Supplementary Information for "Unveiling nontrivial fusion rule of Majorana zero mode using a fermionic mode"

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1 Additional nontrivial fusion loop

As we shown in the main text, the trivial and nontrivial fusion loops can be designed by manipulating the order of fusion and splitting processes. Contrary to the fusion loop in the main text, here we fuse γ_B and γ_1 first. Then, as shown in Fig. S1a, the trivial loop would be denoted as $F_{B1}^{-1}F_{AB}F_{AB}^{-1}F_{B1}$, while the nontrivial loop would be denoted as $F_{AB}F_{B1}^{-1}F_{AB}^{-1}F_{B1}$. The charge transfer for the nontrivial loop denoted by $F_{AB}F_{B1}^{-1}F_{AB}^{-1}F_{B1}$ shows a zero, half, integer charge pumping in Fig. S1b as the corresponding parameters vary as Fig. S1d. While the net charge transfer is always zero, as indicated in Fig. S1c, regardless of whether E_d crosses zero level during the whole process, as can be seen in Fig. S1e. It shows the same charge transfer behavior as the charge pumping in Fig. 2 of the main text, however, the charge pumping is more stable and does not oscillate in the case $E_d = 0$ with $a = 1$. This is because the charge would have no definite way to transfer in and out of the FM states at $E_d = 0$ and display an oscillating behavior when we varying t_c in this situation. While the revised loop can avoid such uncertainty.

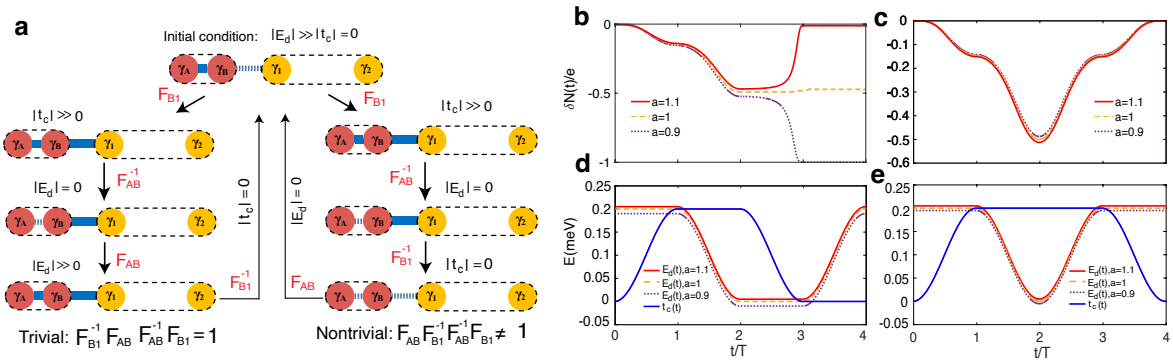

Figure S1: Fusion loops and charge transfer. **a** Another revised trivial loop (left panel), we first fuse γ_B and γ_1 (F_{B1}), followed by the split of γ_A and γ_B (F_{AB}^{-1}), and then reverse the operation to complete the loop. The corresponding nontrivial loop (right panel), two consecutive processes do not commute with each other. **b** The charge transfer for the nontrivial loop $F_{AB}F_{B1}^{-1}F_{AB}^{-1}F_{B1}$. Here F_{AB}^{-1} (F_{AB}) is controlled by $E_d(t) = E_0[a \pm \cos(\omega t)]$ with $\omega = 1/1000\,\text{meV}$ and $E_M = 10^{-9}\,\text{meV}$. After the splitting process, the energy level of the FM reaches exactly to zero for $a = 1$, stays above zero for $a = 1.1$, and changes sign for $a = 0.9$. **c** The charge transfer for the the trivial loop $F_{B1}^{-1}F_{AB}F_{AB}^{-1}F_{B1}$. **d**, **e** The evolution of system parameters corresponding **b**, **c**, respectively.

