Supplemental Material
Topological space-time crystal

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SPACE-TIME CRYSTAL IN TIGHT-BINDING MODELS

In this section, let us derive the tight-binding representation of space-time crystals, based on Wannier functions in the crystal for a set of relevant energy bands, before the space-time translation invariant traveling wave is applied. We consider an isolated group of d consecutive Bloch bands $\{\phi^j_{\boldsymbol{k}}(\boldsymbol{r}) = e^{i\boldsymbol{k}\cdot\boldsymbol{r}}u^j_{\boldsymbol{k}}(\boldsymbol{r}); j = 1, 2, \dots, d\})$ that do not become degenerate with any lower or higher band anywhere in the Brillouin zone, such as the set of occupied valence bands in insulators. Here $u^j_{\boldsymbol{k}}(\boldsymbol{r})$ is the eigenstates of the Bloch Hamiltonian $h_0(\boldsymbol{k})$ defined in the main text, and it has the translation symmetries of the crystal.

The Wannier functions are constructed such that they span the same Hilbert space as the Bloch bands $\phi^j_{\boldsymbol{k}}(\boldsymbol{r})$, with $j = 1, 2, \dots, d$. There are d Wannier functions centered at each lattice site $\boldsymbol{R}$, defined as

$$w_{j\boldsymbol{R}}(\boldsymbol{r}) = \frac{1}{\sqrt{N}}\sum_{\boldsymbol{k}} e^{-i\boldsymbol{k}\cdot\boldsymbol{R}}\tilde{\phi}^j_{\boldsymbol{k}}(\boldsymbol{r}), \tag{S1}$$

where N is the number of unit cells, and $\{\tilde{\phi}^j_{\boldsymbol{k}}(\boldsymbol{r})\}$ are a set of Bloch-like functions that are smooth in $\boldsymbol{k}$ everywhere in the Brillouin zone, and they are related to the energy eigenstates via a unitary transformation as

$$\tilde{\phi}^j_{\boldsymbol{k}}(\boldsymbol{r}) = \sum_i U_{ij}(\boldsymbol{k})\phi^i_{\boldsymbol{k}}(\boldsymbol{r}). \tag{S2}$$

Consider the Hamiltonian

$$H = \xi(\hat{\boldsymbol{p}}) + V_0(\boldsymbol{r}) + \sum_{n\neq 0} e^{in(\delta\boldsymbol{k}\cdot\boldsymbol{r}-\Omega t)}V_n(\boldsymbol{r}), \tag{S3}$$

where the time-independent Hamiltonian $H_0 = \xi(\hat{\boldsymbol{p}}) + V_0(\boldsymbol{r})$ has eigenstates $\phi^j_{\boldsymbol{k}}(\boldsymbol{r})$, which are used to construct the Wannier functions. The Hamiltonian matrix elements in terms of Wannier functions can be written as

$$\langle w_{i\boldsymbol{R}'}|\, H\, |w_{j\boldsymbol{R}}\rangle = \langle w_{i\boldsymbol{R}'}|\, H_0\, |w_{j\boldsymbol{R}}\rangle + \sum_{n\neq 0}\langle w_{i\boldsymbol{R}'}|\, e^{in(\delta\boldsymbol{k}\cdot\boldsymbol{r}-\Omega t)}V_n(\boldsymbol{r})\, |w_{j\boldsymbol{R}}\rangle, \tag{S4}$$

where the first term $[\tilde{h}^0(\boldsymbol{R}'-\boldsymbol{R})]_{ij} \equiv \langle w_{i\boldsymbol{R}'}|\, H_0\, |w_{j\boldsymbol{R}}\rangle$ corresponds to the static hopping/onsite terms in the tight-binding description of the crystal. Inside the summation of the second term, we have

