Majorana Zero Modes Protected by Lattice Symmetry

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We study the lattice-symmetry protection of Majorana zero bound modes (MZBMs) using the recently observed topological crystalline insulator Pb\textsubscript{1-x}Sn\textsubscript{x}Te in proximity to superconductor. With the induced s-wave superconductivity the (001)-surface of the crystalline insulator, which has a C\textsubscript{4} rotational symmetry, characterizes a new class of 2D topological superconductor with four MZBMs obtained in each vortex core, while only two of them are protected by the cyclic symmetry. Furthermore, applying an in-plane external field can break the four-fold symmetry and lifts the MZBMs to finite energy in general. Surprisingly, we show that even the C\textsubscript{4} symmetry is broken, two Majorana modes are restored at zero energy exactly one time whenever the in-plane field varies \(\pi/2\), i.e. 1/4-cycle in the direction. This novel phenomenon has a nontrivial connection to the four-fold cyclic symmetry of the original system and can be adopted to demonstrate the lattice-symmetry protection of the MZBMs. These results can be extended to the generic system with \(C_{2N}\) symmetry.

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There has been much attention attracted in the realization of topological superconductors (SCs) which support non-Abelian Majorana zero bound modes (MZBMs), driven by both the pursuit of exotic fundamental physics and the applications to a building block for fault-tolerant topological quantum computer \cite{1, 2}. While previous studies have been mostly focused on chiral SCs whose topological phases require no symmetry protection, new interests are growing fast in the study of topological SCs, where MZBMs come in pairs due to Kramers' theorem \cite{3, 4–21}, similar as the boundary modes in the low energy physics of the surface states are captured by crystalline topological phases. The initial studies have been considered for insulators \cite{22}. Following the protection of time-reversal symmetry, the Majorana zero bound modes are protected by time-reversal invariant topological insulators \cite{23, 24}. Due to the protection of time-reversal symmetry, the Majorana Kramers' pairs in DIII class 1D wires are shown to obey non-Abelian statistics \cite{25, 26}.

An interesting generalization of the topological states protected by time-reversal symmetry is to consider discrete lattice symmetries, which brings about wide classes of crystalline topological phases. The initial studies have been considered for insulators \cite{27}. Following the theoretical studies, the topological crystalline insulator (TCI) with mirror and rotational symmetries was recently verified in the experiment using 3D rock-salt material Pb\textsubscript{1-x}Sn\textsubscript{x}Te \cite{28, 29}. In particular, the boundary modes at (001)-surface of the material are characterized by four Dirac cones separated in momentum space which exhibit mirror and C\textsubscript{4} four-fold rotational symmetries. A natural consideration might be that, with proximity induced s-wave superconductivity in the lattice-symmetry-protected surface states, a 2D topological crystalline SC should be resulted, with the presence of four MZBMs in each vortex core. An interesting question is, how many MZBMs can be protected by the lattice symmetries? Moreover, while in topological crystalline SCs \cite{22–25} the MZBMs are protected by lattice symmetries, an important questions is how to demonstrate such lattice-symmetry protection of MZBMs in an experiment?

In this work, we propose to study the MZBMs protected by cyclic symmetry using the (001)-surface of the TCI Pb\textsubscript{1-x}Sn\textsubscript{x}Te in proximity to an s-wave SC. We show that a new class of 2D topological crystalline SC with C\textsubscript{4} symmetry is obtained, and such four-fold symmetry only protects two MZBMs in each vortex core. Furthermore, we propose a novel scheme to demonstrate the C\textsubscript{4} lattice-symmetry protection of the topological superconducting phase by inducing couplings in the MZBMs with an in-plane external field. These results can be extended to generic C\textsubscript{2N}-symmetric systems.