Moreover, the initial conditional for $E_d > 0$ and $E_d < 0$ is very important for the whole fusion process. Since we set the initial state composed by MZMs as $|0_{12}\rangle$ in the whole situation. Then the parity of the whole system would determined by the initial conditional of E_d. If $E_d > 0$, the initial state is $|0_{\rm AB}0_{12}\rangle$, which means both the FM and MZM are unoccupied. While if $E_d < 0$, then the initial state is $|1_{\rm AB}0_{12}\rangle$, which means FM is occupied and MZM is unoccupied. Fig. S2a reveals the evolution of wavefunction $\psi_{12}^{+}(t)$ with the nontrivial fusion loop $F_{AB}F_{B1}^{-1}F_{AB}^{-1}F_{B1}$ in the situation $E_d > 0$. Here $\psi_{12}^{+}(t)$ is the evolution state of $\psi_{12}^{+}(0)$ at time t, and $\psi_{AB}^{\pm}(0) = \gamma_A \pm {\rm i}\gamma_B$, $\psi_{12}^{\pm}(0) = \gamma_1 \pm {\rm i}\gamma_2$. As we can see, $\psi_{12}^{+}(t)$ would transform as $\psi_{12}^{-}(0)$ after the whole fusion loop. This means the initial state is $|0_{\rm AB}0_{12}\rangle$, it would gradually switch to state $|1_{\rm AB}1_{12}\rangle$ after the loop finished. During the evolution, an integer charge would be pumped to FM. The pumping is accomplished through TH process. This is consistent with the current plot in Fig. S2c. In the whole process, $J_e(t)$ keeps zero which is the current induced by TE process while $J_h(t)$ is not zero which is the current induced by TH process. Fig. S2b reveals the evolution of wavefunction $\psi_{12}^{+}(t)$ in the situation $E_d < 0$, then the initial state is $|1_{\rm AB}0_{12}\rangle$, it would gradually switch to state $|0_{\rm AB}1_{12}\rangle$ after the loop finished. The corresponding pumping is accomplished through TE process as shown in Fig. S2d.

2 Reduced step for nontrivial fusion

Since the the charge pumping is determined by the number of intersection at zero energy. Then some fusion and splitting steps can be adjusted at the same time. As shown in Figure S3a. For trivial loop, E_d and t_c can be modulated at the same time as $E_d = E_0\cos(\frac{\omega t+\phi_0}{2})$, $t_c = |E_0|[1-\cos(\omega t+\phi_0)]/2$. In this situation, the fusion loop can be reduced to two steps. While for nontrivial loop, the first two steps of F_{AB}^{-1} and F_{B1} are gated individually, and the other two steps can be adjusted at the same time. To be specific, we set $t_c = 0$ and $E_d(t) = E_0(a+\cos(\omega t))$ in the first step with $\omega t \in [0,\pi]$, then $t_c(t) = |E_0|(1+\cos(\omega t))/2$

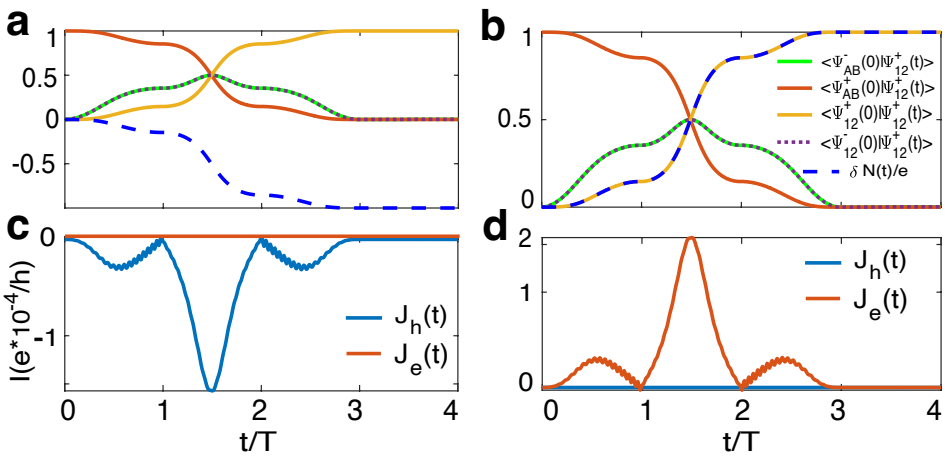

Figure S2: The evolution of wavefunction and charge transfer processes. The charge transfer and the evolution of the wavefunction $\psi^{+}_{B1}(t)$ following the loop $F_{B1}F^{-1}_{AB}F_{AB}F^{-1}_{B1}$ with the initial state $E_d(0) > 0$ in **a** and $E_d(0) < 0$ in **b**. Here the fusion and split process of F^{-1}_{AB} (F_{AB}) is controlled by $E_d(t) = E_0[a \pm \cos(\omega t)]$ with $a = 0$. E_0 is a positive value in **a** and a negative value in **b**. The other parameters are the same as Fig. S1. Although the evolution of wavefunction are the same in both situations, but they choose different transfer process. The transfer process in **a** is TH process as shown in **c** since the initial state is even parity with $E_d(0) > 0$, while the transfer process in **b** is TE process as shown in **d** since the initial state is odd parity with $E_d(0) < 0$

