Band-gap-engineered spin-phonon, and spin-spin interactions with defect centers in diamond coupled to phononic crystals

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We study a spin-phononic system where diamond defect centers are interfaced with a quasi-one-dimensional phononic crystal. We show that, a single defect center, coupled to the phonon modes of a phononic crystal waveguide near the band gap, can seed its own phononic cavity mode with an exponentially decaying envelope around the defect center’s position. The spin-induced phononic cavity, with a greatly reduced and tunable mode volume, allows coherent phonon-mediated interactions between distant spins with a highly tunable range, enabling access to a variety of long-range interacting spin models. This work opens prospects for exploring quantum many-body physics and quantum information processing with defect centers and periodic phononic nanostructures.

Introduction.– Electronic spins associated with defect centers in diamond comprise an outstanding platform for both fundamental research and practical applications [1–7]. Prominent defect centers in diamond include silicon-vacancy (SiV) [8–14], nitrogen-vacancy (NV) [15] and germanium vacancy (GeV) [16] color centers, which possess the advantage of long coherence times [17, 18] and perfect compatibility with other solid-state setups [19–24].

For the realization of practical quantum technologies, coherent and controllable interactions between distant solid spins play an essential role. To achieve this goal, schemes for interfacing solid spins via mechanical degrees of freedom have been extensively investigated [25–41], where a conventional acoustic cavity (waveguide) [42–45] or mechanical resonator is often employed to mediate effective spin-spin interactions. Nevertheless, there are two challenges in complete quantum control of both spin and mechanical degrees of freedom [46, 47]. First of all, the phonon-mediated spin-spin interaction is often too weak due to the weak intrinsic strain coupling of spins to vibrational modes [48, 49]. Second and more importantly, complete control on spin-spin interactions still remains a challenge. In particular, the spatial range of phonon-mediated spin-spin interactions cannot be tuned or controlled, and is set solely by the dimension of the setup.

In this work, we propose that by utilizing phononic crystals that interface with defect centers, the problem mentioned above can be overcome. Phononic crystals [50–60] naturally enable interactions with a strength potentially much greater, owing to the much tighter confinement of the mediating phonon. The ability to tailor the modal properties and dispersion relation of a phononic crystal waveguide significantly goes beyond that of a conventional acoustic waveguide or cavity, which offers a greatly expanded toolbox for controlling spin-phonon interactions. Particularly, the band gap of a phononic crystal provides a tunable interaction range, a feature which is unique to this kind of nanostructures, and makes phononic crystals remarkably different from either acoustic cavities or unstructured waveguides [50–60]. We investigate the band gap engineered spin-phonon, and spin-spin interactions with defect centers in diamond interfaced to a quasi-one-dimensional (1D) phononic crystal. We show that, when the transition frequency of the defect center lies within the band gap, the defect center can seed its own phononic cavity mode with an exponentially decaying envelope around its position. This leads to an enhanced spin-phonon coupling due to the much tighter confinement of the phonon. The band-gap interaction between defect centers and phononic crystal modes can realize coherent spin-spin coupling with a highly tunable spatial range, which is not readily achievable using other interaction mechanisms. This work indicates that hybrid systems [61] composed of defect centers and periodic phononic nanostructures comprise a promising platform for the investigation of quantum many-body physics [62] and quantum information processing.

Model.– We consider the setup shown in Fig. 1, where separated defect centers (SiV, NV, and GeV centers) in diamond are coupled to the phonon modes of a 1D phononic crystal waveguide near a band gap. Without loss of generality, we assume that the defect center is coupled via strain to a continuum of compression modes propagating along the phononic crystal (along the x axis). Local lattice distortions associated with internal compression modes of the phononic crystal affect the defect’s electronic structure, which induces a strain coupling between these phonons and the orbital degrees of freedom of the center [11, 39].

The phononic crystal, a quasi-1D periodic structure, has a spatially periodic structure with lattice constant a, a cross section A, and total length L \( \gg a, \sqrt{A} \). We assume that the transverse dimensions of the phononic crystal are much smaller than the characteristic phonon
The phononic crystal waveguide supports phonon modes of frequency $\omega_{n,k}$ and mode profile $\tilde{Q}_{n,k}(\vec{r})$ [63], where $k$ is the wave vector along the waveguide, and $n$ is the band index. Because of the periodicity of the phononic crystal, the phononic modes are of Bloch form [51]. In the limit of a quasi-1D crystal, $\tilde{Q}_{n,k}(\vec{r}) \sim e^{i k \cdot \vec{r}} \tilde{q}_{n,k}(\vec{r})$, where $\tilde{q}_{n,k}(\vec{r})$ is a periodic function associated with the shape of the Bloch modes, with periodicity given by the lattice constant $a$. Figure 2 shows finite-element-method (FEM) simulations of the mechanical band structures, and displacement patterns of the symmetric modes at the band edge frequency for the two types of phononic crystal waveguides. The band structure of the phononic crystal waveguide shows a sizable band gap for the mechanical modes, which allows the defect center’s transition frequency to lie within the bandgap.

