Controlled manipulation of light by cooperative response of atoms in an optical lattice: Supplementary Online Material

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In this supplementary information, we provide some of the technical details of the optical lattice system and the incident field used to excite it. In Section I, we describe the optical lattice potential. In Section II, we describe the dynamics of the atomic dipoles interacting with both the incident and scattered electric fields. In Section III, we describe how one can construct the approximate phase modulated driving field used to illuminate the optical lattice system and excite collective atomic excitations that were discussed in the text. Finally in Section IV, we discuss how one can obtain effective two-level atoms, which produce the collective response we investigate, from realistic atoms whose energy levels may be degenerate.

I. THE OPTICAL LATTICE TRAPPING POTENTIAL

We consider a two-dimensional square optical lattice of periodicity a, centered on the point $(x_0, y_0, 0)$. Four intersecting beams produce the optical confining potential

$$V = sE_R \left[\sin^2 \left(\pi \frac{x - x_0}{a} \right) + \sin^2 \left(\pi \frac{y - y_0}{a} \right) \right]$$
 (1)

where $E_R = \pi^2 \hbar^2/(2ma^2)$ is the lattice recoil energy [1], and the dimensionless confinement strength s controls the width of the vibrational ground-state wavefunction in each site (Wannier functions) that results from single-particle quantum fluctuations. An additional potential tightly confines the atoms in the z=0 plane. The lattice resides in a Mott-insulator state with precisely one atom per lattice site. Each lattice site, labeled by index j, has a potential minimum located at position \mathbf{R}_j , and the Wannier function $\phi_j(\mathbf{r}) \equiv \phi(\mathbf{r} - \mathbf{R}_j)$. When the confinement is sufficiently tight, the potential V in the neighborhood of each lattice site is roughly harmonic with

$$V(\mathbf{r}) \approx \frac{m}{2} \sum_{\mu=x,y,z} \omega_{\mu}^2 (\Delta r_{\mu})^2 \tag{2}$$

where $\omega_x = \omega_y = 2\sqrt{s}E_R/\hbar$, ω_z is the trapping frequency along the z direction, and $\Delta r_{\mu} \equiv \hat{\mathbf{e}}_{\mu} \cdot (\mathbf{r} - \mathbf{R}_j)$ is the displacement of the μ th component of \mathbf{r} from the lattice site \mathbf{R}_j . An atom in each site occupies the ground state of the harmonic oscillator potential

$$\phi(\mathbf{r}) = \frac{1}{(\pi^3 \ell^4 \ell_z^2)^{1/4}} \exp\left(-\frac{x^2 + y^2}{2\ell^2} - \frac{z^2}{2\ell_z^2}\right), \quad (3)$$

where the width of the of the wave function is $\ell = as^{-1/4}/\pi$, and its thickness $\ell_z = \sqrt{\hbar/(m\omega_z)}$. The atomic density, $\rho_j(\mathbf{r}) \equiv |\phi_j(\mathbf{r})|^2$, at site j thus has a Gaussian profile with a 1/e radius ℓ in the xy plane. This width is directly proportional to the lattice spacing and narrows with increased trapping strength s. It is possible to adjust the lattice spacing by using accordion lattices [2]. Moreover, the relationship between the lattice spacing and the Wannier wavefunction confinement may be controlled by magnetic field dressing [3].

II. DYNAMICS OF ATOMIC EXCITATIONS IN THE LATTICE

In this section, we elaborate on the dynamics of the atomic electric dipoles interacting with light. We show that the evolution of the system can be described as in Eq. (2) of the main text. We then discuss the Monte-Carlo method used to compute the average excitation energies $|e_i|^2$ displayed in Fig. 1 of the text.