for $\omega t \in [\pi, 2\pi]$, and finally the split and fusion process realized at the same time as $E_d(t) = E_0(a - \cos(\omega t))$ and $t_c(t) = |E_0|(1 + \cos(\omega t))/2$ at $\omega t \in [2\pi, 3\pi]$. Clearly, the charge transfer displays the same behavior as we manipulate each step individually in the main text. In the case of $a = 1$, which means E_d is tuned exactly to zero energy after the first step, as shown by the dashed line in Fig. S3b, the system would have no definitive way to evolve in the following step. As we increase t_c to $t_c \gg E_d \approx 0$, the system would be a superposition state of $|0_{\rm AB}0_{12}\rangle$ and $|1_{\rm AB}1_{12}\rangle$. After the couplings recover the initial values through the final step, such a nontrivial fusion process would introduce a half charge transfer, as revealed by the dashed line in Fig. S3b. A little deviation with $a = 1.05$ would result in zero charge transfer as revealed by the red dot line shown in Fig. S3b (The corresponding $E_d(t)$ is shown by the red dot line in Fig. S3d). However, if $a = 0.95$, FM's energy would change sign and the system chooses $|1_{\rm AB}1_{12}\rangle$, resulting in an integer charge transferred from FM to MZMs after one period as the black solid line in Fig. S3b shows.

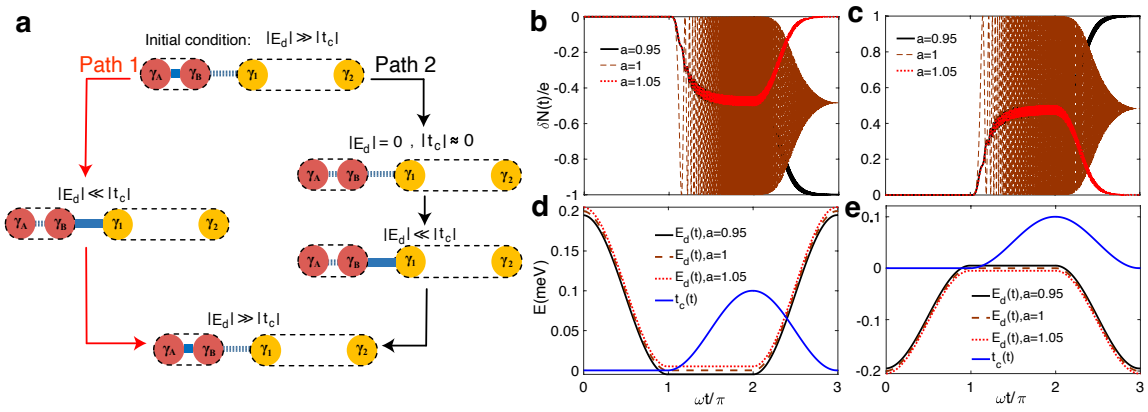

Figure S3: Reduce steps in fusion loops and charge transfer. Since the the charge pumping determined by the number of intersection at zero energy, then some fusion and splitting steps can be adjust at the same time. **a** Path 1 is the trivial fusion loop with only two steps and Path 2 is the non-trivial fusion loop with three steps. For Path 2, we set the parameters as $E_d(t) = E_0(a + \cos(\omega t))$ for $\omega t \in [0, \pi]$, and then $t_c(t) = |E_0|(1 + \cos(\omega t))/2$ for $\omega t \in [\pi, 2\pi]$, and finally $E_d(t) = E_0(a - \cos(\omega t))$ and $t_c(t) = |E_0|(1 + \cos(\omega t))/2$ for $\omega t \in [2\pi, 3\pi]$. **b** Charge transfer at $a = 1.05$, 1, and 0.95 with $E_0 = 0.1\,\mathrm{eV}$. Since the charge choose different fusion channel for $a > 1$ and $a < 1$, the final charge transfer is different (zero for $a > 1$ and one for $a < 1$. **c** The charge transfer for $E_0 = -0.1\,\mathrm{eV}$. The current following direction is reverse. **d** and **e** The correspond manipulation of E_d and t_c in **b** and **c**, respectively.

