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

Ahad K. Ardabili, Tekin Dereli, and Ö E. Müstecaplıoğlu
Department of Physics, Koç University, Sarıyer, Istanbul, 34450, Turkey

We investigate the effect of a strong bichromatic deformation to the $\mathbb{Z}_2$ topological insulator in a fermionic 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 consider bichromatic perturbation along all axes on a triangular optical lattice. We find that $\mathbb{Z}_2$ topological character of the system is robust up to a certain depth of the deformation. The lowest band can become topologically trivial while the lowest two bands are always protected.

PACS numbers:

I. INTRODUCTION

Topological insulators are insulating in the bulk but have metallic states on 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 [5–9]. 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 fermionic 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, 13]. The proposal utilizes interactions which preserves time reversal symmetry (TRS), analogous to synthesized spin-orbit coupling [14], so that the insulators are classified by the so called $\mathbb{Z}_2$ topological invariant [9].

Our aim in this article 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 [22] 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,

$$H = \frac{\mathbf{p}^2}{2m} + \hat{V}(\mathbf{r}), \tag{1}$$

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,

$$\hat{V}(\mathbf{r}) = \begin{pmatrix} (A+B)\mathbb{1}_2 & C\mathbb{1}_2 - i\sigma\cdot\mathbf{D} \\ C\mathbb{1}_2 + i\sigma\cdot\mathbf{D} & (A-B)\mathbb{1}_2 \end{pmatrix}. \tag{2}$$

Here A,B and C are real numbers, $\mathbf{D}$ is a 3-vector with real components and $\mathbb{1}_2$ is 2×2 identity matrix.

This Hamiltonian can be realized using an atom with four internal states as proposed by [11]. Ytterbium ^{171}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 λ_{magic} [23] 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. 1(a), 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 $\mathbf{E} = \epsilon e^{-i\omega t} + \epsilon^* e^{i\omega t}$. The potential in the rotating wave approximation then can be expressed as [24],

$$\hat{V} = \begin{pmatrix} (\frac{\hbar}{2}\Delta + V_{\text{am}})\mathbb{1}_2 & -i\sigma.\epsilon d_r \\ i\sigma.\epsilon d_r & -(\frac{\hbar}{2}\Delta + V_{\text{am}})\mathbb{1}_2 \end{pmatrix}, \tag{3}$$

where $\Delta = \omega - \omega_0$ and d_r is the reduced dipole moment of the atom [25].

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

$$d_r\epsilon = [V\delta, V\cos(\mathbf{r}.\mathbf{k}_1), V\cos(\mathbf{r}.\mathbf{k}_2)], \quad (4)$$

$$\frac{\hbar}{2}\Delta + V_{\rm am}(\mathbf{r}) = V\cos(\mathbf{r}.(\mathbf{k}_1+\mathbf{k}_2)) \quad (5)$$

with $\mathbf{k}_1 = k(1,0,0)$ and $\mathbf{k}_2 = k(\cos(\theta), \sin(\theta), 0)$. Since $\omega \simeq \omega_0$, we have $k \simeq 2\pi/\lambda_0$ with $\lambda_0 = 578$ nm the wavelength of the $e-g$ transition. The spatial dependence of $V_{\rm am}$ is set by a standing wave at the antimagic wavelength $\lambda_{\rm am}$ which creates a state-dependent potential with $|\mathbf{k}_1+\mathbf{k}_2| = 4\pi/\lambda_{\rm am}$ that leads to $\theta = 2\arccos(2\pi/3)$. For simplicity, in all the following discussions we fix $\theta = 2\pi/3$ and define $a \equiv 4\pi/(\sqrt{3}k)$. Therefore the optical potential has the symmetry of a triangular lattice with lattice vectors $\mathbf{a}_1 = (\sqrt{3}/2, -1/2)a$ and $\mathbf{a}_2 = (0,1)a$. The Hamiltonian Eq. (1) is invariant under translation by the lattice vectors $\mathbf{a}_i$. Therefore using the associated reciprocal vectors we can define the Bloch Hamiltonian,

$$\hat{H}_{\mathbf{k}} = \frac{(\hat{p}+\hbar\mathbf{k})^2}{2m}\mathbb{1}_N + V'(\mathbf{r}), \quad (6)$$

here $\mathbf{k}$ is the conserved momentum. $V' = U^{-1}VU$ where $U = 2^{-1/2}(\mathbb{1}_4 - i\Sigma_3\sigma_2)$ is a unitary transformation. The potential V' takes the following form:

$$V' = c_1\Sigma_1 + c_2\Sigma_2\sigma_3 + c_{12}\Sigma_3 + \delta\Sigma_2\sigma_1. \quad (7)$$

