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To cite this article: Ping Xiang *et al* 2013 *New J. Phys.* **15** 063015

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Non-adiabatic control of quantum energy transfer in ordered and disordered arrays

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New Journal of Physics **15** (2013) 063015 (24pp)

Received 27 February 2013

Published 12 June 2013

Online at <http://www.njp.org/>

doi:10.1088/1367-2630/15/6/063015

Abstract. An elementary excitation in an aggregate of coupled particles generates a collective excited state. We show that the dynamics of these excitations can be controlled by applying a transient external potential which modifies the phase of the quantum states of the individual particles. The method is based on an interplay of adiabatic and sudden time scales in the quantum evolution of the many-body states. We show that specific phase transformations can be used to accelerate or decelerate quantum energy transfer and spatially focus delocalized excitations onto different parts of arrays of quantum particles. We consider possible experimental implementations of the proposed technique and study the effect of disorder due to the presence of impurities on its fidelity. We further show that the proposed technique can allow control of energy transfer in completely disordered systems.



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1. Introduction

Experiments with ultracold atoms and molecules trapped in optical lattices have opened a new frontier of condensed-matter physics research. The unique properties of these systems—in particular, large (>400 nm) separation of lattice sites, the possibility of tuning the tunneling amplitude of particles between lattice sites by varying the trapping field and the possibility of controlling interparticle interactions with external electric or magnetic fields—offer many exciting applications ranging from quantum simulation of complex lattice models [1–14] to the study of novel quasi-particles [15] that cannot be realized in solid-state crystals. In the limit of strong trapping field, each site of an optical lattice is populated by a fixed number of ultracold atoms or molecules. Such states can be produced with either bosonic or fermionic particles [7, 16]. Here, we consider an optical lattice fully or partially filled with one particle per lattice site, and assume that tunneling between lattice sites is completely suppressed. Such an array can be thought of as a prototype of a system, in which a single lattice site (or a small number of lattice sites) can be individually addressed by an external field of a focused laser beam. This can be exploited for engineering the properties of quantum many-body systems by changing the energy of particles in individual lattice sites [17].

In this paper, we consider the generic problem of energy transfer—i.e. the time evolution of an elementary quantum excitation—in such a system. In particular, we explore the possibility of controlling energy transfer through an array of coupled quantum monomers by applying monomer-specific external perturbations. This is necessary for several applications. Firstly, collective excitations in molecular arrays in optical lattices have been proposed as high-fidelity candidates for quantum memory [18]. The ability to manipulate collective excitations is necessary for building scalable quantum computing networks [19]. Secondly, ultracold atoms and molecules in optical lattices can be perturbed by a disorder potential with tunable strength [20]. Engineering localized and delocalized excitations in such systems can be used to investigate the role of disorder-induced perturbations on quantum energy transfer, a question of central importance for building efficient light-harvesting devices [21]. Thirdly, the possibility of controlling energy transfer in an optical lattice with ultracold atoms or molecules can be used to realize inelastic scattering processes with both spatial and temporal control. Finally, control

over energy transfer in quantum systems can be used for studying condensed-matter excitations and energy transport without statistical averaging.

An excitation of a coupled many-body system generates a wave packet representing a coherent superposition of single-particle excitations. The method proposed here is based on shaping such many-body wave packets by a series of sudden perturbations, in analogy with the techniques developed for strong-field alignment and orientation of molecules in the gas phase [22]. Alignment is used in molecular imaging experiments and molecular optics [22–25], and is predicted to provide control over mechanical properties of molecular scattering [26, 27]. Here, we consider the use of similar techniques for controlling quantum energy transfer in an interacting many-body system. When applied to a completely ordered system, the proposed method is reminiscent of the techniques used to move atoms in optical lattices, where a uniform force is applied for a short period of time [28]. The conceptual difference comes from the fact that in the present case the momentum is acquired by a quasi-particle—a collective excitation distributed over many monomers. During the subsequent evolution, the particles do not move—rather, the excitation is transferred from one monomer to another. In order to control such excitations, we exploit an interplay of the adiabatic and sudden time scales, which correspond to single-monomer and multi-monomer evolution. We also exploit the wave-like nature of the excitation wave function to draw on the analogy with wave optics. This analogy, too, is not complete due to the discrete nature of the lattice.

