Exotic quantum light-matter interactions in bilayer square lattices

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We investigate quantum emitters (QEs) interacting with a photonic structured bath made of bilayer square lattices, where the resonance anticrossing between the energy bands opens a symmetric middle energy gap. Due to the intrinsic chiral symmetry of the bath and interactions with the squarelike band edges, the QE-photon dressed states generated in this inner band gap are odd neighbor, robust, and anisotropic, when the emitters' transition frequencies lie in the middle of the band gap. We also use giant artificial atoms to engineer and modify the dressed states' patterns. Exotic bound states can lead to spin models with symmetry protection, resulting in fascinating many-body phases. As an example, we show that this proposal can be used to generate both edge states and corner states in the generalized two-dimensional Su-Schrieffer-Heeger model. This work opens up different avenues for research into innovative quantum many-body physics and quantum simulations with photonic or phononic multilayer structures.

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I. INTRODUCTION

Bilayer two-dimensional (2D) materials offer a flexible platform for studying strongly correlated electron movements near electronic flat bands in moiré superlattices [1–4]. A rapidly emerging field is to examine the optical and acoustic analogs of bilayer 2D materials [5–12]. In this field, numerous theoretical works have predicted the localization and condensation of light in bilayer photonic crystals [10,13,14]. The photonic counterparts have a distinct advantage in terms of flexibility, which includes the ability to construct a variety of lattice shapes and tune the coupling strength between layers via interlayer separation or other methods [8,10,15]. Beyond fundamental research focused on photonics, it is also very appealing to investigate light-matter interactions with quantum emitters (QEs) in photonic layered structures [12,16,17].

Long-range tunable coherent dipole interactions, on the other hand, mediated by bound states (BSs) produced within the band gap of structured photonic baths, have attracted considerable interest due to their possible applications in quantum simulations [18–23]. Floquet engineering spin-spin interactions by periodic driving [24,25], tailoring the geometry of photonic interfaces [26–30], and exploiting giant atoms with nonlocal coupling to several positions of the bath [31–38] are some of the approaches proposed to develop more innovative spin models. Remarkably, QEs interacting with topological photonic lattices produce exotic BSs that can be chiral, resilient, and exhibit power-law scaling [39–49]. However,

previous works mostly focus on single-layer 2D or multilayer 3D photonic structures; in stark contrast, photonic bilayer structures possess very distinct band shapes and new features that have yet to be explored for light-matter interactions.

In this paper, we predict another type of QE-photon dressed states and coherent interactions between QEs in photonic bilayer square lattices. By taking advantage of only band crossing in a bilayer structure, we can open a middle energy gap around 2D van Hove singularities without breaking the chiral symmetry of the lattices. The intrinsic chiral symmetry of the bath together with the square geometries of the band edges give rise to the emergence of odd-neighbor (the photon profile vanishes to the even-neighbor sites of the QE), robust, and anisotropic BSs when tuning the QE's frequency to the van Hove points of the bare bands. We also use giant atoms in 2D to consider quasi-1D patterns and purify the anisotropy of the odd-neighbor BSs, which cannot be implemented by pointlike emitters. These BSs can mediate chiral symmetric and anisotropic spin-spin interactions, which have wide applications ranging from robust entanglement distributions to the simulation of nontrivial spin models. Through a specific spin array arrangement, we can simulate a generalized 2D Su-Schrieffer-Heeger (SSH) model that can support both edge modes and corner-localized modes.

II. MODEL AND HAMILTONIAN

As illustrated in Fig. 1(a), we consider a photonic doublelayer structure, where J and ηJ respectively describe the hopping amplitudes between the nearest-neighbor lattices in the top and bottom layers, and G denotes the interlayer

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FIG. 1. (a) Schematics of emitters in bilayer square lattices. The yellow and green disks represent lattice sites consisting of bosonic modes. Here, J and ηJ denote the intracouplings and G is the intercoupling strength. Emitters are coupled to the lattice sites with the interaction strength g. (b) Corresponding energy band structure of the bath shown in (a), with the middle band gap $\varepsilon_{gap} = 2G$. Here, $\eta = -1$ and G = J/4.

coupling strength. Here, we mainly focus on the parameter regime $\eta < 0$. In this regime, we are particularly interested in the $\eta = -1$ case (without loss of generality) and this bosonic Hamiltonian with antisymmetric coupling corresponds to an antiferromagnetic coupling, which is given by ($\hbar = 1$)

$$\hat{H}_{B} = J \sum_{\langle n,m \rangle} \left(\hat{a}_{1m}^{\dagger} \hat{a}_{1n} - \hat{a}_{2m}^{\dagger} \hat{a}_{2n} \right) + G \sum_{n} \hat{a}_{1n}^{\dagger} \hat{a}_{2n} + \text{H.c.}, \quad (1)$$

where \hat{a}_{1n} and \hat{a}_{2n} are the annihilation operators of bosonic modes at the position $\mathbf{n} = (n_x, n_y)$ in layer 1 and layer 2, respectively. Here, we write the bath Hamiltonian in a frame rotating at the frequency $\omega_1 = \omega_2$, with $\omega_{1,2}$ being the cavity's resonance frequency in the two arrays. We also ignore polarization and consider the case for photon fields with a particular polarization (we assume that the E-field vector in a direction perpendicular to the x-y plane). Note that this bath is equal to the one with $\eta = +1$ and alternating phases $(-1)^{n_x+n_y}$ in the interlayer couplings [50], where a photon with momentum k in the top layer is coupled to a photon with momentum $k - (\pi, \pi)$ in the bottom layer. One can easily check that the energy band with such a momentum shift is the same as the one with negative hopping rates. In fact, both of them correspond to the introduction of a uniform effective flux of π in each plaquette { $\hat{a}_{1n}, \hat{a}_{2n}, \hat{a}_{1n_p}, \hat{a}_{2n_p}$ }, with $\boldsymbol{n}_p - \boldsymbol{n} = (0, \pm 1)$ or $(\pm 1, 0)$. We next transform the Hamiltonian into k space by introducing the Fourier transformation $\hat{a}_k = 1/\sqrt{N} \sum_n e^{-ik \cdot n} \hat{a}_n$, with k being the wave vector (for convenience, we assign the lattice constant $d_0 = 1$ here). In terms of $\hat{V}_{k}^{\dagger} = (\hat{a}_{1k}^{\dagger}, \hat{a}_{2k}^{\dagger})$, the bath Hamiltonian in momentum space can be written as $\hat{H}_B = \sum_k \hat{V}_k^{\dagger} \hat{H}(k) \hat{V}_k$, with the kernel