$$\begin{aligned}
\langle w_{i\boldsymbol{R}'}|\, e^{in(\delta\boldsymbol{k}\cdot\boldsymbol{r}-\Omega t)}V_n(\boldsymbol{r})\, |w_{j\boldsymbol{R}}\rangle &= \int d\boldsymbol{r}\, w^*_{i\boldsymbol{R}'}(\boldsymbol{r})e^{in(\delta\boldsymbol{k}\cdot\boldsymbol{r}-\Omega t)}V_n(\boldsymbol{r})w_{j\boldsymbol{R}}(\boldsymbol{r}) \\
&= \int d\boldsymbol{r}\, e^{in(\delta\boldsymbol{k}\cdot\boldsymbol{r}-\Omega t)}w^*_{i,\boldsymbol{0}}(\boldsymbol{r}-\boldsymbol{R}')V_n(\boldsymbol{r})w_{j,\boldsymbol{0}}(\boldsymbol{r}-\boldsymbol{R}) \\
&= e^{in(\delta\boldsymbol{k}\cdot\boldsymbol{R}'-\Omega t)}\int d\boldsymbol{r}\, w^*_{i,\boldsymbol{0}}(\boldsymbol{r})V_n(\boldsymbol{r})w_{j,\boldsymbol{0}}(\boldsymbol{r}+\boldsymbol{R}'-\boldsymbol{R})e^{in\delta\boldsymbol{k}\cdot\boldsymbol{r}},
\end{aligned} \tag{S5}$$

where we have used the fact that the Wannier functions $w_{i,\boldsymbol{R}}(\boldsymbol{r}) = w_{i,\boldsymbol{0}}(\boldsymbol{r}-\boldsymbol{R})$, and $V_n(\boldsymbol{r}) = V_n(\boldsymbol{r}+\boldsymbol{R})$. If we define

$$[\tilde{h}^n(\boldsymbol{R}'-\boldsymbol{R})]_{ij} = \int d\boldsymbol{r}\, w^*_{i,\boldsymbol{0}}(\boldsymbol{r})V_n(\boldsymbol{r})w_{j,\boldsymbol{0}}(\boldsymbol{r}+\boldsymbol{R}'-\boldsymbol{R})e^{in\delta\boldsymbol{k}\cdot\boldsymbol{r}}, \tag{S6}$$

then we obtain Eq. (6) in the main text.

We can introduce the annhilation operator $\psi_{j,\boldsymbol{R}}$ for the jth Wannier function at site $\boldsymbol{R}$, and group $\{\psi_{j,\boldsymbol{R}}\}$ for $j = 1, 2, \dots, d$ into a column vector as $\boldsymbol{\psi}_{\boldsymbol{R}}$, and introduce $\boldsymbol{\psi}^\dagger_{\boldsymbol{R}}$ as the corresponding creation operators (in row vectors). Thus, we obtained a space-time crystal described by the following tight-binding Hamiltonian

$$H = \sum_{\boldsymbol{R}',\boldsymbol{R}} \boldsymbol{\psi}^\dagger_{\boldsymbol{R}'} \left[\tilde{h}^0(\boldsymbol{R}'-\boldsymbol{R}) + \sum_{n\neq 0} e^{in(\delta\boldsymbol{k}\cdot\boldsymbol{R}'-\Omega t)} \tilde{h}^n(\boldsymbol{R}'-\boldsymbol{R}) \right] \boldsymbol{\psi}_{\boldsymbol{R}}. \tag{S7}$$

For periodic boundary condition, we can write $\boldsymbol{\psi}_{\boldsymbol{R}} = 1/\sqrt{N}\sum_{\boldsymbol{k}} e^{i\boldsymbol{k}\cdot\boldsymbol{R}}\boldsymbol{a}_{\boldsymbol{k}}$ and $\tilde{h}^n(\boldsymbol{R}) = 1/N\sum_{\boldsymbol{q}} e^{i\boldsymbol{q}\cdot\boldsymbol{R}} h_n(\boldsymbol{q})$, then we have

$$H = \sum_{\boldsymbol{k}} \left[\boldsymbol{a}^\dagger_{\boldsymbol{k}} h_0(\boldsymbol{k})\boldsymbol{a}_{\boldsymbol{k}} + \sum_{n\neq 0} \boldsymbol{a}^\dagger_{\boldsymbol{k}+n\delta\boldsymbol{k}} h_n(\boldsymbol{k})\boldsymbol{a}_{\boldsymbol{k}} e^{-in\Omega t} \right]. \tag{S8}$$