The surface states of the TCI Pb\textsubscript{1-x}Sn\textsubscript{x}Te can be described with even number of Dirac cones protected by lattice symmetries. In particular, for the (001)-surface, the low energy physics of the surface states are captured by four Dirac Hamiltonians respectively centered at four Dirac points \(K_j\) \((j = 1, 2, 3, 4)\), with \(K_1 = -K_3\) and \(K_2 = -K_4\), as sketched in Fig. 1 \cite{32, 33}. Inherited from the TCI Pb\textsubscript{1-x}Sn\textsubscript{x}Te, the surface Hamiltonian preserves mirror symmetries along \(\Gamma X_1\) and \(\Gamma X_2\) directions. Furthermore, the four Dirac cones are transformed according to \(K_j \rightarrow K_{j+1}\) and \(K_4 \rightarrow K_1\) under the \(C_4\) four-fold rotation (Fig. 1). Using \(k_x\) and \(k_y\) to form a right-handed coordinate centered at \(K_1\) on the surface, the surface Dirac Hamiltonian around \(K_1\) reads \(H_{(1)}^{(1)} = v_\perp k_x s_y - v_\parallel k_y s_x\), where \(v_\perp\) (\(v_\parallel\)) represents the anisotropic Fermi velocity in the \(k_x\) (\(k_y\)) direction, and \(s_x, s_y\) are Pauli matrices on the spin space. For the spin system, the \(C_4\) symmetry is defined by \(C_4(\pi/2) = R_z(\pi/2) \exp(-i\pi s_z/4)\), with which the other three Dirac Hamiltonians can be obtained. Here \(R_z(\pi/2)\)
is the 2D rotation transformation on Bravais lattice vector as \((R_x, R_y) \rightarrow (R_y, -R_x)\) \([32]\). In the presence of \(C_4\) symmetry, the four Dirac cones are decoupled from each other and the surface states are topologically stable.

Now we consider an induced s-wave superconductivity in the surface states, which can be achieved with a heterostructure formed by the \((001)\)-surface and a conventional s-wave SC \([5–13]\). Note that the SC pairing occurs between two states related by time-reversal symmetry, which implies that the pairing only occurs between the states respectively belonging to the Dirac cones around \(K_1\) (\(K_2\)) and \(K_3\) (\(K_4\)). Denoting by \(\Delta_s\) the s-wave SC order parameter, we obtain the total Hamiltonian

\[
H = \sum_{k,j=1,3} \left( -iv_{k,x}\hat{n}_x c_{j+1, k}^\dagger c_{j, k} - v_{k,y}\hat{n}_y c_{j+1, k}^\dagger c_{j, k} + H.c. \right) \\
+ \sum_k (\Delta_s c_{1+, k} c_{3-, k} - \Delta_s c_{1-, k} c_{3+, k} + H.c.) \\
- \sum_{k, \sigma, j=1,3} \mu c_{j, k}^\dagger c_{j, k} + \left\{ C_4 \text{ terms} \right\},
\]

(1)

where \(\mu\) is the chemical potential and \(c_{j, k}^\dagger\) \((c_{j, k})\) is the annihilation (creation) operator of a surface electron from the \(j\)-th Dirac cone at and the spin state \(\sigma = \uparrow, \downarrow\). The last term represents the \(C_4\) transformation on all the former terms. The s-wave order parameter may change the symmetry respected by the total Hamiltonian. In particular, to study MZBMs we shall consider a vortex profile of the s-wave order parameter, which breaks mirror symmetry, while the rotational symmetry is still preserved. As shown below, it is convenient to redefine the \(C_4\) four-fold transformation as \(C_4^{(n)} = U(n\pi/4)C_4U(\pi/4)\), with \(U(\phi)\) a \(U(1)\) phase transformation. In the absence of the s-wave superconductivity, the Hamiltonian \(H\) also respects \(C_4^{(n)}\) symmetry. The redefined \(C_4^{(n)}\) symmetry is useful when a vortex profile of \(\Delta_s\) with winding number \(n\) is present.

The Hamiltonian \(H\) can be block diagonalized with a set of new bases \(c_{\pm, \sigma, k} = \frac{1}{\sqrt{2}}(c_{1\sigma, k} \pm c_{3\sigma, k})\) and \(c_{\pm, \sigma, k} = \frac{1}{\sqrt{2}}(c_{2\sigma, k} \pm c_{4\sigma, k})\) with \(\sigma = \uparrow, \downarrow\). In terms of new bases we obtain \(H = \sum_{k, \eta, \pm} [H_{\eta, \pm}(k) + H_{\eta, \pm}(k)]\), where

\[
H_{\eta, \pm}/b_\pm(k) \equiv \left(\begin{array}{cc}
-i\nu_{k,x}\hat{n}_x k_x - v_{k,y}\hat{n}_y k_y c_{\eta, k}^\dagger & \pm \Delta_{\eta, \pm} c_{\eta, k} \kappa a_{\eta, k} / b_{\eta, \pm, \pm, k} + H.c.
\end{array}\right) - \left(\begin{array}{cc}
\Delta_{\eta, \pm} c_{\eta, k} \kappa a_{\eta, k} / b_{\eta, \pm, \pm, k} + H.c.
\end{array}\right)
\]