$$\hat{H}(\boldsymbol{k}) = \begin{pmatrix} f(\boldsymbol{k}) & G\\ G & -f(\boldsymbol{k}) \end{pmatrix},$$
(2)

where the function $f(\mathbf{k}) = 2J(\cos k_x + \cos k_y)$ is the dispersion of a monolayer square lattice. After diagonalization and in terms of eigenoperators $\{\hat{u}_k, \hat{l}_k\}, \hat{H}_B = \sum_k [\omega_u(\mathbf{k})\hat{u}_k^{\dagger}\hat{u}_k + \omega_l(\mathbf{k})\hat{l}_k^{\dagger}\hat{l}_k]$, with the dispersion of hybrid energy bands

$$\omega_{u,l}(\boldsymbol{k}) = \pm \sqrt{f^2(\boldsymbol{k}) + G^2}.$$
(3)

The relation between the $\{\hat{a}_{1k}, \hat{a}_{2k}\}$ and polariton operators $\{\hat{u}_k, \hat{l}_k\}$ is given by

$$\begin{pmatrix} \hat{u}_k \\ \hat{l}_k \end{pmatrix} = \begin{pmatrix} -\sin\theta_k & \cos\theta_k \\ \cos\theta_k & \sin\theta_k \end{pmatrix} \begin{pmatrix} \hat{a}_{1k} \\ \hat{a}_{2k} \end{pmatrix}, \tag{4}$$

with $\sin \theta_k = G/\sqrt{G^2 + [\omega_l(k) + f(k)]^2}$ and $\cos \theta_k = G/\sqrt{G^2 + [\omega_u(k) + f(k)]^2}$. Because of the chiral symmetry protection, the bands are obviously symmetric about zero energy $[\hat{\sigma}_y \hat{H}(k) \hat{\sigma}_y = -\hat{H}(k)]$ and a middle band gap is opened with size $\varepsilon_{gap} = 2G$. When $\eta \neq -1$, the bath is still bipartite (if looking at a suitably enlarged unit cell), and the eigenvalues are in pairs $\omega_u(k) = -\omega_l(k + \Pi)$, with $\Pi = (\pi, \pi)$. The origin of this gap is the resonance anticrossing between the bare energy bands (G = 0) at the van Hove singularities. The dispersion of hybridized energy bands is shown in Fig. 1(b). In particular, the shape of the middle band edges ($\pm G$) is squarelike, where f(k) = 0.

In this paper, we focus on the QE-photon interactions within the middle band gap. We consider one (or several) twolevel systems { $|e\rangle$, $|g\rangle$ } as the QEs which are locally coupled to a single polarization of light of the bath at one or more sites, with transition frequency ω_e . Other polarized light is decoupled from the systems. The free Hamiltonian of these QEs reads $\hat{H}_S = \Delta/2 \sum_j \hat{\sigma}_z^j$, with detuning $\Delta = \omega_e - \omega_1$ and spin operators { $\hat{\sigma}_z$, $\hat{\sigma}^{\dagger}$, $\hat{\sigma}$ }. The QE-bath interaction of a single giant atom (the *j*th spin) can be described as

$$\hat{H}_{\text{int}}^{j} = \hat{\sigma}_{j}^{\dagger} \left(\sum_{\alpha=1}^{N_{p}} g_{\boldsymbol{n}_{\alpha}} \hat{a}_{1\boldsymbol{n}_{\alpha}} + \sum_{\beta=1}^{N_{q}} g_{\boldsymbol{n}_{\beta}} \hat{a}_{2\boldsymbol{n}_{\beta}} \right) + \text{H.c.}, \qquad (5)$$

where $g_{n_{\alpha,\beta}}$ is the QE-bath coupling strength at certain coupling points, and N_p (N_q) is the number of coupling points in the top (bottom) layer. When choosing { N_p , N_q } = {1, 0} or {0, 1}, the interaction recovers the result of a small atom. This QE-bath interaction Hamiltonian can be transformed into k space,

$$\hat{H}_{\text{int}}^{j} = \frac{1}{\sqrt{N}} \hat{\sigma}_{j}^{\dagger} \sum_{k} \left[\sum_{\alpha=1}^{N_{p}} g_{n_{\alpha}} e^{ik \cdot n_{\alpha}} (-\sin\theta_{k} \hat{u}_{k} + \cos\theta_{k} \hat{l}_{k}) + \sum_{\beta=1}^{N_{q}} g_{n_{\beta}} e^{ik \cdot n_{\beta}} (\cos\theta_{k} \hat{u}_{k} + \sin\theta_{k} \hat{l}_{k}) \right] + \text{H.c.} \quad (6)$$

Thus, the Hamiltonian of the whole system can be written as $\hat{H} = \hat{H}_B + \hat{H}_S + \sum_i \hat{H}_{int}^j$.