For defect centers such as SiV, NV, and GeV centers, strong coupling between the orbital degrees of freedom and the mechanical vibrations can be obtained through the ground states or excited states [11, 27, 39, 64]. Here we take SiV centers as an example, but the general model also applies to NV and GeV centers. The SiV center is a point defect in which a silicon atom is positioned between two adjacent missing carbon atoms in the diamond lattice [11]. Its electronic ground state is formed by an unpaired hole of spin $S = 1/2$, which occupies one of the two degenerate orbital states $|e_x\rangle$ and $|e_y\rangle$ [63]. In the presence of spin-orbit interactions and a weak Jahn-Teller effect, the four states are split into two doublets [11], $\{|g\rangle = |e_-\downarrow\rangle, |e_\uparrow\rangle = |e_\uparrow\downarrow\rangle\}$ and $\{|f\rangle = |e_+\downarrow\rangle, |d\rangle = |e_-\uparrow\rangle\}$. Here, $|e_\pm\rangle = (|e_x\rangle \pm i |e_y\rangle)/\sqrt{2}$ are eigenstates of the orbital angular momentum operator $\hat{L}_z$, with the $z$ axis along the symmetry axis of the defect. The energy gap between these doublets is $\Delta/2\pi = 46$ GHz [11].

The interaction Hamiltonian is given by $H_{\text{strain}} = \sum_{ij} V_{ij}\epsilon_{ij}$ [11, 36, 63], where $V_{ij}$ is an operator acting on the electronic states of the defect center, and $\epsilon$ is the strain tensor. The strain Hamiltonian can be projected onto the irreducible representations of the $D_{3d}$ group for SiV centers, which reflects the symmetry of the orbital wavefunctions, i.e., $H_{\text{strain}} = \hbar\sum_{ij} V_{ij}\epsilon_{ij}$. Each $\epsilon_{ij}$ is a linear combination of strain components $\epsilon_{i,j}$, and corresponds to specific symmetries indicated by the subscript $l$, i.e., $\epsilon_{A_{1g}} = t_\perp (\epsilon_{xx} + \epsilon_{yy}) + t_\parallel \epsilon_{zz}$, and $\epsilon_{E_{2g}} = -2d\epsilon_{xy} + f\epsilon_{xx}$, and $\epsilon_{E_{2g}} = -2d\epsilon_{xy} + f\epsilon_{xx}$. Here $t_\perp$, $t_\parallel$, $d$, and $f$ are the four strain-susceptibility parameters that completely describe the strain-responsibility of the orbital states $|e_x\rangle$ and $|e_y\rangle$. The strain Hamiltonian can be rewritten in the basis spanned by the eigenstates of the spin-orbit coupling [30] $H_{\text{strain}} = \hbar\epsilon_{E_{2g}}(L_+ + L_-) - i\hbar\epsilon_{E_{1g}}(L_- - L_+)$, where $L_+ = L_+^\dagger = |f\rangle \langle g| + |e\rangle \langle d|$. The orbital raising operator...
within the ground state.

Upon quantization, the mechanical displacement $\hat{Q}(\vec{r})$ becomes an operator, which can be expressed in terms of the elementary normal modes and annihilation operators as $\hat{Q}(\vec{r}) = \sum_{n,k} [\hat{Q}_{n,k}(\vec{r}) \hat{a}_{n,k} + \text{H.c.}]$ [63, 65]. The resulting strain coupling can be written in the general form $\hat{H}_{\text{strain}} \simeq \sum_{n,k} [\hbar g_{n,k} \hat{a}_{n,k} \hat{J}_x e^{ikx} + \text{H.c.}]$ [63, 66], where the coupling constant $g_{n,k}$ depends on the local strain tensor and can be evaluated for a known mode profile $\hat{Q}_{n,k}(\vec{r})$, and $\hat{J}_+ = |f\rangle \langle g| + |d\rangle \langle e|$. The defect center is coupled predominantly to only a single band of the phononic crystal waveguide, via tuning the transition frequency $\Delta$ of the color center close to the band edge frequency $\omega_{\text{BE}}$, with detuning $\delta_{\text{BE}} = \Delta - \omega_{\text{BE}}$ (where $\delta_{\text{BE}} > 0$, so that the spin frequency lies within the band gap). We assume that the detuning to any other band edge is much larger than $\delta_{\text{BE}}$, so the other bands can be neglected. For clarity, we omit the band index $n$ in the following discussion.

**Phononic bound state and effective acoustic cavity.** When the transition frequency of the defect center is tuned close to the band edge, the spin is dominantly coupled to the modes near the band edge wavevector $k_0 = \pi/a$ due to the van Hove singularity in the density of states, i.e., $\frac{dk}{\omega_{\text{BE}}}|_{k_0} \to \infty$. In this case, the dispersion relation can be approximated to be quadratic $\omega_k \simeq \omega_{\text{BE}} - \alpha a^2 (k - k_0)^2$, with $\alpha$ a parameter characterizing the band curvature. In the presence of a static magnetic field $\vec{B} = B_0 e_z$ and a microwave driving field of frequency $\omega_0$ and Rabi-frequency $\Omega$ along $e_x$, we can implement a Raman transition between the states $|g\rangle$ and $|e\rangle$ via the excited state $|f\rangle$ through coupling the SiV center to the mechanical modes. The Hamiltonian of the whole system can be written as [63]