The charge transfer would be more stable with time increase. As further revealed in Fig. S4b, for an initial state $|0_{\mathrm{AB}}0_{12}\rangle$, E_d would cross zero for $a < 1$ after the first step, then the states would transfer to $|1_{\mathrm{AB}}1_{12}\rangle$ state, which would cause an integer charge pumping from MZM to FM. If $a > 1$, E_d would remain above zero energy all the time, then the states would transfer back to $|0_{\mathrm{AB}}0_{12}\rangle$, with no net charge transfer in the end. We also investigate the charge transfer process for different period $T = 10^4(\mathrm{eV})^{-1}$, $T = 0.5 * 10^4(\mathrm{eV})^{-1}$, $T = 10^3(\mathrm{eV})^{-1}$ with $\omega T = \pi$. We can see that the charge pumping δN_F after the manipulation is definite with a slow oscillation period. Since we should keep t_c at zero in the first step as E_d varies, we further study the case for $t_c \neq 0$. We investigate the parameters as $E_d(t) = E_0(a + \cos(\omega t))$ and $t_c(t) = |E_0|(1 - \cos(\phi_0))/2$ for $\omega t \in [0, \pi]$, and then $t_c(t) = |E_0|(1 - \cos(\omega t + \phi_0))/2$ for $\omega t \in [\pi, 2\pi]$, and finally $E_d(t) = E_0(a - \cos(\omega t))$ and $t_c(t) = |E_0|(1 + \cos(\omega t + \phi_0))/2$ for $\omega t \in [2\pi, 3\pi]$. It is the same as the parameters of Fig. 4 in the main text except that there's an initial deviation ϕ_0 in t_c. we show the final charge transfer versus period T at $a = 0.9$.

We find that the nontrivial charge transfer can still be distinguished even for $\phi_0 = 0.05\pi$ for $T \in [10^3, 10^4](\text{eV})^{-1}$. This suggests that the nontrivial pumping is to be observed when the time period $T \ll 1/\min(t_c)$, where $\min(t_c)$ represents the minimum value of t_c during the fusion loop. Moreover, adiabatic evolution further requires $T \gg 1/\Delta$. As a result, the time window for the nontrivial pumping is $1/\Delta \ll T \ll 1/\min(t_c)$.

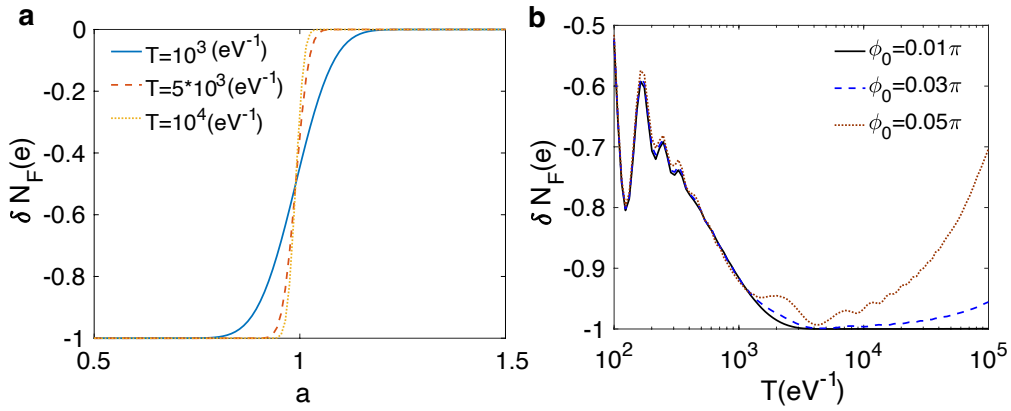

Figure S4: Time scale. a The charge transfer is distinct for $a > 1$ and $a < 1$ with different time period. There's an integer charge transfer if $a < 1$, and no charge transfer if $a > 1$. Since such process is an adiabatic process, the transition region would become more and more steep with time increase. **b** The influence of final charge transfer in the case of $t_c \neq 0$. We set $t_c(t) = |E_0|(1 - \cos(\phi_0))/2$ in the initial time. This means $t_c \neq 0$ for $\phi_0 \neq 0$, It would gradually destroy nontrivial charge transfer process but still sustains in a finite time window.