A. Basic model

We consider an ensemble N two-level atoms placed in harmonic potentials centered at the lattice sites \mathbf{R}_i (i = $1, \ldots, N$). Each atom has an internal ground state $|g\rangle$ and an excited state $|e\rangle$ which differ in energy by $\hbar\omega_{e,g}$. A coherent, monochromatic field $\mathbf{D}_{\text{in}}^{+}(\mathbf{r},t)$ with frequency Ω impinges on the lattice. The field incident on the atoms in the lattice drives the $|g\rangle \leftrightarrow |e\rangle$ transition, inducing a polarization density $\mathbf{P}^{+}(\mathbf{r},t) = \sum_{j} \mathbf{P}_{j}^{+}(\mathbf{r},t)$, where the polarization due to an atom in site j, $\mathbf{P}_{i}^{+} = \mathbf{d}_{j}\delta(\mathbf{r} - \mathbf{r}_{j})$, \mathbf{d}_{j} is the dipole moment of an atom in site j, and \mathbf{r}_{j} is its position coordinate. Interactions between the atoms and the EM field are described by the electric dipole Hamiltonian $H_{\rm dip} = -\int d^3r \, \mathbf{D} \cdot \mathbf{P}/\epsilon_0$. Scattering of light from the atoms produces correlations between the positions of the atoms and the scattered field profile. In this way, continuous measurement of the scattered light yields an effective measurement of the atomic positions. This process simultaneously projects the position coordinates of an atom in each site j onto a specific position \mathbf{r}_j through the projection operator $\hat{Q}(\{\mathbf{r}_j\}) \equiv \bigotimes_{j=1}^N |\mathbf{r}_j\rangle_j \langle \mathbf{r}_j|$ acting on the initial vibrational state of the system, where $\{\mathbf{r}_i\}$ denotes the set $\{\mathbf{r}_1, \dots, \mathbf{r}_N\}$ of realized position coordinates for atoms in lattice sites $\{1, \ldots, N\}$. We therefore characterize the evolution of the polarization density associated with site j in terms of the slowly varying coherence conditioned on the realized atomic position \mathbf{r}_j , and the positions in all other sites $\mathbf{r}_{j'}$ for $j' \neq j$. We define the amplitudes $e_j(\mathbf{r}_j,t;\{\mathbf{r}_{j'\neq j}\}) \equiv e^{i\Omega t} \langle \sigma_j \rangle_{\{\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N\}}$ to be the slowly varying coherence between the ground and excited states of an atom at site j conditioned on the observation of atoms at positions $\{\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N\}$ within their respective sites, where σ_j is the coherence operator for an atom in site j. For a single realization of position coordinates of the atoms, the polarization in site j depends on the position of all the atoms via the amplitudes e_j :

$$\mathbf{P}_{j}(\mathbf{r}, t; \{\mathbf{r}_{j'}\}) = e^{-i\Omega t} \hat{\mathbf{d}} \wp \delta(\mathbf{r} - \mathbf{r}_{j}) e_{j}(\mathbf{r}_{j}, t; \{\mathbf{r}_{j'\neq j}\}), \quad (4)$$

where \wp is the dipole matrix element. In addition to the incident electric field, an atom at site j experiences driving by the fields $\mathbf{D}_{\mathrm{S},j'}^+$ scattered from all other sites $j' \neq j$ in the lattice. The total displacement field arriving at this site is thus

$$\mathbf{D}_{\mathrm{ext},j}^{+}(\mathbf{r},t) \equiv \mathbf{D}_{\mathrm{in}}^{+}(\mathbf{r},t) + \sum_{j'\neq j} \mathbf{D}_{\mathrm{S},j'}^{+}(\mathbf{r},t). \tag{5}$$

When the atomic dynamics evolve on timescales much longer than the time it takes for light to propagate across the optical lattice, the scattered fields can be expressed in the monochromatic limit as [4, 5]

$$\mathbf{D}_{S,j}^{+}(\mathbf{r}) = \frac{k^3}{4\pi} \int d^3r' \mathbf{G}(\mathbf{r} - \mathbf{r}') \cdot \mathbf{P}_{j}^{+}(\mathbf{r}'), \qquad (6)$$

where $k = \Omega/c$, and **G** is the radiation kernel with tensor components

$$\mathbf{G}_{\mu,\nu}(\mathbf{r}) = \frac{1}{k^2} \left(\partial_{\mu} \partial_{\nu} - \delta_{\mu,\nu} \nabla^2 \right) \frac{e^{ikr}}{kr} \,. \tag{7}$$