$$\hat{H} = \sum_k \hbar \omega_k \hat{a}_{k}^\dagger \hat{a}_k + \hbar \omega_s \hat{\sigma}_{ee}$$

$$+ \sum_k \hbar g_{\text{eff}} (\hat{a}_{k}^\dagger \hat{\sigma}_{ge} e^{-ikx_0} + \hat{a}_k \hat{\sigma}_{eg} e^{ikx_0}),$$

where $\sigma_{ij} = |i\rangle \langle j|$, $\omega_s = \Delta - \delta$, $g_{\text{eff}} = g_k \Omega / \delta$, and $g_k$ is the coupling strength between the defect center (with the position $\vec{r}_0$) and phonon modes in the band. Moreover, for the modes near the band edge the coupling strength $g_k$ is approximately independent of $k$, i.e., $g_k \sim g \sim \frac{\pi}{\sqrt{\hbar \omega_{\text{BE}} / 2 \pi \rho a}}$ [63], where $d / 2 \pi \sim 1 \text{ PHz/strain}$ is the strain sensitivity, and $v_t = 1.71 \times 10^4 \text{ m/s}$ is the speed of sound in diamond.

For a single excitation in the system, there exists a bound state $|\varphi_{b}\rangle = \cos \theta |0\rangle |e\rangle + \sin \theta |1\rangle |g\rangle$ within the bandgap with the eigenenergy $\hbar \Omega_b$. Here $|0\rangle$ is the vacuum state for the phonon modes, and $|1\rangle = \int d\vec{k} c_{k} \hat{a}_{k}^\dagger |0\rangle$ is a single phonon excitation of the modes in the band. The bound state and the corresponding eigenenergy are determined by the eigenvalue equation $\hat{H}|\varphi_{b}\rangle = \hbar \Omega_b |\varphi_{b}\rangle$.

Solving this equation yields [63]

$$\Omega_b - \omega_s = \frac{\pi g_{\text{eff}}}{\sqrt{\alpha (\Omega_b - \omega_{\text{BE}})}}$$

$$\tan^2(\theta) = \frac{\omega_s - \Omega_b}{2(\omega_{\text{BE}} - \Omega_b)}$$

$$c_k = \frac{g_{\text{eff}} e^{-ikx_0}}{\tan \theta (\Omega_b - \omega_{\text{BE}}).}$$

In real space, the phononic part of the bound state is exponentially localized around the spin with spatial mode envelope

$$E(x) = \int dk c_k Q_k(x) = \sqrt{\frac{2\pi}{L_c}} e^{-|x-x_0|/L_c} Q_{k_0},$$

where the localization length $L_c$ is given by

$$L_c = a \frac{\alpha}{\Omega_b - \omega_{\text{BE}}}.$$}

This localized phononic cloud has the same properties as a confined acoustic cavity mode. The localization of the phononic wavefunction is determined predominantly by the properties of the band edge, and the frequency detunings, leading to the possibility of dynamic tuning of the localization length.

The coupling between the defect center and the phononic crystal modes near the band edge can be well understood by mapping to the Jaynes-Cummings model in cavity quantum-electrodynamics [66, 67] or spin-mechanics. In particular, the eigenstate $|\varphi_{b}\rangle$ looks identical in form to one of the dressed eigenstates of the Jaynes-Cummings model. This mapping can be made formal: the phonon confined around the defect center has the same functionality as the mode of an actual acoustic cavity. We can associate an effective spin-phonon coupling strength $g_{\text{c}} = g_{\text{eff}} \sqrt{2\pi \alpha / L_c}$ with the bandgap setup. The effective vacuum-Rabi splitting $g_{\text{c}}$ is identical to that of a real cavity whose mode volume is the same as the bound phonon size $V_{\text{eff}} = 4L_c$. This effective spin-phonon interaction can be much stronger than that of defect centers coupling to a conventional phononic waveguide [30], via tuning the effective acoustic cavity mode volume to a much smaller value such that the phonons are confined much tighter. The effective acoustic cavity frequency is the average frequency of the phonon modes, i.e., $\int d\vec{k}|c_k|^2 \omega_k = \omega_{\text{BE}} - \delta_b$, and the effective spin-cavity detuning is $\Delta_{\text{E}} = \Delta_{\text{BE}} + \delta_b$.

In Fig. 3(a)-(c), we present the numerical simulations for the dependence of the bound-state eigenfrequency $\Omega_b$, the defect center’s excited state population $P_e = \cos^2 \theta$, and the length of the effective phononic cavity $L_c$ on detuning $\Delta_{\text{BE}}$. Fig. 3(a) shows that when $\Delta_{\text{BE}} / g_{\alpha} \ll -1$, then $\Omega_b$ approaches $\omega_{\text{BE}}$, while $\Omega_{b}$ approaches $\omega_{\text{BE}} + \Delta_{\text{BE}}$ when $\Delta_{\text{BE}} / g_{\alpha} \gg 1$. Fig. 3(b) shows that when $\Delta_{\text{BE}} / g_{\alpha} \ll -1$, the state becomes mostly phononic: a cavity mode dressed by the spin. From Fig. 3(c), one
can see that localized phonon arises with larger detuning $\Delta_{BE}$ or flatter bands, giving rise to an enhancement of the effective spin-phonon coupling. From Fig. 3(d), we find that the phononic component of the hybrid spin-phonon state extends over multiple sites.