III. IMPLEMENTATIONS

Before proceeding, we make a simple discussion about possible physical implementations for examining the singleparticle physics of our Hamiltonian model, in which particle statistics plays a negligible role. As we ignore the polarization degree of freedom, the double-layer square lattices (i.e., the bath Hamiltonian) can be realized in various platforms, such as cold atoms in optical lattices [51,52] and optomechanical systems [53,54]. The two-level emitters (small atoms) can be deeply trapped atom internal states [55–57] and color centers [58–61], respectively. Taking cold atom realizations as an example, we may consider alkaline-earthmetal atoms with different internal states trapped by optical potentials [62], which mimic the bilayer square lattices and the QE behavior. The bath Hamiltonian can be obtained and controlled using laser-assisted tunneling [63–67], while an empty bath corresponds to the Fermi level $E_F = \min[\omega_k]$. For typical temperatures T of a few 100 nK and hopping rates $J/2\pi \sim \text{kHz}$ [64,68], the initial mean thermal excitation number obeying Fermi-Dirac distribution is about $\langle \hat{a}_{k}^{\dagger} \hat{a}_{k} \rangle = (1 + 1)^{2}$ $e^{\hbar(\omega_k - E_F)/k_BT})^{-1} \sim 0.1$ for modes near the van Hove singularities. Lower-temperature fulfilling $k_B T \ll \hbar G$ is preferable. Moreover, matter-wave waveguide QED setups have already been reported in experiments [69,70]. Therefore, we can restrict ourselves to the ideal case of T = 0 in the following sections. As for the impurities, a theoretical proposal for engineering giant atoms in 2D dynamical state-dependent optical lattices has recently been put forward [33].

IV. BOUND STATES WITH SMALL ATOMS

In this work, we are particularly interested in the BS produced in the inner band gap of manufactured bilayer structures. We first consider a small atom coupled to the site $\mathbf{n}_0 = (0, 0)$ in the top layer, with the Hamiltonian $\hat{H}_{sys} = \Delta/2\hat{\sigma}_z + g(\hat{a}_{1n_0}\hat{\sigma}^{\dagger} + \text{H.c.})$. Then we can calculate the eigenvalue and the wave function by solving the stationary Schrödinger equation $(\hat{H}_B + \hat{H}_{sys})|\psi\rangle = E_{\text{BS}}|\psi\rangle$ in momentum space, with a general one-particle state

$$|\psi\rangle = \left(C_e \hat{\sigma}^{\dagger} + 1/\sqrt{N} \sum_{k} \sum_{\beta=a_1, a_2} C_{k,\beta} \beta_k^{\dagger}\right) |g\rangle |0\rangle.$$
(7)

Here, $|0\rangle$ represents the ground state of the bath, and the coefficients C_e , $C_{k,a_1} = -gC_ef(\mathbf{k})/\omega^2(\mathbf{k})$ and $C_{k,a_2} = [G/f(\mathbf{k})]C_{k,a_1}$ are the probability amplitudes. Though the energy $E_{\rm BS} \in (-G, G)$ can be exactly solved by the pole equation $E_{\rm BS} = \Delta + \Sigma_e(E_{\rm BS})$, with self-energy Σ_e [71], $E_{\rm BS} \approx \Delta$ is a good approximation when $\{g, \Delta\} \ll G$. In particular, $E_{\rm BS} = \Delta$ when the spin is resonant with the cavity mode. Finally, we obtain the spatial distribution of the photonic part of the BS by means of the inverse Fourier transform $C_{n,a_{1(2)}} \propto \sum_n e^{i\mathbf{k}\cdot\mathbf{n}}C_{k,a_{1(2)}}$.

Different from the common BSs induced by the band edge at $\mathbf{k}_{edge} = (0, 0)$ or $\pm(\pi, \pm \pi)$ in a monolayer square lattice [20], the BS shown in parallel arrays is derived from the interactions with the band edges around $\mathbf{k}_{edge} = \pm(k_x, \pi \pm k_x)$ [see Fig. 1(b)]. Returning to real space, the superposition of exponentials resulting from interactions with the opposite side of the square band edges can provide an interference effect, which causes the wave function to be enhanced or suppressed in certain neighboring sites. The maximum interference is observed when the QE's transition frequency is at the middle of the band gap.

In Fig. 2, we plot the spatial distribution of the photonic part of the BSs, when a single small atom with frequency $\Delta = 0$ is coupled to the n = 0 site in the top layer. We list the main features of these BSs as follows: First, in the top layer, the wave function only emerges at the odd lattices, while in the bottom layer, it appears at the even lattices. We denote this exotic dressed state odd-neighbor BS because they are both



FIG. 2. Spatial distributions (a), (c) C_{n,a_1} and (b), (d) C_{n,a_2} of the odd-neighbor, robust, and anisotropic BSs with G = J/4, when the emitter with interaction strength g = 0.1J is coupled to the n = 0 site in the top layer. There are no disorders in (a), (b) and off-diagonal disorders in (c), (d).

odd-neighbor sites with regard to the site to which the QE is coupled. Second, the wave-function phases alternate with ± 1 , with the exception of the vicinity around the QE. Third, the BS has an anisotropic nature [20,33], with the wave function predominantly distributed along the $n_x \pm n_y = \pm(\mp)1$ directions in the top layer and along the $n_x \pm n_y = 0$ directions in the bottom layer, due to the squarelike dispersion of the band edges.

Another interesting feature of these odd-neighbor BSs is the robustness to off-diagonal disorders (i.e., disorders in the hopping amplitudes). To illustrate this effect, we plot odd-neighbor BSs under the off-diagonal disorders in Figs. 2(c) and 2(d), where we add random perturbations $\hat{H}_{dis} = \sum_{\langle n,m \rangle} (\varepsilon_{1n} \hat{a}_{1n}^{\dagger} \hat{a}_{1m} + \varepsilon_{2n} \hat{a}_{2n}^{\dagger} \hat{a}_{2m} + \varepsilon_{3n} \hat{a}_{1n}^{\dagger} \hat{a}_{2n} + \text{H.c.})$ to the bath Hamiltonian \hat{H}_B , with disorder strengths $\{\varepsilon_{1n}, \varepsilon_{2n}\} \in [-J/4, J/4]$ and $\varepsilon_{3n} \in [-G/4, G/4]$. With respect to the n = 0 site, we discover that there is no distribution in the evenneighbor sites, and the BSs' energy is fixed at zero.