In the absence of the bichromatic lattice the Hamiltonian in Eq. (6) is invariant under the half translational symmetries $T_1 = \Sigma_2 T_{\mathbf{a}_1/2}$ and $T_2 = \Sigma_1\sigma_3 T_{\mathbf{a}_2/2}$ where $T_{\mathbf{a}_i}$ is translation operator along the lattice vector $\mathbf{a}_i$.

In order to examine the robustness of the $\mathbb{Z}_2$ topological insulator to strong perturbations we introduce bichromatic deformations. For simplicity, we do not change the angular orientation of the lattice so that the angular variable θ is not affected by the deformation. This can be accomplished by not deforming the element introduced in Eq. (5). In addition, we do not deform the first component in the element Eq. (4). The δ 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

$$\begin{aligned} d_r\epsilon &= [V\delta, V\cos(\mathbf{r}.\mathbf{k}_1) + V'\cos(2\mathbf{r}.\mathbf{k}_1+\phi), \\ &\quad V\cos(\mathbf{r}.\mathbf{k}_2) + V'\cos(2\mathbf{r}.\mathbf{k}_2+\phi)], \\ \frac{\hbar}{2}\Delta + V_{\rm am}(\mathbf{r}) &= V\cos(\mathbf{r}.(\mathbf{k}_1+\mathbf{k}_2)) \\ &\quad + V''\cos(2\mathbf{r}.(\mathbf{k}_1+\mathbf{k}_2)+\phi'). \end{aligned}$$

Here we examine the case where $\phi = \phi' = 0$. 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 $\mathbf{k}_1$ direction. We explore its effect on the topological character of the insulator in the next section.

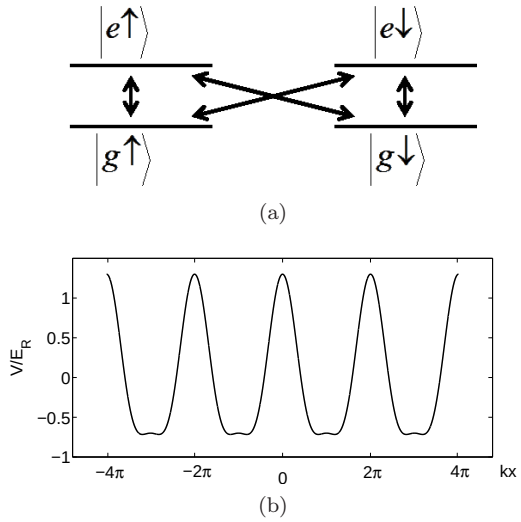
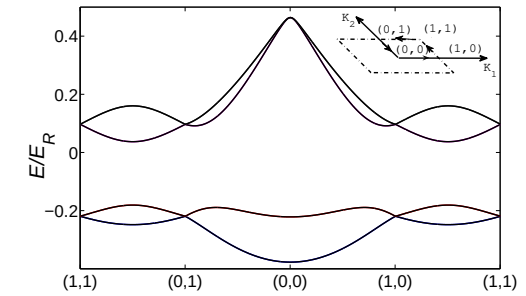


FIG. 1: (Color online) (a) Optical transitions between the ground (g) and excited (e) energy levels. Two-fold nuclear spin degeneracy yields the manifold of states $|g\uparrow\rangle$, $|g\downarrow\rangle$, $|e\uparrow\rangle$ and $|e\downarrow\rangle$ used to define the potential matrix in Eq. (3) (b) The schematic view of the cross section of the bichromatic optical lattice along the $\mathbf{k}_1$ direction, for the case $V' = 0.2V$.(All quantities plotted are dimensionless)