**Spin-spin interactions mediated by phononic crystals.**

The band-gap interaction allows us to use the phononic crystal modes as a quantum bus to perform more complex tasks. Analogous to the spin-exchange interaction in cavity QED, two defect centers that are separated by a distance on the order of the length $L_c$ can exchange a phonon excitation via the induced acoustic cavity mode. Based on this effective interaction, it is possible to implement quantum information processing and a variety of interacting spin models [62] with distant defect spins.

We consider two separated SiV centers coupled to the same phononic crystal modes near the band edge, through Raman transitions between the states $|g\rangle$ and $|e\rangle$. In the interaction picture, we can obtain the interaction between the defect centers and phononic crystal modes $\hat{H} = \sum_{j=1,2} \sum_k \hbar g^j_e(a_k^\dagger g|e\rangle e^{-i\omega_k t - ikx_j} + a_k e^{i\omega_k t + ikx_j})$, with $\delta_k = \omega_s - \omega_k$. In the dispersive regime $\delta_k \gg g^j_e$, this will lead to an effective spin-spin interaction via the exchange of virtual phonons [63],

$$\hat{H}_{s-s} = \hbar J_{12} \hat{\sigma}_e^1 \hat{\sigma}_g^2 + \text{H.c.}$$

with the effective coupling strength $\lambda_{\text{eff}} = g_e^2/2\Delta_{BE}$. Here the spatial range reflects the shape of the localized phononic cloud.

Different from the dipole-dipole interactions mediated by a conventional cavity, the form of the band-gap-mediated interactions between spins is to decay exponentially with spin separation [68], as shown in Fig. 4. Furthermore, the range of the interaction can be tuned through the effective interaction length $L_c$, the length scale of which can be on the order of the length of experimental setups, and thus effectively long-range over the system size. Therefore, the band gap interaction can realize coherent spin-spin interactions with a highly tunable range, which cannot be readily achieved using other interaction mechanisms. This potentially enables the study of a variety of interacting spin models [63], and the deterministic generation of entanglement and quantum state transfer between spins at a distance of several lattice constants though a phononic channel.

We assume that the two defect centers are initially prepared in the state $\psi(0) = |g\rangle|e\rangle$. Then under the Hamiltonian $\hat{H}_{s-s}$, the state evolution of the system is given by $\psi(t) = \cos(J_{12}t)|g\rangle|e\rangle - i\sin(J_{12}t)|e\rangle|g\rangle$, which is an entangled state for the two centers. If we choose $J_{12} = \pi/4$, we can obtain the maximally entangled two-particle state $\psi(\tau) = \frac{1}{\sqrt{2}}(|g\rangle|e\rangle - i|e\rangle|g\rangle)$, which is the well-known Einstein-Podolsky-Rosen state. The interaction (5) between the two defect centers can also be used to transfer arbitrary quantum information encoded in ground spin states from one center to the other: $(a|g\rangle + \beta|e\rangle)|e\rangle \rightarrow (a|g\rangle + \beta|e\rangle)|e\rangle$.

Fig. 5 displays the numerical results for the time evolution of the concurrence and populations for two defect centers under ideal and realistic conditions through solving the master equation using the QuTiP library [69]. We find that, the concurrence and populations are significantly affected by the distance between the centers, even though the other conditions are the same. Moreover, if the decoherence of the defect centers is taken into account, for distances between the centers larger than $L_c$,
the produced entangled states and the quantum state transfer efficiency will be significantly spoiled.

For the setups illustrated in Fig. 1, the band edge frequency is \( \omega_{BE}/2\pi = 45.5 \) GHz, and the quality factor of a phononic crystal mode can reach \( Q_m \sim 10^7 \), resulting in a mechanical damping rate \( \gamma_m/2\pi \sim 5 \) kHz. This high mechanical quality factor should be achievable with the use of phononic crystal shields and with the state-of-the-art nanofabrication technologies [56, 70, 71]. At mK temperatures, the thermal phonon number is far below 1 and the spin dephasing rate of SiV centers is about \( \gamma_s/2\pi \sim 0.1 \) kHz with dynamical decoupling [10]. Even taking into account the surface effect on SiV centers’ decoherence, the spin dephasing rate is still expected to be about \( \gamma_s/2\pi \sim 100 \) kHz. The coupling strength for the design in Fig. 1(a) can be calculated as \( g/2\pi \sim 178 \) MHz. If we choose \( \Omega \sim g, \delta \sim 10g, \) and \( \Delta_{BE} = 43g_0 \), then we have \( g_{eff} \sim 0.1g, g_c/2\pi \sim 21.2 \) MHz, and \( \lambda_{eff}/2\pi \sim 1.27 \) MHz. The time for generating the entangled state and implementing quantum state transfer is about \( \tau \leq 1\mu s \), which is smaller than the coherence time of the setup.