To further understand the odd-neighbor profiles and the robustness, we turn to consider a unit cell including more sites such that the bath Hamiltonian is bipartite. When the QEs with a transition frequency $\Delta = 0$ are only coupling to the odd sites defined by sum $(n) \equiv (n_x + n_y) \in \mathbb{Z}_{odd}$, the full Hamiltonian in terms of the block matrix can be formally written as

$$\boldsymbol{H} = \begin{pmatrix} 0 & \boldsymbol{\mathcal{Q}}_{p} & \boldsymbol{g} \\ \boldsymbol{\mathcal{Q}}_{p}^{\dagger} & 0 & 0 \\ \boldsymbol{g}^{\dagger} & 0 & 0 \end{pmatrix}, \tag{8}$$

with the submatrix Q_p describing the bipartite interactions and the submatrix g being the atom-photon coupling term in the odd-site subspace. By solving $H\Psi = E\Psi$ with eigenvector $\Psi = (\Psi_{\text{odd}}^T, \Psi_{\text{even}}^T, \Psi_{\text{QE}}^T)^T$, we can find an eigenvalue E = 0with $\Psi_{\text{odd}} = 0$ for this block matrix since det(H) = 0. Obviously, E = 0 persists when only adding off-diagonal disorders dQ_p to the lattice, while $\Psi_{\text{odd}} = 0$ manifests a vanishing wave function in the odd-site subspace (i.e., odd-neighbor



FIG. 3. Wave-function distribution of the odd-neighbor BSs formed by a giant atom coupling to bilayer square arrays. (a), (b) The giant atom is coupled to two sites $n_{1,2} = (0,0)$ and (1,1) in layer 1. (c), (d) The giant atom is coupled to four sites $n = (\pm 1, \pm 1), (\pm 1, \mp 1)$ in layer 1.

property). This general conclusion can be applied to arbitrary dimensions. Indeed, this phenomenon has already been observed in the 1D and 3D chiral symmetric photonic lattices [28,40,41].

V. BOUND STATES WITH GIANT ATOMS

The pattern of the BSs can be further engineered by taking advantage of giant atoms. To protect the BSs' odd-neighbor property, the coupling sites of a single giant atom should be even neighbor. Quantum interference between nonlocal coupling points can result in the cancellation of the spatial distribution of the BSs in certain lattice sites or directions.

We first consider the case when a giant atom is coupled to two sites $n_{1,2} = (0, 0)$ and (1,1) in the top layer with identical coupling strength g. Then the QE-bath interaction Hamiltonian in k space simplifies to

$$\hat{H}_{\text{int}} = \frac{g}{\sqrt{N}} \hat{\sigma}^{\dagger} \sum_{k} [1 + e^{i(k_x + k_y)}] \times (-\sin\theta_k \hat{u}_k + \cos\theta_k \hat{l}_k) + \text{H.c.}, \qquad (9)$$

where the interference term $I(\mathbf{k}) = 1 + e^{i(k_x+k_y)}$ results in destructive interferences for band-edge modes $\mathbf{k}_{edge} = \pm (k_x, \pi - k_x)$. This is reflected in the cancellation of one branch of the anisotropic BS pattern, as shown in Figs. 3(a) and 3(b). Another example is to homogenize the anisotropy of the BS through coupling to four positions in the top layer. The four sites are $\mathbf{n} = (\pm 1, \pm 1), (\pm 1, \mp 1)$ and the interference term in \mathbf{k} space can be chosen as $I(\mathbf{k}) = 4 \sin k_x \sin k_y$. Clearly, for the band-edge modes $\mathbf{k}_{edge} = (0, \pm \pi)$ and $(\pm \pi, 0)$, this term approaches zero. As a result, the non-Markovian part in the BS stemmed from van Hove singularities is filtered, as plotted in Figs. 3(c) and 3(d).



FIG. 4. (a) Bipartite spin model with all the QEs at even lattices, that is $sum(n) \in \mathbb{Z}_{even}$. The QEs in layer 1 (blue) are only coupled to the QEs in layer 2 (red) and vice versa. (b) Spin interactions of (a) along the diagonal directions. (c) Vertical view of the configuration of a generalized 2D SSH model in the trivial phase, with QEs alternately and dimerically placed in the double layers. (d) Spin model energy spectrum of a finite system with 144 small atoms inside the 35×35 bilayer square arrays. (e), (f) One of the edge modes and corner modes extracted from the spectrum of the second-order topological insulator shown in (d). Here, we choose G = 4J and g = 0.1J.

VI. BIPARTITE SPIN MODEL

The odd-neighbor, robust, and anisotropic BSs can mediate long-range tunable, chiral symmetric, and anisotropic spin-spin interactions when involving multiple QEs. In the Markovian limit, the coherent interactions can be described as $\hat{H}_S = \sum_{i < j} (g_{ij} \hat{\sigma}_i^{\dagger} \hat{\sigma}_j + \text{H.c.})$, where the coupling strength g_{ij} vanishes for sum $(\mathbf{n}_{ij}) \in \mathbb{Z}_{\text{even}} (\mathbb{Z}_{\text{odd}})$ when two QEs are in the same (different) layer(s), with relative position $\mathbf{n}_{ij} = \mathbf{n}_j - \mathbf{n}_i$. In fact, a general analysis in Ref. [72] has shown that the emitter Hamiltonian can inherit chiral symmetry of the photonic bath in a one-emitter-per-resonator case, when setting $\Delta = 0$. A direct application of this spin model can realize high-fidelity entanglement of multiple QEs located at the odd lattices via an auxiliary one at the even lattice, where the unwanted crosstalk is reduced (see Ref. [26] and Appendix D).