3 Exact solution of FM-MZM hybrid system

In the main text, we have shown a simple criterion for nontrivial charge pumping: if $E_d(t)$ and $t_c(t)$ intersect at zero energy an odd number of times, the charge pumping becomes nontrivial, and the opposite is true for even intersections. Such rule is different from Thouless pumping. In Thouless pumping, the charge pumping is determined by the winding number encircled by the parameters. However, we can still find an exact solution for this system. We start with the Hamiltonian H_M in the representation of the Majorana operators, given by:

$$H_M = \mathrm{i}E_d\gamma_A\gamma_B + \mathrm{i}|t_c|\gamma_B\gamma_1. \tag{1}$$

In the qubit operator representation: $\sigma_z = i\gamma_A\gamma_B$ and $\sigma_x = \mathrm{i}\gamma_B\gamma_1$, and the Hamiltonian exactly describes a typical two-level system. Since σ_z and σ_x do not commute with each other, tuning E_d and t_c in different order would lead to distinct results. However, since the charge pumping is not relevant to the concrete path it experienced. The nontrivial loop can be can be homotopy to a loop with two periods: in the first period, we vary E_d from E_0 to $-E_0$ with t_c keeps zero. While in the second part, we vary $E_d = -E_0\cos(\omega t)$ and $t_c = E_0\sin(\omega t)$ from $\omega t = 0$ to $\omega t = \pi$. This is right a half circle in the parameter space. For the first part, the evolution would induce a dynamical phase $\phi = \int_0^T E_d(t)\sigma_z dt$. While for the second part, it is just a nuclear magnetic resonance system with $H_N(t) = -E_0\cos(\omega t)\sigma_z + E_0\sin(\omega t)\sigma_x$. This Hamiltonian can be exactly calculated through unitary transformation $\hat{U}(t) = \exp(-\mathrm{i}\frac{\omega t}{2}\sigma_y)$. Then the effective Hamiltonian would become time independent:

$$H_{eff} = \hat{U}(t)H_N(t)\hat{U}(t)^{-1} - \hat{U}(t)(-i\frac{\partial}{\partial t}\hat{U}(t)^{-1}) = -E_0\sigma_z - \frac{\omega}{2}\sigma_y. \tag{2}$$

Now, the time evolution operator U is easily seen to be given by:

$$U(t) = \hat{U}(t)e^{-\mathrm{i}H_{eff}t} = \exp(-\mathrm{i}\frac{\omega t}{2}\sigma_y)[\cos(\Omega t) - \mathrm{i}\sin(\Omega t)(\frac{E_0}{\Omega}\sigma_z - \frac{\omega}{2\Omega}\sigma_y)] \tag{3}$$

Here, $\Omega = \sqrt{E_0^2 + (\omega/2)^2}$. If $\omega \ll E_0$, then $\Omega \simeq E_0$ and $U(t) \simeq \exp(-\mathrm{i}\frac{\omega t}{2}\sigma_y)\exp(\mathrm{i}E_0 t\sigma_z)$. In this situation, the states would be slowly rotated with frequency $\omega/2$. Then the state would change from $|0_{\mathrm{AB}}0_{12}\rangle$ to $|1_{\mathrm{AB}}1_{12}\rangle$ after the loop finished.