**Conclusions.**—We have investigated the band gap engineered spin-phonon, and spin-spin interactions with defect centers in diamond coupled to a quasi-1D phononic crystal. We show that, when the transition frequency of the defect center lies within a band gap, the defect center can seed its own phononic cavity mode with an exponentially decaying envelope around its position. The band-gap interaction allows coherent phonon-mediated interactions between spins with a tunable spatial range. The scheme presented in this work is general and can be applied to other defect centers or solid-state systems such as SiC-based systems [72] and hexagonal boron nitride emitters [73]. This work opens prospects for exploring quantum many-body physics and quantum information processing with defect centers and phononic nanostructures.

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SUPPLEMENTAL MATERIAL:

Phononic crystals

Calculation of mechanical compression modes in diamond phononic crystals

In the main text, we study a quasi-1D periodic structure with lattice constant $a$, a cross section $A$, and total length $L \gg a, \sqrt{A}$. With the framework of elastic mechanical theory, mechanical modes can be treated as a continuum field with time-dependent displacement at the position $\vec{r}$, given by $\vec{Q}(\vec{r}, t)$. The field $\vec{Q}(\vec{r}, t)$ obeys the equation of motion [S1]

$$\rho \frac{\partial^2}{\partial t^2} \vec{Q}(\vec{r}, t) = (\lambda + \mu) \nabla (\nabla \cdot \vec{Q}(\vec{r}, t)) + \mu \nabla^2 \vec{Q}(\vec{r}, t).$$

(S1)

Here $\rho$ is the mass density, and $\lambda$ and $\mu$ are the Lamé constants. Waves in periodic structures are best understood in terms of band theory. From Bloch’s theorem, we have that in a structure with periodic variation, the time-harmonic solutions to the mechanical wave equations can be expressed as a product of a plane-wave solution $e^{ikx}$ and a periodic function $\vec{u}_{n,k}(\vec{r})$, i.e., $\vec{Q}_{n,k}(\vec{r}) = e^{ikx} \vec{u}_{n,k}(\vec{r})$, with the eigenfrequencies $\omega_{n,k}$. The Lamé constants can be expressed in terms of the Young’s modulus $E$ and the Poisson ratio $\nu$

$$\lambda = \frac{\nu E}{(1 + \nu)(1 - 2\nu)}, \quad \mu = \frac{E}{2(1 + \nu)}.$$ (S2)

The frequencies $\omega_{n,k}$ and field patterns of the normal modes can be determined by solving the corresponding eigenvalue equations using finite element simulations [S2]. The material properties of diamond we used are $E = 1050$ GPa, $\nu = 0.2$, and $\rho = 3539$ kg/m$^3$, while for silicon the material properties are $E = 170$ GPa, $\nu = 0.28$, and $\rho = 2329$ kg/m$^3$. All modes considered in this work have even mirror symmetry under reflection $R_z$ about the plane perpendicular to the axis $z$.

Quantization of the displacement fields in diamond phononic crystals

The motion can be quantized following an approach similar to that used for the electromagnetic field in quantum optics [S3]. We define phonon creation and annihilation operators $\hat{a}^\dagger_{n,k}$ and $\hat{a}_{n,k}$ respectively, for each modal solution $\vec{Q}_{n,k}(\vec{r})$ of the equations of elasticity in the structure. Then the field operator can be expressed as

$$\vec{Q}(\vec{r}) = \sum_{n,k} [\vec{Q}_{n,k}(\vec{r})\hat{a}_{n,k} + \text{H.c.}].$$ (S3)

To calculate the proper normalization of the field profiles, we assume a single-phonon Fock state $|\Psi\rangle = \hat{a}^\dagger_{n,k}|0\rangle$ and calculate the expectation value of additional field energy above vacuum. We find

$$E_{\text{mech}} = 2\omega_{n,k}^2 \int d^3\vec{r} \rho(\vec{r}) \vec{Q}_{n,k}^*(\vec{r}) \cdot \vec{Q}_{n,k}(\vec{r})$$

$$= 2\rho V_{\text{eff}} \omega_{n,k}^2 \max(|\vec{Q}_{n,k}|^2),$$ (S4)

where the last equality defines the effective mode volume for mode $\{n, k\}$. Setting $Q_0 = \max(|\vec{Q}_{n,k}|)$ and assuming the phonon energy as $E_{\text{mech}} = \hbar \omega_{n,k}$, we arrive at the general result for a phonon mode, $Q_0 = \sqrt{\hbar/2\rho V_{\text{eff}} \omega_{n,k}}$.