A potentially interesting configuration based on parity properties is that the photonic lattice is half filled by the QEs, in which the QEs only interact if they are coupled to the lattice sites in different layers, as shown schematically in Figs. 4(a) and 4(b). The anisotropic spin-spin interactions are mainly along the diagonal directions of the lattice arrays [see Fig. 4(b)]. At this time, the spin model is bipartite in the layer space, with the Bloch Hamiltonian

$$\hat{H}_{\mathcal{S}}(\boldsymbol{k}) = \begin{pmatrix} 0 & f_{\mathcal{S}}(\boldsymbol{k}) \\ f_{\mathcal{S}}^{*}(\boldsymbol{k}) & 0 \end{pmatrix},$$
(10)

where $f_S(\mathbf{k}) = \sum_n J_{1,2}^n \exp(-i\mathbf{k} \cdot \mathbf{n})$ is the off-diagonal term and $J_{1,2}^n$ denotes the coupling between the QEs coming from the different layers at a distance \mathbf{n} . The system also has inversion symmetry $\hat{H}_S(\mathbf{k}) \rightarrow \hat{H}_S(-\mathbf{k})$, with $\hat{\sigma}_x$ the corresponding local operator [73]. The spin model protected by chiral symmetry can be harnessed to simulate exotic many-body phases, such as double Néel ordered states [40,45].

VII. GENERALIZED 2D SSH MODEL

Apart from the key symmetries that provide topological protection, bond order is another crucial ingredient required for entering topology. We selectively position the QEs in a dimeric and alternating manner in the bipartite spin model whose vertical view is plotted in Fig. 4(c). This specific spin array arrangement can investigate the topological phases of a generalized 2D SSH model [74–82].

We consider a system composed of 35×35 bilayer square lattices and a 12×12 spin array, with a configuration similar to that shown in Fig. 4(c). The energy spectrum of the spin interactions is plotted in Fig. 4(d), with G = 4J. Here, the inner band gap of 8J occupies most of the entire range of $8\sqrt{2J}$. We point out that the ratio between out-of-plane coupling and in-of-plane coupling G/J mainly influences the localization length of the BSs. For a given light-matter coupling $g \ll \{G, J\}$, the increasing of the detuning to band edges reduces the localization length of the BSs and thereby the spin couplings. The anisotropy is weakened as well even though $f(\mathbf{k}) = 0$ for $\omega(\mathbf{k}) = \pm G$ is still satisfied, as compared to the patterns under weak interlayer coupling G = J/4. However, the odd-neighbor and robust properties stemming from chiral symmetry are independent of the ratio G/J. The profiles of the BSs are more localized such that we can approximate emitter interactions to the third-neighbor or even nearest-neighbor hoppings. In this regime, the edge modes are spectrally isolated from the bulk energy bands, as shown in Fig. 4(d). Despite the challenges, we believe that $10^{-4}J$ for the energy eigenvalues is likely at finite temperatures in cold atom realizations. This is because the spin frequencies are far away from the Fermi level of an empty bath, and the bath modes are traced out for arriving at spin-spin interactions.

By expanding the spin couplings up to the third-neighbor hoppings, the nondiagonal term $f_S(k)$ in Eq. (10) can be rewritten as

$$f_{\rm SSH}(\bar{k}) \simeq \begin{pmatrix} f_0(\bar{k}_x) & f_0(\bar{k}_y) \\ f_0^*(\bar{k}_y) & f_0^*(\bar{k}_x) \end{pmatrix},\tag{11}$$

with $f_0(\bar{k}_j) = t_1 + t_2 e^{i\bar{k}_j} + t_3 e^{-i\bar{k}_j} + t_4 e^{2i\bar{k}_j}$ (j = x, y) and wave vector $\bar{k} = (\bar{k}_x, \bar{k}_y)$ for the spin array. In the topological phase, one finds $|t_2| \gg |t_1| \gg |t_4| \gg |t_3|$. To characterize the existence of edge modes, we should calculate the topological

polarization through the integral [77]

$$\mathbf{P} = \frac{1}{2\pi} \int_{\mathrm{BZ}} d\bar{\boldsymbol{k}} \operatorname{Tr}[\mathcal{A}_m(\bar{\boldsymbol{k}})], \qquad (12)$$

where $\mathcal{A}_m(\bar{k}) = i \psi_m^{\dagger}(\bar{k}) \partial_{\bar{k}} \psi_m(\bar{k})$ is the non-Abelian Berry connection and $\psi_m(\bar{k})$ represents the eigenfunction of a spin Hamiltonian with band index m. In addition to numerical calculation, another method is based on symmetry analysis [83]. Because the spin model respects C_4 symmetry, the values of the polarization are either (0,0) or $(\frac{1}{2}, \frac{1}{2})$ for a system being in the trivial or topological phase, respectively. The existence of corner states can be further characterized by the secondary topological index $Q_{\text{corner}} = \frac{1}{4}$. Note that the corner modes here are also known as bound states in the continuum with the protection of the simultaneous C_{4v} and sublattice symmetries. A detailed analysis can be found in Ref. [84]. In Fig. 4(e), we extract and plot one of the edge states distributed along the boundary of the 2D spin array. While in Fig. 4(f), we give a topological corner state with distributions localized at the four corners of the square array, direct evidence of nontrivial second-order topological insulating phases [85,86].

VIII. CONCLUSION

In summary, we developed a photonic bath with a symmetric middle band gap caused by parallel array interlayer hybridization. In this band gap, the quantum optical properties of small and giant atoms are investigated. Interactions with squarelike band-edge modes of a chiral symmetric photonic lattice, in particular, result in odd-neighbor, robust, and anisotropic BSs, which can mediate spin-spin interactions that inherit the BSs' properties. We have demonstrated the capability of our system in the simulation of nontrivial many-body phases, such as topological phases of high-order topological insulators.

