $D$ |
|--------|-----|
| 0      | 1   |
| 0.01   | 0   |
| 0.02   | 1   |
| 0.03   | 1   |
| 0.04   | 1   |
| 0.05   | 1   |
| 0.06   | 1   |
| 0.07   | 1   |
| 0.08   | 0   |
| 0.09   | 0   |
| 0.1    | 1   |
| 0.2    | 1   |
| 0.3    | 1   |

We consider the $\mathbb{Z}_2$ topological insulator of ultracold atomic system on a triangular optical lattice, introduced in Ref. [11], deformed globally by bichromatic potentials. We examine the effect of this deformation which can be as large as the insulating gap, on the topological character of the system. We find that the system retains its topological character robustly against this kind of perturbation. The large insulating gap of such topological bichromatic insulators with deep bichromatic deformation can be used for disorder and relativistic dynamics studies in the nearly free electron regime.

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