The monochromatic dipole radiation kernel, representing the radiated field at \mathbf{r} from a dipole residing at \mathbf{r}' , can be expressed as [6]

$$\mathbf{G}(\mathbf{r}) = \left[\frac{2}{3} + \left(\frac{\mathbf{r}\mathbf{r}}{r^2} - \frac{1}{3}\right) \left(\frac{3 - 3ikr - k^2r^2}{k^2r^2}\right)\right] \frac{e^{ikr}}{kr} + \frac{8\pi}{3}\delta(k\mathbf{r}). \tag{8}$$

B. Stochastic simulations

In the simulations we solve the cooperative optical response of the atomic sample to the incident field using a Monte-Carlo approach in which the position coordinates of the atoms are sampled according to their position correlation functions, and the optical response is calculated for each stochastic realization [7]. We assume that the atoms form a Mott-insulator state of precisely one atom per lattice site. The position coordinates of atoms within each site j are therefore independent stochastic variables, sampled from Gaussian distributions $\rho_j(\mathbf{r})$. The

atoms reside at the vibrational ground states of the lattice sites and the Gaussian distribution $\rho_i(\mathbf{r})$ results from the single-particle quantum fluctuations, determined by the Wannier wavefunction density in the particular site j. The atomic position in the site j is centered at \mathbf{R}_{j} . The width of the Wannier wavefunction is determined by the lattice confinement. Since each stochastic realization of position coordinates for the atoms in the N lattice sites $\{\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N\}$ can be interpreted as an outcome of a continuous measurement process of scattered light that localizes the atoms, each stochastic Monte-Carlo trajectory also represents a possible outcome of a single experimental run. We evaluate the ensemble averages of the atomic optical excitations by computing the excitations for each of many stochastic realizations of position coordinates of the atoms and then calculating their ensemble average. The numerically calculated ensemble average then corresponds to the experimentally measured ensemble average over many experimental runs and provides quantum mechanical expectation values of the observables.

In order to calculate the optical response for each stochastic realization of position coordinates for the atoms in the N lattice sites, $\{\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N\}$, we assume here that the incident light is sufficiently weak that we can neglect the excited state saturation of the atoms. In this limit, the coherence amplitude for an atom in site j obeys the equations of motion [7]

$$\frac{d}{dt}e_j = (i\delta - \Gamma/2)e_j + e^{i\Omega t} \frac{\wp}{i\hbar\epsilon_0} \hat{\mathbf{d}}^* \cdot \mathbf{D}_{\mathrm{ext},j}^+(\mathbf{r}_j, t), \quad (9)$$

where $\delta \equiv \Omega - \omega_{e,g}$ is the detuning of the incident light from the resonance of the atomic transition and Γ is the atomic spontaneous emission rate. For each stochastic realization of atomic positions, the light impinging on an atom in a particular site consists of the incident field and the scattered light from all the other N-1 sites. Because light scattered from an atom is directly proportional to its coherence amplitude, we obtain

$$\frac{d}{dt}e_{j} = (i\delta - \Gamma/2)e_{j} + \sum_{j'\neq j} C_{j,j'}e_{j'} + e^{i\Omega t} \frac{\wp}{i\hbar\epsilon_{0}} \hat{\mathbf{d}}^{*} \cdot \mathbf{D}_{\mathrm{in}}^{+}(\mathbf{r}_{j}, t),$$
(10)

where $C_{j,j'}$ is the coupling matrix element representing the effect of dipole radiation from the atom in site j' on the coherence amplitude of the atom in site j;

$$C_{j,j'} = \frac{3\Gamma}{2i} \hat{\mathbf{d}}^* \cdot \mathbf{G}(\mathbf{r}_j - \mathbf{r}_{j'}) \cdot \hat{\mathbf{d}}. \tag{11}$$