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APPENDIX A: BILAYER SQUARE LATTICES OF $\eta \neq -1$

Although we particularly focus on the $\eta = -1$ case in the main text, we present some results in the $\eta \neq -1$ case in this Appendix. The dispersion relations of two hybrid energy



FIG. 5. (a) Dispersion relationship of hybrid energy bands. (b) Corresponding density of states. (c)–(f) Wave-function spatial distribution of the BS with a small random off-diagonal disorder. In (c), (d) $\Delta = 0$ and (e), (f) $\Delta = 0.5J$. Here, $\eta = -4$, G = J, and g = 0.1J.

bands read

$$\omega_{u/l}(\mathbf{k}) = \frac{(1+\eta)f(\mathbf{k})}{2} \pm \sqrt{\frac{(1-\eta)^2 f^2(\mathbf{k})}{4} + G^2}.$$
 (A1)

It is obvious that the solutions are no longer strictly symmetric $\mathbf{k} \to -\mathbf{k}$ with respect to the zero energy, but still come in pairs $\omega_u(\mathbf{k}') = -\omega_l(\mathbf{k})$, with $\mathbf{k}' = (k_x + \pi, k_y + \pi)$. Besides, the energy gap opened around van Hove singularities persists as long as $G \neq 0$ and $\eta < 0$, even though the band-edge modes no longer entirely satisfy $f(\mathbf{k}) = 0$. Nevertheless, the shape of the middle band edges is still squarelike. To clarify it, we plot the energy bands in Fig. 5(a), with $\eta = -4$ and G = J. The corresponding density of states is also given in Fig. 5(b), which shows a divergency in the middle band edges.

APPENDIX B: DETAILS OF BOUND STATES WITH A SINGLE COUPLING POINT

As discussed in the main text, the full Hamiltonian is given by $\hat{H} = \hat{H}_B + \hat{H}_{sys}$. The QE-photon dressed state formed in the single-excitation subspace can be solved based on the secular equation $\hat{H}|\psi\rangle = E_{BS}|\psi\rangle$, with the eigenvalue E_{BS} and one particle ansatz

$$|\psi\rangle = \left(C_{e}\hat{\sigma}^{\dagger} + \sum_{n}\sum_{\beta=a_{1},a_{2}}C_{n,\beta}\beta_{n}^{\dagger}\right)|g\rangle|0\rangle.$$
 (B1)

To obtain the coefficients, we solve the stationary Schrödinger equation in k space and do the inverse Fourier transform, which yields

$$C_{\boldsymbol{n},a_1} = \frac{gC_e}{4\pi^2} \iint_{\mathrm{BZ}} d\boldsymbol{k} e^{i\boldsymbol{k}\cdot\boldsymbol{n}} C_{\boldsymbol{k},a_1}, \tag{B2}$$

$$C_{\boldsymbol{n},a_2} = \frac{gC_e}{4\pi^2} \iint_{\mathrm{BZ}} d\boldsymbol{k} e^{i\boldsymbol{k}\cdot\boldsymbol{n}} C_{\boldsymbol{k},a_2}, \tag{B3}$$

with wave functions in reciprocal space

$$C_{k,a_1} = \frac{\sin^2 \theta_k}{E_{\rm BS} - \omega_u(k)} + \frac{\cos^2 \theta_k}{E_{\rm BS} - \omega_l(k)},\tag{B4}$$

$$C_{k,a_2} = \frac{-\sin\theta_k\cos\theta_k}{E_{\rm BS} - \omega_u(k)} + \frac{\sin\theta_k\cos\theta_k}{E_{\rm BS} - \omega_l(k)}.$$
 (B5)

Here, $\sin \theta_k = G/\sqrt{G^2 + [\omega_l(k) - \eta f(k)]^2}$ and $\cos \theta_k = G/\sqrt{G^2 + [\omega_u(k) - \eta f(k)]^2}$. Though the probability amplitude C_e can be obtained by imposing the normalization condition, $C_e \approx 1$ is a good approximation in the Markovian limit $g \ll \varepsilon_{gap}/2$, with ε_{gap} the size of the middle band gap. When considering $\eta = -1$ and $E_{BS} = 0$, we arrive at

$$C_{\boldsymbol{n},a_1} = \frac{gC_e}{4\pi^2} \iint_{\mathrm{BZ}} d\boldsymbol{k} e^{i\boldsymbol{k}\cdot\boldsymbol{n}} \frac{-f(\boldsymbol{k})}{f^2(\boldsymbol{k}) + G^2}, \qquad (\mathrm{B6})$$

$$C_{n,a_2} = \frac{gC_e}{4\pi^2} \iint_{\rm BZ} dk e^{ik \cdot n} \frac{-G}{f^2(k) + G^2},$$
 (B7)

which are used in the main text. One can easily check that $C_{n,a_1} = 0$ for sum $(n) \equiv (n_x + n_y) \in \mathbb{Z}_{even}$ and $C_{n,a_2} = 0$ for sum $(n) \in \mathbb{Z}_{odd}$ due to the interference between the k mode and the k' mode, with $k' = (k_x + \pi, k_y + \pi)$. The intrinsic chiral symmetry of the bath Hamiltonian is responsible for the odd-neighbor profiles and the robustness.