SiV centers

As discussed in the main text, the SiV center is a point defect in which a silicon atom is positioned between two adjacent missing carbon atoms in the diamond lattice. Its electronic ground state is formed by an unpaired hole of spin $S = \frac{1}{2}$, which occupies one of the two degenerate orbital states $|e_x\rangle$ and $|e_y\rangle$. The spin and orbital degeneracy is lifted by the spin-orbit coupling and by the Jahn-Teller effect. In the presence of an external magnetic field $\vec{B}$, the Hamiltonian for the electronic ground state of the SiV center is [S4]

$$\hat{H}_{\text{SiV}} = -\hbar \lambda_{\text{SO}} \hat{L}_z \hat{S}_z + \hat{H}_{\text{JT}} + \hbar \gamma_L \hat{B}_z \hat{L}_z + \hbar \gamma_S \vec{B} \cdot \vec{S},$$

(S5)
where \( \hat{L}_z \) and \( \hat{S}_z \) are the projections of the angular momentum and spin operators onto the symmetry axis of the defect center (along \( z \) axis). \( \lambda_{SO} \) is the spin-orbit coupling strength while \( \gamma_L \) and \( \gamma_s \) are the orbital and spin gyromagnetic ratios respectively. In the basis defined by the degenerate eigenstates \( \{|e_x \uparrow\}, |e_x \downarrow\}, |e_y \uparrow\}, |e_y \downarrow\}\), the different contributions to the SiV energy levels, introduced in Eq. (S5), read

\[
\begin{align}
(Y_s B_0 - \lambda_{SO} \hat{L}_z)\hat{S}_z &= \frac{1}{2} \begin{bmatrix}
Y_s B_0 & i\lambda_{SO} \\
-i\lambda_{SO} & Y_s B_0
\end{bmatrix} \otimes \begin{bmatrix}
1 & 0 \\
0 & -1
\end{bmatrix} \\
\hat{H}_{JT} &= \hbar \begin{bmatrix}
K_x & K_y \\
K_y & -K_x
\end{bmatrix} \otimes \begin{bmatrix}
1 & 0 \\
0 & 1
\end{bmatrix}.
\end{align}
\] (S6)

\[
\begin{align}
\tan \theta &= \frac{2K_x + \Delta}{\sqrt{\lambda_{SO}^2 + 4K_y^2}}, \\
\tan \phi &= \frac{2K_y}{\lambda_{SO}}.
\end{align}
\] (S7)

In the above equation \( K_i \) represents an energy shift due to local strain in the crystal along axis \( i \). Diagonalizing Eq. (S5) leads to the eigenstates

\[
\begin{align}
|g\rangle &= (\cos \theta |e_x\rangle - i e^{-i\phi} \sin \theta |e_y\rangle) \downarrow \\
|e\rangle &= (\cos \theta |e_x\rangle + i e^{i\phi} \sin \theta |e_y\rangle) \uparrow \\
|f\rangle &= (\sin \theta |e_x\rangle + i e^{-i\phi} \cos \theta |e_y\rangle) \downarrow \\
|d\rangle &= (\sin \theta |e_x\rangle - i e^{i\phi} \cos \theta |e_y\rangle) \uparrow,
\end{align}
\] (S8)

(S9)

(S10)

(S11)

with

\[
\begin{align}
E_{f,g} &= (-Y_s B_0 \pm \Delta)/2, \\
E_{d,e} &= (Y_s B_0 \pm \Delta)/2
\end{align}
\] (S12)

with \( \Delta \simeq 2\pi \times 46 \text{ GHz} \). In this work, we can neglect the small distortions of the orbital states by the JT effect and in the remainder of this work, use the approximation \(|g\rangle \simeq |e_\downarrow\rangle, |e\rangle \simeq |e_\uparrow\rangle, |f\rangle \simeq |e_\downarrow\rangle, |d\rangle \simeq |e_\uparrow\rangle\).

**Strain coupling of SiV centers to phononic crystal modes**

As discussed in the main text, local lattice distortions associated with internal compression modes of the phononic crystal affect the defect’s electronic structure, which induces a strain coupling between these phonons and the orbital degrees of freedom of the center. The interaction Hamiltonian is given by

\[
H_{\text{strain}} = \sum_{ij} V_{ij} \epsilon_{ij}
\] (S13)

where \( V_{ij} \) is an operator acting on the electronic states of the defect center, and \( \epsilon \) is the strain tensor defined by

\[
\epsilon_{ij} = \frac{1}{2} \left( \frac{\partial Q_j}{\partial \epsilon_{ij}} + \frac{\partial Q_i}{\partial \epsilon_{ij}} \right).
\] (S14)

In this work we assume that the symmetry axis of the defect center is along the \( z \) direction while the phononic crystal is along the \( x \) axis. The strain Hamiltonian can be projected onto the irreducible representations of the \( D_{3d} \) group for SiV centers, which reflects the symmetry of the orbital wavefunctions, i.e.,

\[
H_{\text{strain}} = \hbar \sum_i V_i \epsilon_i.
\] (S15)