Note that \(C_4^{(n)} - c_{\pm, \sigma, k} c_{\eta, k}^{(n)} = e^{i(n-s)\pi/4} b_{\eta, \pm, \pm, k}\) and \(C_4^{(n)} - c_{\pm, \sigma, k} c_{\eta, k}^{(n)} = e^{i(n-s)\pi/4} b_{\eta, \pm, \pm, k}\), where the momenta \(k = (k_x, k_y)\), \(k' = (-k_y, k_x)\), and \(s = 1(-1)\) for \(\sigma = \uparrow, \downarrow\). On the other hand, the superconducting vortex transforms via \(R_x^{-1}(\pi/2)\Delta_{\eta}(r) R_x(\pi/2) = (-\mu R_x^{(n)}\Delta_{\eta}(r))\), where the vortex profile is described by \(\Delta_{\eta} = \Delta_0(r) e^{i\theta(r)}\). With these results it can be verified that the total Hamiltonian is invariant under the \(C_4^{(n)}\) transformation. From Eq. \(2\) we know that the Hamiltonian \(H\) describes four decoupled Dirac cones with induced s-wave orders \(\pm \Delta_s\), respectively, which render four copies of \(p + ip\) SC and support MZBMs \([5]\). However, the bases \(c_{\pm} \) and \(c_{\pm}\) are connected to each other by the \(C_4^{(n)}\) transformation, which distinguishes our system from a trivial four-copy version of \(p + ip\) chiral SCs, and can lead to new physics in the present 2D topological crystalline SC.
\[ e^{-\int_0^d \Delta \phi(t')dt'} \] the other two MZBSs for \( H_{\text{bs}} \) are obtained by \( C_4^{(n)} \) rotation and the relations read
\[ \gamma^{(n)}_h = C_4^{(n)-1} \gamma^{(n)}_a C_4^{(n)}, \quad C_4^{(n)-1} \gamma^{(n)}_h C_4^{(n)} = \eta \gamma^{(n)}_a. \] (3)

Note the result \( C_4^{(n)-1} e^{i\theta} C_4^{(n)} = -e^{i\theta} \) has been used. These relations can be reorganized in a more transparent way by redefining that \( \gamma_1 = (\gamma^{(+)}_a + \gamma^{(-)}_a)/\sqrt{2}, \gamma_2 = (\gamma^{(+)}_b + \gamma^{(-)}_a)/\sqrt{2}, \gamma_3 = (\gamma^{(+)}_a - \gamma^{(-)}_a)/\sqrt{2}, \) and \( \gamma_4 = (\gamma^{(+)}_b - \gamma^{(-)}_b)/\sqrt{2} \). Then we have
\[ \gamma_{j+1} = C_4^{(n)-1} \gamma_{j} C_4^{(n)}, \quad \gamma_1 = C_4^{(n)-1} \gamma_4 C_4^{(n)}. \] (4)

The Eq. 4 reflects the cyclic properties of the four Majorana modes, with which we know that the only possible perturbation respecting \( C_4^{(n)} \) symmetry takes the following form \( V_{\text{pert}} = \Gamma_1 (i \gamma_1 \gamma_2 + i \gamma_2 \gamma_3 + i \gamma_3 \gamma_4 + i \gamma_4 \gamma_1) = i 2 \Gamma_0 \eta^\dagger \gamma_a^\dagger \gamma_a \). Thus an infinitesimal perturbation without breaking \( C_4^{(n)} \) symmetry can gap out \( \gamma_a \). However, the rest two MZBs \( \gamma_b^\dagger \) and \( \gamma_b \) can be protected by the \( C_4^{(n)} \) symmetry. Furthermore, even the four-body interaction cannot lift the rest degeneracy, since the four-operator interaction \( \gamma_1 \gamma_2 \gamma_3 \gamma_4 \) is forbidden by the \( C_4 \) symmetry. Therefore, the four-fold cyclic symmetry group protects only two MZBSs, which tells that the present topological crystalline SC with \( C_4 \) symmetry is classified by a \( Z_2 \) invariant.