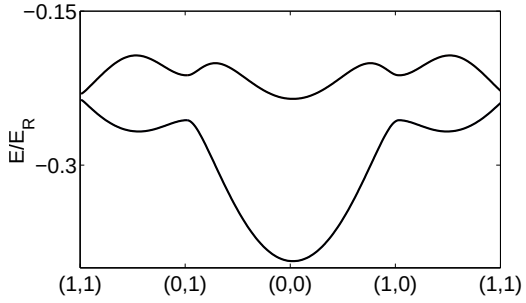
III. RESULTS

We determine the topological character of the insulator directly using the band structure to calculate the $\mathbb{Z}_2$ invariant. The Hamiltonian in Eq. (1) can be numerically diagonalized using plane-wave method. The band structure is shown in Fig. 2. The Lowest twofold degenerate energy bands for the lattice without disorder Fig. 2(a) has no gap between first and second bands. As we introduce the bichromatic lattice along different direction the fourfold degeneracies at special points in k-space are lifted. For the cases when the potential strength are as large as $V' = 0.5V$ and $V'' = 0.5V$, Fig. 2(b) shows a gap opening between first and second bands but it is very narrow. Fig. 2(b) shows a gap opening for the case $V' = 0.5V$and $V'' = 0.5V$.

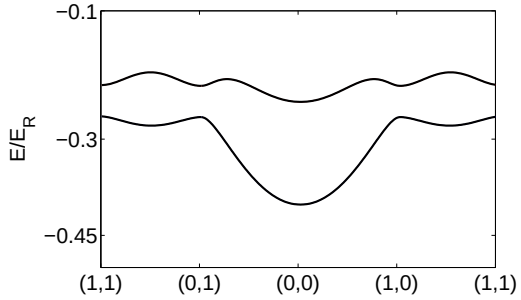
In order to investigate the topological state of the system we use the method in Ref. [22]. There are other methods to determine the topological characteristic of the systems where the detailed discussion and the relevant mathematical methods and the advantages and shortcoming of different approaches on the calculation of $\mathbb{Z}_2$ invariant can be found in the literature [2, 22, 26–29]. In the case of inversion symmetric materials, finding the



(a)

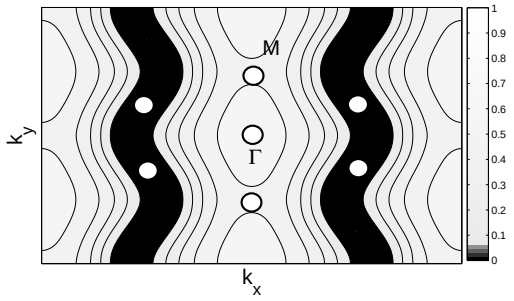


(b)

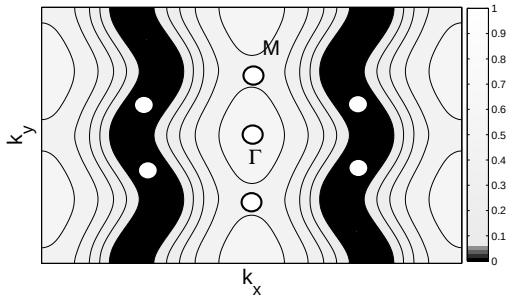


(c)

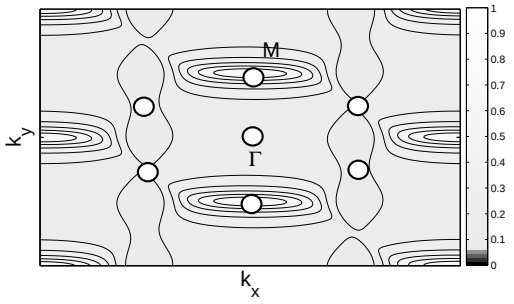
FIG. 2: (Color online) Lowest energy bands for the lattice with $V = 0.5E_R$ are shown for the cases of (a) $V' = V'' = 0$ and (b) $V' = 0.5V$ and $V'' = 0$ (c) $V' = 0.5V$and $V'' = 0.5V$. The $\mathbf{k}$-points are labeled as ($\mathbf{\Gamma}_{pq} = (p\mathbf{k}_1 + q\mathbf{k}_2)/2$) and indicated in the figure by (p, q) with $p, q \in \{0, 1\}$. At the special points (1,0), (1,1) and (0,1) the fourfold degeneracy is reduced to twofold by the presence of bichromatic lattice potential.