Each \( \epsilon_i \) is a linear combination of strain components \( \epsilon_{i,j} \), and corresponds to specific symmetries indicated by the subscript \( t \), i.e.,

\[
\begin{align}
\epsilon_{A_{1g}} &= \ell_\perp (\epsilon_{xx} + \epsilon_{yy}) + \ell_\parallel \epsilon_{zz} \\
\epsilon_{E_{g}} &= d(\epsilon_{xx} - \epsilon_{yy}) + f \epsilon_{zz} \\
\epsilon_{E_{g}} &= -2d \epsilon_{xy} + f \epsilon_{yz}.
\end{align}
\] (S16)
Here $t_\perp, t_\parallel, d,$ and $f$ are the four strain-susceptibility parameters that completely describe the strain-response of the orbital states $|e_x\rangle$ and $|e_y\rangle$. The effects of these strain components on the electronic states are described by

$$V_{A_{xy}} = |e_x\rangle\langle e_x| + |e_y\rangle\langle e_y|$$  \hspace{1cm} (S18)
$$V_{E_{xx}} = |e_x\rangle\langle e_x| - |e_y\rangle\langle e_y|$$  \hspace{1cm} (S19)
$$V_{E_{yy}} = |e_y\rangle\langle e_y| + |e_y\rangle\langle e_x|$$  \hspace{1cm} (S20)

The strain Hamiltonian can be rewritten in the basis spanned by the eigenstates of the spin-orbit coupling

$$H_{\text{strain}} = \hbar \epsilon E_x (L_- + L_+) - i \hbar \epsilon E_y (L_- - L_+)$$  \hspace{1cm} (S21)

where $L_+ = L_-^\dagger = |f\rangle\langle g| + |e\rangle\langle d|$ is the orbital raising operator within the ground state. Upon quantization, the mechanical displacement $\tilde{Q}(\vec{r})$ becomes an operator, which can be expressed in terms of the elementary normal modes and annihilation operators as

$$\tilde{Q}(\vec{r}) = \sum_{n,k} [Q_0 e^{ikx} \tilde{u}_{n,k}(\vec{r}) \hat{a}_{n,k} + \text{H.c.}].$$  \hspace{1cm} (S22)

The resulting strain coupling can be written as

$$\hat{H}_{\text{strain}} \simeq \sum_{n,k} [\hbar g_{n,k} \hat{a}_{n,k} \tilde{J}_x e^{ikx} + \text{H.c.}],$$  \hspace{1cm} (S23)

with the spin-phonon coupling strength given by

$$g_{n,k} = \frac{d}{\psi_l} \sqrt{\frac{\hbar \omega_{BE}}{2\pi paA}} s_{n,k}(\vec{r}).$$  \hspace{1cm} (S24)

Here the dimensionless profile is given by

$$s_{n,k}(\vec{r}) = \frac{1}{k} \left\{ (iku^x_{n,k} + \partial_x u^x_{n,k} - \partial_y u^y_{n,k} + \frac{f}{2d} \partial_z u^z_{n,k} + \frac{f}{2d} \partial_y u^y_{n,k}) - i \left[ (-iku^y_{n,k} - \partial_x u^y_{n,k} - \partial_y u^z_{n,k} + \frac{f}{2d} \partial_y u^y_{n,k}) \right] \right\}.$$  \hspace{1cm} (S25)

For compression modes along the phononic crystal direction $x$, the mode function can be approximated as $\tilde{u}_{n,k}(\vec{r}) \sim \epsilon_x \cos(\omega_{n,k} x/v_l)$, leading to $|s_{n,k}(\vec{r})| = 1$.

**Band-gap interactions between single SiV centers and acoustic modes**

As discussed in the main text, we consider the case where the transition frequency of the defect center is tuned close to the band edge. Then the spin is dominantly coupled to the modes near the band edge wavevector $k_0 = \pi/a$ due to the van Hove singularity in the density of states, i.e., $\lim_{k \to \pm \pi/a} |\psi_k| \to \infty$. In this case, the dispersion relation can be approximated to be quadratic $\epsilon_k \simeq \omega_{BE} - \alpha \alpha^2 (k - k_0)^2$, with $\alpha$ a parameter characterizing the band curvature. In the presence of a static magnetic field $\vec{B} = B_0 \hat{e}_z$ and a microwave driving field of frequency $\omega_0$ and Rabi-frequency $\Omega$ along $\hat{e}_x$, we can implement a Raman transition between the states $|g\rangle$ and $|e\rangle$ via the excited state $|f\rangle$ through coupling the SiV center to the mechanical modes. In the interaction picture, the full Hamiltonian is given by

$$\hat{H} = \sum_k \hbar g_k \hat{a}_k e^{ikx_0} (\hat{\sigma}_f + \hat{\sigma}_d) e^{\delta_{\text{diss}} t} + \hbar \Omega \hat{\sigma}_f e^{i\Omega t} + \text{H.c.}$$  \hspace{1cm} (S26)

In the dispersive limit, i.e., $\Delta_{\text{BE}} \delta \gg g_k, \Omega$, and after adiabatic elimination of the excited states $|f\rangle$ and $|d\rangle$, we obtain the effective interaction Hamiltonian

$$\hat{\mathcal{H}} = \sum_k \hbar g_{\text{eff}} (\hat{a}_k \hat{\sigma}_{eg} e^{ikx_0} e^{i\Delta_{\text{BE}} t} + \text{H.c.}),$$  \hspace{1cm} (S27)

with $\Delta_{\text{BE}} = \Delta - \delta - \omega_{\text{BE}}$. In the Schrödinger picture, we have