The existence of MZBSs can lead to zero bias peak in the tunneling transport from a normal lead to the vortex core of the SC \( \text{[11][13][33][37]} \). Without breaking the \( C_4 \) symmetry, due to the two symmetry protected MZBSs, the height of zero bias peak is expected to be double of that induced by a single MZBM under the same conditions. In particular, at zero temperature, the zero bias peak is of height \( 4e^2/h \) [39]. These results can reflect the number of Majoranas localized in each vortex core.

By showing the existence of two protected Majorana modes, it is important to study how to demonstrate in an experiment the protection by the lattice symmetry. For this we consider an external field to induce controllable lattice-symmetry-breaking terms in the Hamiltonian. In particular, with the consideration of a distortion by strain or an in-surface magnetic field \( \pm \) (or an electric field by a gate \( \pm \)) one can break the four-fold symmetry and introduce mass terms for the four Dirac cones in the form \( m_j = \alpha (u \times K_j) \cdot \hat{e}_z \) or \( m_j = \alpha (u \cdot K_j) \), where \( u \) represents the direction of the displacement vector due to distortion or the applied external field. It follows that \( m_1 = -m_3 = m_0 \cos \phi \) and \( m_2 = -m_4 = m_0 \sin \phi \), where \( \phi \) represents the angle of the external field. By a straightforward derivative one can find that the mass terms generate couplings between the MZBSs \( \gamma_a^\dagger \) and \( \gamma_b^\dagger \), and the coupling Hamiltonian takes the following form
\[ V_c(\phi) = i 2 \Gamma_0 \gamma_a^\dagger \gamma_b^\dagger + i 2 \Gamma_1 \sin (2\phi + \beta) \gamma_a^\dagger \gamma_b^\dagger + i 2 m_0 \cos \phi \gamma_a^\dagger \gamma_b^\dagger + i 2 m_0 \sin \phi \gamma_a^\dagger \gamma_b^\dagger. \] (5)

It is noteworthy that since the \( C_4^{(n)} \) symmetry is broken, an additional \( \Gamma_1 \)-coupling term between \( \gamma_a^\dagger \) and \( \gamma_b^\dagger \) is now allowed. On the other hand, the variation of \( \phi \) by \( \pi/2 \) is equivalent to do a \( C_4^{(n)}(\pi/2) \) rotation, which transforms \( \gamma_a^\dagger \leftrightarrow \gamma_b^\dagger \), and should change the sign of the coupling coefficient. Therefore this coupling term must be proportional to \( \sin (2\phi + \beta) \), with \( \beta \) an arbitrary constant which should be material-dependent. We note that in general the perturbation by an in-plane vector- or pseudovector-type field always induces the symmetry-breaking couplings as given in Eq. 4.

The spectra of the coupling Hamiltonian \( \gamma \) can be numerically solved, with two positive and two negative eigenvalues obtained for a fixed \( \phi \). It is interesting that for any input parameters of \( \Gamma_0/\Gamma_1, \beta, \) and \( m_0 \), as long as \( m_0^2 \neq 2 \Gamma_0 \Gamma_1 \) (or \( \beta \neq 0 \)), one can always find that spectra for the two lowest Andreev Bound states cross zero energy four times when the angle \( \phi \) varies a cycle from 0 to \( 2\pi \). Several cases are shown in Fig. 2 (a). This phenomenon has a profound reason which is intrinsically