The operator $K(t) = H(t) - i\partial_t$ can be Block diagonalized if we introduce $\boldsymbol{A}_{\boldsymbol{k}}(t) = (\dots, e^{i\Omega t}\boldsymbol{a}^T_{\boldsymbol{k}-\delta\boldsymbol{k}}, \boldsymbol{a}^T_{\boldsymbol{k}}, e^{-i\Omega t}\boldsymbol{a}^T_{\boldsymbol{k}+\delta\boldsymbol{k}}, \dots)^T$. This leads to

$$K(t) = \sum_{\boldsymbol{k}} \boldsymbol{A}^\dagger_{\boldsymbol{k}}(t) \left[\mathscr{H}(\delta\boldsymbol{k},\boldsymbol{k}) - i\partial_t \right] \boldsymbol{A}_{\boldsymbol{k}}(t), \tag{S9}$$

where we obtain the effective enlarged *time-independent* Hamiltonian $\mathscr{H}(\boldsymbol{k})$, which we have derived using the Bloch functions in the main text.

Particle-hole symmetries in $\mathscr{H}(k)$

In the main text, we have shown that the effective Hamiltonian $\mathscr{H}_{\rm eff}(k)$ for the 1D model proposed in class D has a particle-hole symmetry realized via $\rho_x \mathscr{H}_{\rm eff}(k)\rho_x = -\mathscr{H}_{\rm eff}(\pi - \delta k - k)^*$. Here, we generalize this result by showing that any truncation of the frequency-domain-enlarged Hamiltonian $\mathscr{H}(k)$ has a particle-hole symmetry with respect to the energy, say $-\Omega/2$, as long as the truncation is symmetric about this energy.

To make a truncation symmetric around $-\Omega/2$, we write

$$\mathscr{H}(k) \simeq \mathscr{H}_N(k) - \mathbb{I}\Omega/2 \tag{S10}$$

where the $2N$-by-$2N$ matrix

$$\mathscr{H}_N(k) = \begin{pmatrix} h_0(k-(N-1)\delta k) + (N-\frac{1}{2})\Omega & h_1^\dagger(k-(N-1)\delta k) & & \\ h_1(k-(N-1)\delta k) & \ddots & \ddots & \\ & \ddots & \ddots & h_1^\dagger(k+(N-1)\delta k) \\ & & h_1(k+(N-1)\delta k) & h_0(k+N\delta k) - (N-\frac{1}{2})\Omega \end{pmatrix} \tag{S11}$$

and $\mathbb{I}$ is the identity matrix of the same size of $\mathscr{H}_N(k)$. For $h_0(k) = -2w\cos(ka)$ and $h_1(k) = \Delta\cos(ka + \delta ka/2)$, one can easily verify that $\mathscr{H}_N(k)$ has a particle-hole symmetry realized via $X_N\mathscr{H}_N(k)X_N = -\mathscr{H}_N(\pi - \delta k - k)^*$, with the $2N$ by $2N$ matrix

$$X_N = \begin{pmatrix} & & 1 \\ & \iddots & \\ 1 & & \end{pmatrix}. \tag{S12}$$

SIGNATURE OF TOPOLOGICAL EDGE STATES IN TUNNELING CONDUCTANCE

In this section, we will show that the topologically protected edge modes in space-time crystals can be probed by measuring tunneling conductance, via either a scan tunneling microscope (STM) tip or a lead in a quantum transport setup. The existence of edge quasienergy eigenstates will produce a nonzero conductance [1] between the edge of the space-time crystal, and the STM tip (or lead).