For each stochastic realization of position coordinates of the atoms, Eq. (10) represents a collective response of the atomic sample to the incident light. Repeated exchanges of a photon between the same atoms lead to cooperative response of the atoms. The system exhibits collective eigenmodes with each eigenmode associated with a specific resonance frequency and a radiative linewidth. In the text, we considered an 18×18 array with lattice spacing 0.55λ ($\lambda = 2\pi c/\Omega$), and dipole orientations

 $\hat{\mathbf{d}} \approx \hat{\mathbf{e}}_z + 0.1\hat{\mathbf{e}}_y$. For this configuration, when the atoms are placed precisely at the centers of the lattice sites \mathbf{R}_j , the collective mode spontaneous emission rates range from a very subradiant $3 \times 10^{-3}\Gamma$ to the superradiant 5Γ , while their collective frequency shifts from the single atom resonance range from -2Γ to 0.9Γ .

In each stochastic realization of position coordinates of atoms within their respective lattice sites, we solve the steady-state solution of the excitation amplitudes of the atom in each lattice site e_j by setting $de_j/dt=0$ in Eq. (10). The results for a single stochastic realization of $|e_j|^2$ are displayed in the main text. We then compute the ensemble average of the atomic excitation $\overline{|e_j|^2}$ by averaging over a sufficiently large number of stochastic realizations. That is, we take $\mathcal N$ stochastic realizations of the position coordinate of an atom within each site j. For the ν th realization ($\nu=1,\ldots,\mathcal N$) we have sampled the position coordinates of an atom in site j, $\mathbf r_j^{(\nu)}$. For these atomic positions, we solve the steady state of Eq. (10) to obtain the atomic amplitudes $e_j^{(\nu)}$ and calculate the ensemble average

$$\overline{|e_j|^2} = \frac{1}{\mathcal{N}} \sum_{\nu=1}^{\mathcal{N}} \left| e_j^{(\nu)} \left(\mathbf{r}_j^{(\nu)}; \left\{ \mathbf{r}_{j'\neq j}^{(\nu)} \right\} \right) \right|^2. \tag{12}$$

C. Many-particle correlations

In this paper we consider a specific many-particle atom state: the bosonic Mott-insulator state with precisely one atom per site. The atoms reside in the lowest vibrational state of each lattice site. Vacuum fluctuations for the position of the single-particle state of the atoms are incorporated in the Monte-Carlo sampling of the atomic positions from the Gaussian density distribution, determined by the Wannier wavefunctions of each lattice site. As we will show below, for the specific Mott-state of one atom per site, the sampling procedure also represents all the many-particle correlations of the system.

The joint probability distribution $P(\bar{\mathbf{r}}_1, \dots, \bar{\mathbf{r}}_N)$ for the positions of the N atoms is given by the absolute square of the normalized many-particle wavefunction

$$P(\bar{\mathbf{r}}_1, \dots, \bar{\mathbf{r}}_N) = |\Psi(\bar{\mathbf{r}}_1, \dots, \bar{\mathbf{r}}_N)|^2$$
(13)

$$P(\bar{\mathbf{r}}_1, \dots, \bar{\mathbf{r}}_N) \simeq \frac{1}{N!} \sum_{j_1 \dots j_N} |\phi_{j_1}(\bar{\mathbf{r}}_1)|^2 \dots |\phi_{j_N}(\bar{\mathbf{r}}_N)|^2 \quad (14)$$