**FIG. 2**: (Color online) (a) Spectra of the lowest two Andreev bound states by breaking \( C_4^{(n)} \) symmetry and (b) Pfaffian versus \( \phi \), with the parameters \( \Gamma_1 = 0 \) (blue curves); \( \Gamma_1 = 0.5 \Gamma_0, \beta = 0.5 \) (black curves); and \( \Gamma_1 = 0.5 \Gamma_0, \beta = 1.0 \) (red curves), respectively. (c) Critical angle \( \phi_c \) versus \( m_0 \) for different magnitudes of \( \beta \). (d) The differential tunneling conductance in unit of \( e^2/h \) at zero temperature, with the parameter regime \( \Gamma_0 = m_0 = 2 \Gamma_1, \beta = 0 \), and the tunneling energy chosen to be 0.2\( \Gamma_0 \). The upper bright band represents the higher Andreev bound state spectrum. Only the results with bias \( V_0 \geq 0 \) are shown here.
related to the $C^{(n)}_2$ symmetry of the original system. Actually, when $\phi$ advances $\pi/2$, we can see that coupling Hamiltonian $V_c(\phi + \pi/2) = i2\Gamma_0\gamma_{\alpha\beta}^{(-)} + 2\Gamma_1 \sin(2\phi + \beta)\gamma_{\alpha\beta}^{(+)}$, and such that $\gamma_{\alpha\beta}^{(+)} = i2m_0 \sin \phi \gamma_{\alpha\beta}^{(-)} \gamma_{\alpha\beta}^{(+)\gamma_{\alpha\beta}^{(-)}} + i2m_0 \cos \phi \gamma_{\alpha\beta}^{(+)} \gamma_{\alpha\beta}^{(-)}$, which can return to $V_c(\phi)$ by $C^{(n)}_2$ rotation that $\gamma_{\alpha\beta}^{(+)\gamma_{\alpha\beta}^{(-)}} = \gamma_{\alpha\beta}^{(+)\gamma_{\alpha\beta}^{(-)}}$ and $\gamma_{\alpha\beta}^{(+)} = \pm \gamma_{\alpha\beta}^{(+)}$. On the other hand, note that the four MZBMs can form two complex fermions (Andreev Bound states) as $f_{\alpha\beta} = \gamma_{\alpha\beta}^{(+)\gamma_{\alpha\beta}^{(-)}} + i\gamma_{\alpha\beta}^{(+)\gamma_{\alpha\beta}^{(-)}}$. Then the variation of $\pi/2$ in $\phi$ equivalently transforms $f_{\alpha\beta} \rightarrow f_{\alpha\beta}^*$ and $f_{\alpha\beta} \rightarrow f_{\alpha\beta}^*$ according to Eq. (3), which implies that the ground state of the system changes fermion parity. This result can be quantitatively confirmed by calculating the Pfaffian for the coupling Hamiltonian $V_c(\phi)$, which can be written as $V_c(\phi) = i \sum_{\alpha,\alpha',\eta,\eta'} \gamma_{\alpha\beta}^{(+)\eta} \gamma_{\alpha'\beta}^{(+)\eta'}$ with $\alpha, \alpha' = a, b$ and $\eta, \eta' = \pm$. The matrix $V_c(\phi)$ is skew-symmetric, with the Pfaffian satisfying

$$\frac{\text{Pf} [V_c(\phi)]}{\det [V_c(\phi)]^{1/2}} = \text{sgn} \left[ \sin(2\phi) - \frac{2\Gamma_0 \Gamma_1}{m_0^2} \sin(2\phi + \beta) \right],$$

which reverses sign when varying $\phi$ by $\pi/2$, with $m_0^2 \neq 2\Gamma_0 \Gamma_1$ (or $\beta \neq 0$) [Fig. 2(b)]. Therefore, there must be one zero-energy crossing in the Andreev Bound state spectra during this variation. Finally, when the angle $\phi$ advances $2\pi$, we always get four crossings for the lowest two Andreev Bound states, and the four angles of the crossing points are given by

$$\phi_c' = \frac{1}{2} \tan^{-1} \left[ \frac{2\Gamma_0 \Gamma_1}{m_0^2 - 2\Gamma_0 \Gamma_1} \tan \beta \right] + \frac{l}{2} \pi, \ l = 0, \ldots, 3, (7)$$

where two Majorana modes are obtained [Fig. 2(c)]. The cyclic zero-energy crossings can be measured by the differential tunneling conductance, as shown in Fig. 2(d). This novel phenomenon can be adopted to demonstrate the symmetry-protection for MZBMs by $C_4$ group of the original system.