In the following, for concreteness, let us focus on the STM-type setup. Let us consider a (movable) tip is tunnel-coupled to the sample (the space-time crystal) at a location $\boldsymbol{r}$. The sample is further weakly connected to a bath, which may locate beneath a layer of insulating substrate. Let us denote the tunneling rate between the sample and the tip (bath) as γ_T (Γ_B). It has been shown in Ref. [1] that in the tunneling regime when $\Gamma_T \ll \Gamma_B \ll$ the band width of the space-time crystal, the DC conductance at bias voltage V can be written as

$$G(V) \propto \frac{e^2\Gamma_T}{h}\mathrm{Im}[G_0^r(eV)]_{\boldsymbol{r},\boldsymbol{r}}, \tag{S13}$$

where $G_n^r(\omega)$ is the sample's Floquet retarded Green function evaluated at spatial point $\boldsymbol{r}$, defined as

$$G_n^r(\omega) = \frac{1}{T}\int_0^T dt \int_{-\infty}^{\infty} d\tau e^{in\Omega t} e^{i\omega\tau} G^r(t, t-\tau), \tag{S14}$$

with the retarded Green function written in terms of fermion creation and annihilation operators

$$[G^r(t,t')]_{\boldsymbol{r},\boldsymbol{r}'} = -i\theta(t-t')\left\langle \{\psi_{\boldsymbol{r}}(t), \psi^\dagger_{\boldsymbol{r}'}(t')\}\right\rangle. \tag{S15}$$

The $G_0^r(\omega)$ can be computed from,

$$G_0^r(\omega) = \sum_n \frac{\left|\phi_n^{(0)}(\boldsymbol{r})\right|^2}{\omega - \epsilon_n + i\gamma_B}, \tag{S16}$$

where ε_n is quasienergy obtained by solving the eigenvalue problem for the enlarged Hamiltonian (written in coordinate space),

$$\begin{pmatrix} \ddots & \ddots & & & \\ \ddots & h_0+\Omega & h_1^\dagger & \ddots & \\ & h_1 & h_0 & h_1^\dagger & \ddots \\ & \ddots & h_1 & h_0-\Omega & \\ & & & \ddots & \ddots \end{pmatrix} \begin{pmatrix} \vdots \\ \phi_n^{(-1)} \\ \phi_n^{(0)} \\ \phi_n^{(1)} \\ \vdots \end{pmatrix} = \epsilon_n \begin{pmatrix} \vdots \\ \phi_n^{(-1)} \\ \phi_n^{(0)} \\ \phi_n^{(1)} \\ \vdots \end{pmatrix}. \tag{S17}$$

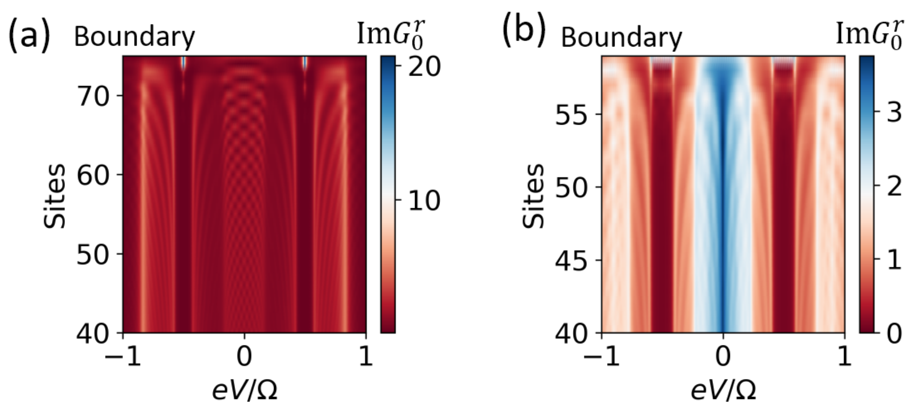

FIG. S1. (a). Imaginary part of G_0^r (in arbitrary unit) as a function of energy eV at different spatial locations, in the 1D model of class D. We took the same parameters that generate Fig. 2(b) of the main text. (b) Same for the 2D model of class A, where we assume periodic boundary condition along x and the vertical axis denotes the position along y direction, at a fixed x. We took the same parameters that generate Fig. 3 of the main text. Additionally, we took $\gamma_B/\Omega = 10^{-2}$.