Here the coordinates of the N atoms are denoted by $(\bar{\mathbf{r}}_1, \ldots, \bar{\mathbf{r}}_N)$. The summation runs over all possible N-tuples (j_1, \ldots, j_N) of the state labels $j = (1, \ldots, N)$ referring to the lattice sites j with precisely one atom per site. The Wannier wavefunctions for each lattice site ϕ_j in Eq. (14) are assumed to have a negligible overlap with the neighboring sites, so that $\phi_j(\mathbf{r})\phi_k(\mathbf{r}) \simeq 0$, whenever $j \neq k$. Since we have exactly one atom per site, we may

rewrite the joint probability distribution of Eq. (14) as

$$P(\bar{\mathbf{r}}_1, \dots, \bar{\mathbf{r}}_N) \simeq \frac{1}{N!} \sum_{i_1 \dots i_N} |\phi_1(\bar{\mathbf{r}}_{i_1})|^2 \dots |\phi_N(\bar{\mathbf{r}}_{i_N})|^2$$
 (15)

where the summation runs over all possible permutations of the atomic coordinates i = (1, ..., N). Since there are N! such permutations, we can express the joint probability distribution in terms of the positions of an atom in the jth lattice site \mathbf{r}_j , instead of the position coordinates of the jth atom $\bar{\mathbf{r}}_j$. Each N! term contributes equally in the sum and we obtain for the joint probability distribution of the position of an atom in the lattice sites j = (1, ..., N) in the coordinate representation $(\mathbf{r}_1, ..., \mathbf{r}_N)$

$$P'(\mathbf{r}_1, \dots, \mathbf{r}_N) \simeq |\phi_1(\mathbf{r}_1)|^2 \dots |\phi_N(\mathbf{r}_N)|^2$$
 (16)

In the resulting joint probability distribution the position coordinates of atoms within each site j are independent stochastic variables that are sampled from the Gaussian distributions $\rho_j(\mathbf{r}) = |\phi_j(\mathbf{r})|^2$, corresponding to the stochastic Monte-Carlo sampling procedure implemented in the previous section.

III. THE INCIDENT LIGHT

By exploiting interactions between the atoms, one can tailor the incident field so that it drives specific linear combinations of collective modes, providing a desired collective response. In the text, for example, we consider phase modulated driving that can excite an array of isolated atoms arranged in a checkerboard pattern on an optical lattice. A spatial light modulator is employed to produce an incident field approximately of the form

$$\mathbf{E}_{\text{in}}^{+}(\mathbf{r},t) = \hat{\mathbf{e}}_{y} E_{0} e^{i(kz - \Omega t)} e^{i\varphi(x,y)}, \tag{17}$$

where

$$\varphi(x,y) = \varphi_{\max} \sin(\kappa x) \sin(\kappa y). \tag{18}$$

A field profile of this form, however, contains evanescent plane wave components whose transverse wavevectors excede the the carrier wave number k. We therefore approximate this phase modulated field through the truncated Fourier expansion

$$\mathbf{E}_{\text{in}}^{+} = \sum_{m,n} C_{m,n} \hat{\mathbf{e}}_{m,n} e^{i(\mathbf{k}_{m,n} \cdot \mathbf{r} - \Omega t)}, \tag{19}$$

where $\mathbf{k}_{m,n} = m\kappa\hat{\mathbf{e}}_x + n\kappa\hat{\mathbf{e}}_y + q_{m,n}\hat{\mathbf{e}}_z$, $q_{m,n} \equiv \sqrt{(\Omega/c)^2 - \kappa^2(m^2 + n^2)}$, and $\hat{\mathbf{e}}_{m,n}$ is the normalized projection of the vector $\hat{\mathbf{e}}_y$ onto the plane perpendicular to $\mathbf{k}_{m,n}$. We have truncated the expansion for values of m and n for which $q_{m,n}^2 \geq 0$.