4 The Hamiltonian and parameters for tight-binding model

The tight binding Hamiltonian of the NS system is given by

$$\begin{aligned} H_{NS} &= \sum\nolimits_{\mathbf{R},\mathbf{d},\alpha} -t_0(\psi^\dagger_{\mathbf{R}+\mathbf{d},\alpha}\psi_{\mathbf{R},\alpha} + h.c.) - \mu\psi^\dagger_{\mathbf{R},\alpha}\psi_{\mathbf{R},\alpha} \\ &+ \sum\nolimits_{\mathbf{R},\mathbf{d},\alpha,\beta} -\mathrm{i}U_R\psi^\dagger_{\mathbf{R}+\mathbf{d},\alpha}\hat{z}\cdot(\vec{\sigma}\times\mathbf{d})_{\alpha\beta}\psi_{\mathbf{R},\beta} \\ &+ \sum\nolimits_{\mathbf{R},\alpha} \Delta(R)e^{\mathrm{i}\phi}\psi^\dagger_{\mathbf{R},\alpha}\psi^\dagger_{\mathbf{R},-\alpha} + h.c. \\ &+ \sum\nolimits_{\mathbf{R},\alpha,\beta} \psi^\dagger_{\mathbf{R},\alpha}(V_x\vec{\sigma}_x)_{\alpha\beta}\psi_{\mathbf{R},\beta}. \end{aligned} \tag{4}$$

Here, the subscript $\mathbf{R}$ denotes the lattice site; $\mathbf{d}$ is the unit vector and $\mathbf{d}_x$ connects the nearest neighbor sites along x- direction; α and β are the spin indices; t_0 denotes the hopping amplitude; μ is the chemical potential; U_R is the Rashba coupling strength; and V_x is the Zeeman energy. The superconducting pairing amplitude is denoted as Δ, and ϕ is the pairing phase. In the numerical simulations, the effective mass $m^* = 0.026m_e$, the Rashba spin-orbit coupling strength $\alpha = 30\,\mathrm{meV}\cdot\mathrm{nm}$, the superconducting pairing strength $\Delta = 0.25\,\mathrm{meV}$, the g factor $g = 15$, the length of nanowire is $N_x = 120a$ with he lattice constant $a = 20\,\mathrm{nm}$, The quantum dot which connects with the nanowire is described by

$$H_d = \sum\nolimits_\alpha 2E_d d^\dagger_\alpha d_\alpha + \sum\nolimits_{\alpha,\beta} d^\dagger_\alpha(V_x\vec{\sigma}_x)_{\alpha\beta}d_\beta, \tag{5}$$

where E_d represents the on-site energy of the QD and d_α is the fermionic annihilation operator with spin α. The coupling between the nanowire and the QD is described by the hopping term

$$H_{Sd} = \sum\nolimits_\alpha t_{cN}\psi^\dagger_{1,N_x,\alpha}d_\alpha + h.c., \tag{6}$$

where t_{cN} is the coupling strength between QD and nanowire.

In experiment, the trivial Andreev bound states (ABSs) could appear at zero energy and

blend with MZMs. It is necessary to investigate the fusion rule of trivial ABSs. Such ABS is usually induced by a hard-wall confined potential at the interface, which can be modeled by a square quantum well confinement at the end of the nanowire [1–3]. We simulate the square quantum well by setting $\mu(R) = -2t$, $\Delta(R) = 0$ for $\mathbf{R} < 20a$ and $\mu(R) = -2t + 0.45\,\mathrm{meV}$, $\Delta(R) = \Delta$ for $\mathbf{R} > 20a$. When an external magnetic field V_{x1} and a smooth confinement are applied in the nanowire, as shown in Fig. 4b of the main text, ABS will be trapped in the confinement region before the topological phase transition occurs ($0.2\,\mathrm{meV} < V_{x1} < 0.45\,\mathrm{meV}$). In contrast to the MZMs that distribute non-locally at both ends of the nanowire, the quasi-MZM can be viewed as two strongly overlapped MZMs γ_1 and γ_2 which are both localized inside the confinement region. To numerically simulate the fusion process in a NS wire, we follow the traditional time-evolution method of trotter decomposition [4].

References

[1] Albrecht, S. M. *et al.* Exponential protection of zero modes in Majorana islands. *nature* **531**, 206 (2016).

[2] Prada, E., San-Jose, P. & Aguado, R. Transport spectroscopy of NS nanowire junctions with Majorana fermions. *Phys. Rev. B* **86**, 180503(R)(2012).

[3] Liu, C.-X., Sau, J. D. & Das Sarma, S. Distinguishing topological Majorana bound states from trivial Andreev bound states: Proposed tests through differential tunneling conductance spectroscopy. *Phys. Rev. B* **97**, 214502 (2018).

[4] Wang, L., Troyer, M. & Dai, X. Topological charge pumping in a one-dimensional optical lattice. *Phys. Rev. Lett.* **111**, 026802 (2013).