To clarify it, we consider a chiral symmetric system with multiple quantum emitters. The full Hamiltonian in terms of the block matrix can take the form

$$\boldsymbol{H} = \begin{pmatrix} \boldsymbol{H}_p & \boldsymbol{g}_{oe} \\ \boldsymbol{g}_{oe}^{\dagger} & \boldsymbol{\Delta} \end{pmatrix}, \quad \text{with} \quad \boldsymbol{H}_p = \begin{pmatrix} 0 & \boldsymbol{Q}_p \\ \boldsymbol{Q}_p^{\dagger} & 0 \end{pmatrix}. \quad (B8)$$

Here, the submatrix H_p is the bath's Hamiltonian, $g_{oe} = (g_{odd}, g_{even})$ is the coupling term and $\Delta/\Delta = I$. Assuming $\Delta = 0$ and no emitters in even sites $g_{even} = 0$, and using the formula for the block matrices

$$\det\begin{pmatrix} A & B \\ C & D \end{pmatrix} = \det(A)\det(D - CA^{-1}B), \quad (B9)$$

the determinant of the full Hamiltonian is zero, that is $\det(\boldsymbol{H}) = 0$. By solving $\boldsymbol{H}\boldsymbol{\Psi} = E\boldsymbol{\Psi}$ with eigenvector $\boldsymbol{\Psi} = (\boldsymbol{\Psi}_{\text{odd}}^T, \boldsymbol{\Psi}_{\text{even}}^T, \boldsymbol{\Psi}_{\text{QE}}^T)^T$, we can always find an eigenvalue E = 0 with $\boldsymbol{\Psi}_{\text{odd}} = 0$, in the presence of off-diagonal disorders $d\boldsymbol{Q}_p$.

In Figs. 5(c) and 5(d), we plot the photonic part of the BS with $\eta = -4$, G = J, and $\Delta = 0$. We still find odd-neighbor and robust properties when off-diagonal disorders are included. As a contrast, we give the BS pattern in Figs. 5(e) and 5(f) with $\Delta = 0.5J$, in which the full Hamiltonian (the emitter part together with the lattice part) is no longer protected by chiral symmetry. As a result, the single-emitter BS can have weights in both odd and even sites.

APPENDIX C: BOUND STATES WITH MULTIPLE COUPLING POINTS

1. Some details

We now detail the results of the light-matter interaction beyond the dipole approximation. In this case, the so-called "giant atom" features nonlocal coupling to the optical lattices. In terms of intralayer interference factors

$$\mathbf{I}(\boldsymbol{k}) = \sum_{\alpha=1}^{N_p} g_{\boldsymbol{n}_{\alpha}} e^{i\boldsymbol{k}\cdot\boldsymbol{n}_{\alpha}}, \quad \mathbf{I}'(\boldsymbol{k}) = \sum_{\beta=1}^{N_q} g_{\boldsymbol{n}_{\beta}} e^{i\boldsymbol{k}\cdot\boldsymbol{n}_{\beta}}, \quad (C1)$$

which reflect the interference effects stemmed from multiple coupling points of the giant atom, the interaction Hamiltonian in k space can be rewritten as

$$\hat{H}_{\text{int}} = \frac{1}{\sqrt{N}} \hat{\sigma}^{\dagger} \sum_{k} [\mathbf{I}(k) \times (-\sin\theta_{k}\hat{u}_{k} + \cos\theta_{k}\hat{l}_{k}) + \mathbf{I}'(k) \times (\cos\theta_{k}\hat{u}_{k} + \sin\theta_{k}\hat{l}_{k})] + \text{H.c.}$$
(C2)

From the view of the wave-function distribution of the BS, the interference pattern is a superposition of multiple BSs based on small atoms

$$C_{\mathbf{n},a_{1}}^{g} = \sum_{n_{\alpha}} (g_{n_{\alpha}}/g) C_{\mathbf{n}-n_{\alpha},a_{1}}^{s} + \sum_{n_{\beta}} (g_{n_{\beta}}/g) C_{\mathbf{n}-n_{\beta},a_{2}}^{s}, \quad (C3)$$

$$C_{n,a_2}^{g} = \sum_{n_{\alpha}} (g_{n_{\alpha}}/g) C_{n-n_{\alpha},a_2}^{s} - \sum_{n_{\beta}} (g_{n_{\beta}}/g) C_{n-n_{\beta},a_1}^{s}.$$
 (C4)

To protect the parity property, we assume that the coupling points are even neighbor with each other.

2. Other patterns

In addition to the unconventional patterns of two examples shown in Fig. 3, we present some other results in this Appendix. First, we consider four coupling points $n_{1,2,3,4} = (1,0)/(-1,0)/(0,1)/(0,-1)$ in the top layer with identical coupling strength *g*. In this case, the interference factor can be expressed as

$$\mathbf{I}(\boldsymbol{k}) = 2g(\cos k_x + \cos k_y),\tag{C5}$$

which is zero for all the band-edge modes. This corresponds to the trap of the photon population around giant atom, which is plotted in Figs. 6(a) and 6(b).

We may further consider a single giant atom with coupling points distributing in two layers. For simplicity, we assume that the QE is simultaneously coupled to the $n_1 = (0, 0)$ lattice site of the top layer and the $n_2 = (1, 0)$ lattice site of the bottom layer, with identical coupling strength g. In this case, I(k) = g and $I'(k) = ge^{i(k_x+k_y)}$ in the interaction Hamiltonian. In Figs. 6(c)-6(e), we plot the BS pattern of such a configuration and show the chiral feature in some directions, such as the $n_x = n_y + 1$ direction. Next, we attempt to understand how it occurs. Taking the spatial distribution in the top layer for example, the expression of C_{n,a_1}^g can be rewritten as

$$C_{n,a_1}^{g} = C_{n-n_1,a_1}^{s} + C_{n-n_2,a_2}^{s} = Ae^{i\theta_1} + Be^{i\theta_2}, \quad (C6)$$

where A/B denotes the amplitude and θ_1/θ_2 is the phase. We recall that the BS for a small atom has alternating phases ± 1 in real space. Thus, the phase difference $\delta\theta = \theta_1 - \theta_2$ plays