Because our goal was to produce a phase modulated driving of the meta-atoms, we choose $C_{m,n}$ so as to reproduce a phase modulated driving, i.e.

$$\hat{\mathbf{d}}^* \cdot \mathbf{E}_{\text{in}}^+ = \sum_{m,n} C_{m,n} (\hat{\mathbf{d}}^* \cdot \hat{\mathbf{e}}_{m,n}) e^{i(\mathbf{k}_{m,n} \cdot \mathbf{r} - \Omega t)}$$
(20)

$$\approx \hat{\mathbf{d}}^* \cdot \hat{\mathbf{e}}_y e^{i\varphi(x,y)} e^{i(kz - \Omega t)}, \tag{21}$$

The coefficients $C_{m,n}$ are obtained from the discrete Fourier transform of the phase modulation $\exp(i\varphi(x,y))$ and dividing by $\hat{\mathbf{e}}_{m,n} \cdot \hat{\mathbf{d}}$.

IV. REALIZING AN EFFECTIVE TWO-LEVEL ATOMIC LEVEL STRUCTURE

The simulations of the cooperative response were performed using two-level atoms. In this section we show how an effective two-level system can be realized using atoms both with and without degenerate electronic ground state manifold. In the first case a $J=0 \rightarrow J=1$ transition represents an effective two-level system when only one of the excited states is resonant to the incident field and the other levels are tuned off-resonant using magnetic fields. In the second case, one may use a cycling transition that decouples all except one electronic ground state and excited state.

Specifically, the atoms in the lattice are initially trapped in a stable electronic ground state $|g\rangle$. The incident field with frequency Ω drives transitions between the ground state and an excited state $|e\rangle$. This excited state energy level must be shifted so that a field of frequency Ω , independently of its polarization, only drives the $|g\rangle \leftrightarrow |e\rangle$ electronic transition. Furthermore, one must choose $|e\rangle$ so that it can only spontaneously decay into the designated ground state $|g\rangle$.

One way to realize a two-level atom is to employ the cycling transition. That is, choose $|g\rangle$ to be the Zeeman state that maximizes the projection of angular momentum onto the z axis in the hyperfine ground level with the largest total angular momentum F_g . For an alkali metal atom, this would be the state $|g\rangle=|^2S_{1/2};F_g,m_g=F_g\rangle$, where m_q is the angular momentum along the z axis. Then, $|e\rangle$ would be in a level with total atomic angular momentum $F_e = F_g + 1$ with the z component of angular momentum $m_e = F_e$. Selection rules guarantee that an atom in state $|e\rangle$ could only decay into $|g\rangle$. The $|g\rangle \leftrightarrow |e\rangle$ transition could be shifted out of resonance with all other atomic transitions by applying a uniform dc magnetic field along the z direction. For example, in ⁸⁷Rb, the Zeeman shift from a magnetic field of 65 G would shift the $|g\rangle \leftrightarrow |e\rangle$ transition out of resonance with all other transitions by about 10 linewidths. This would produce an effective two level atom whose coherent excitation produces a circularly polarized dipole $\mathbf{d}_{\text{cycling}} = -(\mathbf{\hat{e}}_x + i\mathbf{\hat{e}}_y)/\sqrt{2}$.

In the manuscript, we considered a transition which produced a linearly polarized dipole $\hat{\mathbf{d}} \approx \hat{\mathbf{e}}_z + 0.1\hat{\mathbf{e}}_y$. To attain this, one could trap a species of alkaline-earth or rare-earth metal atom with zero nuclear spin so as to eliminate superfluous hyperfine levels which could result in unwanted Raman scattering. The electronic ground state $|g\rangle$ of this atom would be the non-degenerate ${}^{1}S_{0}$ state, possessing zero angular momentum. The excited state $|e\rangle$ would then reside in an excited level with angular momentum $J_e = 1$, and have a zero projection of angular momentum along the desired dipole orientation d. For instance, the Mott insulator transition has been experimentally observed using bosonic ¹⁷⁴Yb [8]. As with the cycling transition, the atomic states with angular momentum projections ± 1 could be shifted out of resonance by applying a uniform dc magnetic field parallel to d.

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