In Fig. S1, we show the imaginary part of G_0^r as a function of energy, or bias voltage eV, at different spatial locations of the sample, for both the 1D model of class D and the 2D model of class A introduced in the main text. It can be seen that the appearance of the quasienergy edge modes can be seen as nonzero conductance measured via tunneling into the boundary of the sample (top of the figures), whereas the conductance drops to zero if the tunneling is inside the bulk (bottom of the figures).

STABILITY OF 2D CLASS A SPACE-TIME CRYSTAL

Like the topological edge modes in a strong topological insulator, spatial disorder that weakly breaks the space-time translation symmetry cannot distroy the edge modes in space-time crystals, as long as the disorder does not break the onsite AZ symmetries and the bulk gap does not close. For class A models in particular, as there are no additional AZ symmetries, the topologically protected edge modes will be very stable against an arbitrary weak perturbation.

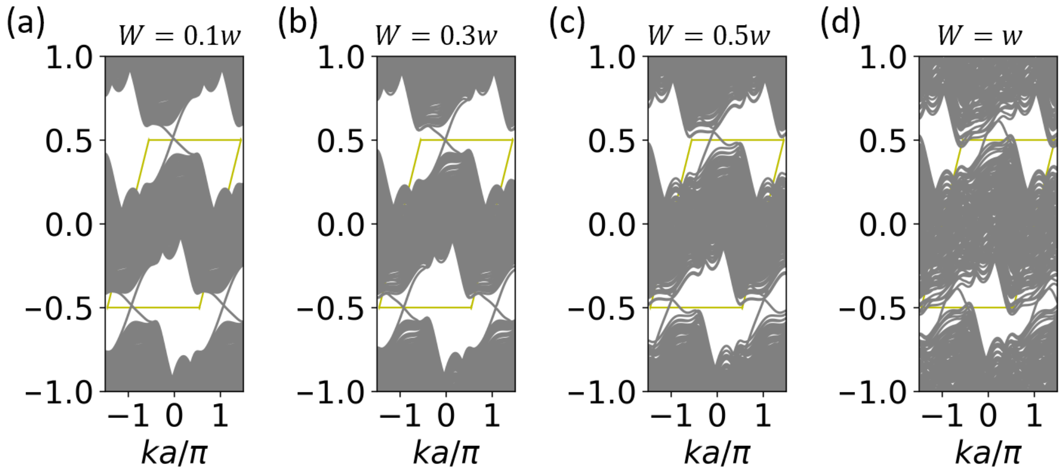

FIG. S2. One dimensional band structure for the 2D model when periodic boundary condition is assumed only along x, with the same parameters that generate the Fig. 3 (b) of the main text. In addition, we add onsite random potentials of strength (a) $W = 0.1w$, (b) $W = 0.3w$, (c) $W = 0.5w$, (d) $W = w$.

To illustrate this, let us consider the 2D model introduced in the main text. For simplicity, let us take the periodic boundary condition along x and add to Eq. (10) of the main text an independently identically distributed (i.i.d.) onsite random potential along the y direction, drawn from uniformly from the interval $[-W, W]$. In Fig. S2, we plot the 1D band structure along k_x with different disorder strength W, with other parameters same as the ones for Fig. 3(b) in the main text. It can be seen that the topologically protected edge modes are stable up to disorder strength $W \simeq 0.5w$, where w is the static nearest neighbor hopping strength. Note that for class A model the gapless edge may not cross at energy $\Omega/2$, in contrast to systems with particle-hole or chiral symmetries.

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[1] B. M. Fregoso, J. P. Dahlhaus, and J. E. Moore, Dynamics of tunneling into nonequilibrium edge states, Phys. Rev. B **90**, 155127 (2014).