$$\hat{H} = \sum_k \hbar \omega_k \hat{a}_k^{\dagger} \hat{a}_k + \hbar \omega_0 \hat{\sigma}_{ee} + \sum_k \hbar g_{\text{eff}} (\hat{a}_k^{\dagger} \hat{\sigma}_{ge} e^{-ikx_0} + \hat{a}_k \hat{\sigma}_{ge} e^{ikx_0}).$$  \hspace{1cm} (S28)
For a single excitation in the system, there exists a bound state

$$|\varphi_b\rangle = \cos \theta |0\rangle + \sin \theta |1\rangle$$

within the bandgap with the eigenenergy $h \Omega_b$. Here $|0\rangle$ is the vacuum state for the phonon modes, and $|1\rangle = \int d k c_k |0\rangle$ is a single phonon excitation of the modes in the band. The bound state and the corresponding eigenenergy are determined by the eigenvalue equation

$$\hat{H} |\varphi_b\rangle = h \Omega_b |\varphi_b\rangle.$$  \hspace{1cm} (S30)

From this equation we have

$$\cos \theta (\Omega_b - \omega_s) = \sin \theta \sum_k g_{eff} c_k e^{ikx_0}$$

and

$$c_k \sin \theta (\Omega_b - \omega_k) = g_{eff} e^{-ikx_0}.$$  \hspace{1cm} (S32)

Solving these equations yields

$$c_k = g_{eff} e^{-ikx_0} \tan \theta (\Omega_b - \omega_k)$$

and

$$\Omega_b - \omega_s = \sum_k \frac{g_{eff}^2}{(\Omega_b - \omega_k)^2}.$$  \hspace{1cm} (S35)

When we take $\omega_k \simeq \omega_{BE} - \alpha a^2 (k - k_0)^2$, and change from a discrete modes to a continuous distribution, we can obtain

$$\Omega_b - \omega_s = \frac{\pi g_{eff}^2}{\sqrt{\alpha (\Omega_b - \omega_{BE})} L_c}$$

and

$$\tan^2 \theta = \frac{\omega_s - \Omega_b}{2(\omega_{BE} - \Omega_b)}.$$  \hspace{1cm} (S37)

In real space, the phononic part of the bound state is exponentially localized around the spin with spatial mode envelope

$$\mathcal{E}(x) = \int d k c_k Q_k(x) = \sqrt{\frac{2 \pi}{L_c}} e^{-|x-x_0|/L_c} Q_{k_0}.$$  \hspace{1cm} (S39)

**Band gap engineered spin-spin interactions between distant SiV centers**

As discussed in the main text, the band-gap interaction allows us to use the phononic crystal modes as a quantum bus to perform more complex tasks. Analogous to the spin-exchange interaction in cavity QED, two defect centers that are separated by a distance on the order of the length $L_c$ can exchange a phonon excitation via the induced acoustic cavity mode. We consider two separated SiV centers coupled to the same phononic crystal modes near the band edge, through Raman transitions between the states $|g\rangle$ and $|e\rangle$. In the interaction picture, we can obtain the interaction between the defect centers and phononic crystal modes

$$\hat{H} = \sum_{j=1,2} \sum_k h g_{eff}^j (\hat{a}_k^+ \hat{a}_j e^{-i \delta_k t - ikx_j} + \hat{a}_k \hat{a}_j^+ e^{i \delta_k t + ikx_j})$$

with $\delta_k = \omega_s - \omega_k$. In the dispersive regime $\delta_k \gg g_{eff}^j$, this will lead to an effective spin-spin interaction via the exchange of virtual phonons. With the phononic modes eliminated, the interaction is described by the effective Hamiltonian

$$\hat{H} = h \hat{\sigma}_{eg} \hat{\sigma}_{ge} g_{eff}^2 \int \frac{d k e^{i(kx_1-x_2)}}{\omega_s - \omega_k} + \text{H.c.}.$$  \hspace{1cm} (S41)
We can integrate over the phononic modes and apply the same approximation near the band edge as used to derive the bound state. To first order in $\Delta_{\text{BE}}^{-1}$, the interaction becomes

$$\hat{H}_{s-s} = \frac{\hbar g_c^2}{2\Delta_{\text{BE}}} e^{-|x_1-x_2|/L_c} \hat{\sigma}_{eg}^1 \hat{\sigma}_{ge}^2 + \text{H.c.} \quad (S42)$$

We can generalize the above results to the case where an array of distant defect centers are coupled with the band-gap mediated interaction. This opens another exciting perspective for quantum simulation, with spin-spin Hamiltonians for quantum magnetism of the general form

$$\hat{H}_{\text{spin}} = \sum_{\alpha=x,y,z} \sum_{i,j} J_{\alpha}^{i,j} \hat{\sigma}_{i\alpha} \hat{\sigma}_{j\alpha}, \quad (S43)$$

where $\hat{\sigma}_{i\alpha}$ are Pauli operators and $J_{\alpha}^{i,j}$ are the spin-spin interaction energies in the $\alpha$ direction for sites $i$ and $j$. Here, the range of interactions has an exponentially decaying envelope, i.e., $J_{\alpha}^{i,j} \sim e^{-|x_i-x_j|/L_c}$, and is restricted to nearest neighbours.

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