(a)



(b)



(c)

FIG. 3: (Color online) The pfaffian $|Pf(\mathbf{k})|$ in $\mathbf{k}$-space for different potentials in Eq. (8). Γ and M are high symmetry points. (a) $V' = 0$ and $V'' = 0$ are used to calculate the $|Pf(\mathbf{k})|$ of the the lowest twofold degenerate two bands. (b) $|Pf(\mathbf{k})|$ for $V' = 0.5V$ and $V'' = 0$. As one goes along the path C which includes the half of the first Brillouin zone one cut the line of zeros of $|Pf(\mathbf{k})|$ twice. This shows that system is still in non trivial topological state, which is the case for Fig. 3(a) as well. (c) $|Pf(\mathbf{k})|$ for lowest 2 bands for $V' = 0.5V$ and $V'' = 0.5V$ where there is no line of zeros therefore the system has trivial topology.

$\mathbb{Z}_2$ can be done using the Fu and Kane method [30]. Since the parity and time-reversal operators commute, we only need to check the parity eigenvalues in four time-reversal invariant points in k-space for all bands below the gap. The result for the system, without bichromatic deformation, turns out to be non-trivial so that it is either a $\mathbb{Z}_2$ insulator or a quantum spin Hall insulator, depending on the presence or absence of δ coupling, respectively [11].

The Hilbert space of the time reversal Hamiltonian can be divided into two subspaces which can be called as even and odd depending on the relation between the vectors and their time reversal partners. In the even subspace the Hamiltonian transforms under the time reversal operator as $H_k = \Theta H_k \Theta^{-1}$ and therefore the eigenvectors have this property that the $\Theta|v_i>$ is equivalent to $|v_i>$ up to a $U(2)$ rotation, here i is the band index. The four special points in half of the 2-D Brillouin zone which are time reversal invariant points belong to even subspace.

The eigenfunctions $|v_i>$ are orthogonal to their time reversal partner $\Theta|v_i>$ in odd subspace. The zeros of the Pfaffian ($Pf(\mathbf{k})$) for the overlap matrix elements $\omega_{ij} =< v_i|\Theta|v_j >$ of the time reversal operator is related to the

topological characteristic of the Hamiltonian. $|Pf(\mathbf{k})|$ vanishes in the odd space whereas in the even subspace is equal to 1 up to a $U(2)$ rotation. The Pfaffian of a skew symmetric matrix $\omega_{2\times 2}$ is its ω_{12} element and it has more complicated form for higher number of bands. Therefore the task of finding the topological characteristic of the Hamiltonain reduces to finding the complex zeros of the Pfaffian. The zeros can occur either in pairs of points in the Brillouin zone or on the lines depending on the symmetry of the system. Odd number of pairs of complex zeros or odd number of two times cutting the line of zeros as we go through half the Brillouin zone, indicates that we have non trivial topological insulator and even is the sign of trivial insulator [22].

In order to find the zeros of Pfaffian for the bichromatic lattice we plot directly the absolute value of the Pfaffian. Since the numerical diagonalization of the Hamiltonian do not return in general the wave functions with the time reversal invariance, we impose this constraint in the special points of the Brillouin zone using the following relation:

$$|v_i(k)>=\Theta|v_{i-1}(k)> . \tag{8}$$

The Pfaffian for lowest bands of the band structure in Fig. 2 are shown in Fig. 3. In the absence of the bichromatic lattice Fig. 2(a) the zeros of Pfaffian $|Pf(k)|$ occur along a line Fig. 3(a). For the case when $V'=0$ and $V''=0.5V$ the system holds its nontrivial topology Fig. 3(b) when we consider two lowest twofold degenerate bands Fig. 2(b) of Hamiltonian Eq. (1). On the other hand for the case $V'=0.5V$ and $V''=0.5V$ since we break the half translational symmetry of the Hamiltonian Eq. (1) Ref. [11], there is a gap opening between the first and second band Fig. 2(c) which allows us to discuss the topological characteristic of the lowest band as well. The line of zero vanishes for the lowest band, which means we have trivial insulator Fig. 3(c). However the lowest two bands together still keep their non-trivial characteristic and we saw similar pattern as in Fig. 3(b) for this case. The lowest band for the case $V'=0.5V$ and $V''=0$ is also trivial but the gap between the lowest bands is very narrow Fig. 2(b).

IV. CONCLUSION

We considered 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 examined the effect of this deformation which can be as large as the insulating gap, on the topological character of the system. We found that the system retains its topological character robustly against this kind of perturbation for two lowest twofold degenerate bands. However the lowest twofold degenerate band has trivial topology. 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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