FIG. 6. Modulus of the wave-function distribution in real space. (a), (b) Four coupling points $n_{1,2,3,4} = (\pm 1, 0)/(0, \pm 1)$ distributing in the top layer, with identical coupling strength *g*. Photon population is trapped. (c), (d) Two coupling points $n_{1,2} = (0, 0)/(1, 0)$ respectively distributing in the two layers, with identical coupling strength *g*. Chiral patterns occur in some directions. (e) Spatial distribution C_{n,a_1} and (f) phase difference $\delta\theta = \theta_1 - \theta_2$ along the $n_x = n_y + 1$ direction [labeled by the blue line in (c)]. A sudden jump of $\delta\theta$ occurs at n_2 . Here, $\eta = -1$, G = J/4, and g = 0.1J.

an important role in the process of two site interferences. In Fig. 6(f), we plot the relative phase $\delta\theta$ along the $n_x = n_y + 1$ direction and find a sudden jump between 0 and the π phase difference. This means the appearance of destructive (constructive) interference on the left (right) side, which accounts for the emergence of chirality.

APPENDIX D: EIGHT-PARTICLE ENTANGLEMENT

When a set of small atoms are taken into account, the BSs can mediate odd-neighbor, robust, and anisotropic dipole-dipole interactions. In the parameter regime of $g \ll G$ (Markovian regime), the effective dynamics is governed by the following Hamiltonian,

$$\hat{H}_{S} = \frac{1}{2} \sum_{i,j} (g_{ij} \hat{\sigma}_{i}^{\dagger} \hat{\sigma}_{j} + \text{H.c.}), \qquad (D1)$$

with coupling strength

$$g_{ij} = \begin{cases} gC_{\mathbf{n}_{ij},a_1}/C_e, & Q_i, Q_j \in \text{layer 1}, \\ -gC_{\mathbf{n}_{ij},a_1}/C_e, & Q_i, Q_j \in \text{layer 2}, \\ gC_{\mathbf{n}_{ij},a_2}/C_e, & Q_i \in \text{layer 1}, Q_j \in \text{layer 2}, \end{cases}$$
(D2)

where $\mathbf{n}_{ij} = \mathbf{n}_j - \mathbf{n}_i$ is the relative position. Based on the parity property of the BS, the coupling strength g_{ij} vanishes



FIG. 7. (a) Configuration for eight-particle entanglement, with nine atoms in the top layer. Eight of them are in the odd sites and an auxiliary one is at the origin. (b) Time evolution of the fidelity of the goal state $|\phi\rangle_{\text{goal}}$, with initial state $|\phi_0\rangle$. Both the ideal result and the situation under dissipation are plotted. Here, $\eta = -1$, G = J/4, and g = 0.1J.

for sum(\mathbf{n}_{ij}) $\in \mathbb{Z}_{even}$ (\mathbb{Z}_{odd}) when two atoms are in the same (different) layers. This means that we can divide the atoms into two manifolds, and in each manifold there is no intercoupling.

A possible direct application, which makes use of this spin-spin interaction, is long-distance entanglement distribution. We consider nine QEs located in the top layer of the bilayer lattices, and eight of them are odd-site QEs along the diagonal directions with $n_{1-8} = (n, \pm n \pm 1)/(-n, \pm n \pm 1)/((-n - 1, \pm n))$, while an auxiliary one is at the origin, as shown schematically in Fig. 7(a). The effective Hamiltonian of this setup can be constructed by

$$\hat{H}_{\text{eff}} = gC_{n_1,a_1}/C_e \hat{\sigma}_a^{\dagger} \sum_{i=1}^{8} \hat{\sigma}_i + \text{H.c.}$$
 (D3)

Here, we assume an identical atom-photon coupling strength and in the weak-coupling limit. In order to prepare the desired

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entanglement state, we consider the initial state $|\phi_0\rangle = |e\rangle_a \otimes |g\rangle^{\otimes 8}$, where the auxiliary atom is initially in the excited state and the other eight atoms are initially in the ground state. After a time interval $\tau = \pi C_e/(4gC_{n_1,a_1})$, the system evolves into the target entanglement state

$$|\phi\rangle_{\text{goal}} = |g\rangle_a \otimes \frac{1}{\sqrt{8}} \sum_{i=1}^8 \hat{\sigma}_i^{\dagger} |g\rangle^{\otimes 8}.$$
 (D4)

Compared with a previous four-particle entanglement scheme discussed in Ref. [26], we can generate an entangled state involving more particles (up to eight), and more importantly avoid the unwanted cross-talk which dominates the infidelity. Thus, our scheme may achieve higher fidelity. The time evolution of the dynamics under dissipation is governed by the following master equation,

$$\frac{d\hat{\rho}}{dt} = -i[\hat{H}_{\text{eff}}, \hat{\rho}] + n_{\text{ph}}\kappa \sum_{\mathbf{n}} (D[\hat{a}_{1,\mathbf{n}}]\hat{\rho} + D[\hat{a}_{2,\mathbf{n}}]\hat{\rho}) + \Gamma \sum_{i=1}^{8} D[\hat{\sigma}_i]\hat{\rho} + \Gamma D[\hat{\sigma}_a]\hat{\rho},$$
(D5)

where $n_{\rm ph}$ is the photonic component of the BS, κ and Γ denote the photon loss of each site and the decay rate of each QE, and $D[\hat{O}]\hat{\rho} = \hat{O}\hat{\rho}\hat{O}^{\dagger} - \frac{1}{2}\hat{O}^{\dagger}\hat{O}\hat{\rho} - \frac{1}{2}\hat{\rho}\hat{O}^{\dagger}\hat{O}$ for a given operator \hat{O} . In the weak-coupling limit, we can neglect cavity damping terms since $n_{\rm ph}\kappa \ll \Gamma$. In Fig. 7(b), we plot the fidelity as a function of evolution time and show a high-fidelity preparation of the target state.

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