Finally, we show how to generalize the above results for a system with $C_4$ symmetry to the system with generic $C_{2N}$ symmetry, in which case the surface has $2N$ Dirac cones related by the $2N$-fold rotational symmetry. Note that the four MZBMs $\gamma_{\alpha\beta}^{(+)\gamma_{\alpha\beta}^{(-)}}$ consist of a 4D reducible representation of $C_4^{(n)}$ group. In the diagonal bases given by $\gamma_{\pm} = \gamma_a^{(+)} \pm \gamma_b^{(+)}$, $f = \gamma_a^{(-)} + i\gamma_b^{(-)}$ and $f^\dagger = \gamma_a^{(-)} - i\gamma_b^{(-)}$, the group element can be represented as $M[C_4^{(n)}] = [1, -1, -i, i]^{\text{diag}}$. Then each of the two Majorana bases and two complex fermion bases consists of a 1D irreducible representation. For a unitary group, it can be shown that only the Majorana bases ($\gamma_{\alpha\beta}^{(+)\gamma_{\alpha\beta}^{(-)}}$) which consist of independent 1D irreducible representations are protected by the symmetry group, while the complex fermion bases are not [39]. This provides an alternative interpretation of the protection of two MZBMs in the $C_4^{(n)}$-symmetric system. Similarly, for a system with $C_{2N}^{(n)}$ symmetry, from the 2N MZBMs we can obtain $2N$ independent 1D irreducible representations of the $C_{2N}^{(n)}$ group, with the representation matrix given by $M[C_{2N}^{(n)}] = [1, e^{i\pi/N}, e^{i2\pi/N}, \ldots, -1, \ldots, e^{i(2N-1)\pi/N}]^{\text{diag}}$. Again only the two real eigenvalues $\pm 1$ correspond to Majorana bases (denoted by $\gamma_{\pm}$) for the representation space, which are protected by the $C_{2N}^{(n)}$ symmetry. The rest bases are complex fermion modes and can be gapped out without breaking $C_{2N}^{(n)}$ symmetry. With this general proof one can also know that a $C_{2N+1}$ symmetry cannot protect any Majorana modes.

For the generic $C_{2N}$-symmetric system, applying an external field can gap out all the Majorana modes but restore two of them $2N$ times when the field varies one cycle in the direction. Actually, when the angle $\phi$ of the field advances $\pi/N$, the new coupling Hamiltonian $V_{\text{couple}}(\phi + \pi/N)$ should generically return to $V_{\text{couple}}(\phi)$ by a $C_{2N}$ transformation. Under this transformation the complex fermion mode, defined by $f = \gamma_a^{(+)} + i\gamma_b^{(-)}$, transforms via $f \rightarrow f^\dagger \rightarrow f$ according to the eigenvalues of the representation matrix $M[C_{2N}^{(n)}]$. Therefore the ground state changes fermion parity and one level crossing occurs. The $2N$-time restoration demonstrates the protection of MZBMs by the $C_{2N}$ symmetry.

In conclusion, we have studied MZBMs protected by 2D cyclic symmetries using the topological crystalline insulator in proximity to superconductor. A new class of 2D topological superconducting phase has been predicted by inducing $s$-wave superconductivity in the (001)-surface of the crystalline insulator Pb$_{1-x}$Sn$_x$Te, with four MZBMs obtained in each vortex core, while only two of them are protected by the $C_4$ lattice symmetry. Furthermore, we have shown a novel phenomenon that with an external field applied in-plane to break the $C_4$ symmetry, the two MZBMs are lifted to finite energy in general, but, surprisingly, they are restored to zero energy exactly four times when the in-plane field varies $2\pi$, i.e. one cycle in the direction. This novel phenomenon has a nontrivial correspondence to the four-fold cyclic symmetry of the original system and can be adopted to experimentally demonstrate the lattice-symmetry protection of the MZBMs. We have extended these results to the generic system with $C_{2N}$ symmetry, where there are always two MZBMs protected by the cyclic lattice symmetry, and the lattice-symmetry protection of the MZBMs can be demonstrated in the $2N$ times of zero-energy crossing by varying one cycle the external field. Our results may provide insights into the study of rich physics about symmetry-protection in the wide classes of topological crystalline SCs.

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Note.-In writing the present manuscript, we note that the result of protection of two Majorana modes by $C_4$ symmetry is also obtained recently in an independent work by C. Fang et al., using a different classification theory [10]. On the other hand, here we have further proposed a novel scheme to demonstrate the lattice-symmetry protection of MZBMs.

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