In order to emphasize the generality of the proposed method, we formulate the problem in terms of the general Hamiltonian parameters. We then describe in detail how the required external perturbations can be realized in experiments with ultracold atoms and molecules. The possibility of using rotational excitations in molecular arrays is particularly interesting due to the long lifetime of rotationally excited states. Electronic excitations of atoms in an optical lattice may also give rise to collective excitations [29]. However, the lifetime of these excited states is limited by fast spontaneous emission [30, 31]. We propose a mechanism for suppressing spontaneous decay by tailoring the properties of the excitation wave packets.

The paper has the following structure. Sections 2 and 3 present the results in terms of the general Hamiltonian parameters. Section 4 addresses the particular case of ultracold atoms and molecules. Section 5 discusses controlled energy transfer in systems with, specifically, dipole–dipole interactions. Section 6 considers the effects of lattice vacancies on the possibility of controlling energy transfer and section 7 extends the proposed technique to control of excitation dynamics in strongly disordered arrays with a large concentration of impurities. Section 8 presents the conclusions.

2. Sudden phase transformation

Consider, first, an ensemble of N coupled identical monomers possessing two internal states arranged in a one-dimensional (1D) array with translational symmetry. The Hamiltonian for such a system is given by

$$H_{\text{exc}} = \Delta E_{e-g} \sum_n |e_n\rangle\langle e_n| + \sum_{n,m} \alpha(n-m) |e_n, g_m\rangle\langle g_n, e_m|, \quad (1)$$

where $|g_n\rangle$ and $|e_n\rangle$ denote the ground and excited states in site n , ΔE_{e-g} is the monomer excitation energy and $\alpha(n-m)$ represents the coupling between two monomers at sites n and m .

The singly excited state of the system is

$$|\psi_{\text{exc}}\rangle = \sum_{n=1}^N C_n |e_n\rangle \prod_{i \neq n} |g_i\rangle. \quad (2)$$

In general, the expansion coefficients C_n are complicated functions of n determined by the properties of the system, in particular, the translational invariance or lack thereof as well as the strength of disorder potential. If an ideal, periodic system with lattice constant a is excited by a single-photon transition, the expansion coefficients are $C_n = e^{iakn}/\sqrt{N}$ and $|\psi_{\text{exc}}\rangle \Rightarrow |\psi_{\text{exc}}(k)\rangle$ represents a quasi-particle called Frenkel exciton, characterized by the wave vector k [33]. The magnitude of the wave vector k is determined by the conservation of the total (exciton plus photon) momentum. The energy of the exciton is given by $E(k) = \Delta E_{e-g} + \alpha(k)$ with $\alpha(k) = \sum_n \alpha(n) e^{-iakn}$. In the nearest neighbor approximation

$$E(k) = \Delta E_{e-g} + 2\alpha \cos ak, \quad (3)$$

where $\alpha = \alpha(1)$.

With atoms or molecules on an optical lattice, it is also possible to generate a localized excitation placed on a single site (or a small number of sites) by applying a gradient of an external electric or magnetic field and inducing transitions in selected atoms by a pulse of resonant electromagnetic field [34]. The presence of a disorder potential, whether coming from jitter in external fields or from incomplete population of lattice sites, also results in spatial localization. Similar to how equation (2) defines the collective excited states in the basis of lattice sites, any localized excitation $|\psi\rangle$ can be generally written as a coherent superposition of the exciton states $|\psi_{\text{exc}}(k)\rangle$ with different k :

$$|\psi\rangle = \sum_k G_k |\psi_{\text{exc}}(k)\rangle. \quad (4)$$

Control over energy transfer in an ordered array can be achieved by (i) shifting the exciton wave packets in the momentum representation (which modifies the group velocity and the shape evolution of the wave packets) and (ii) focusing the wave packets in the coordinate representation to produce localized excitations in an arbitrary part of the lattice. To achieve this, we propose to apply a series of site-dependent perturbations that modify the phases of the quantum states of spatially separated monomers. These phase transformations change the dynamics of the time evolution of the collective excitations. Here we consider the transformations leading to acceleration or deceleration of collective excitations, while the focusing phase transformations are described in section 3.

For modifying the group velocity of a collective excitation, the essential idea is to add a factor $e^{i\delta an}$ to each term in the expansion (2), so that each $|\psi_{\text{exc}}(k)\rangle$ component in a wave packet is transformed into $|\psi_{\text{exc}}(k + \delta)\rangle$. This transformation shifts the wave packets by δ in k -space while preserving their shape. As a result, one can engineer wave packets probing any part of the dispersion $E(k)$ leading to different group velocity and shape evolution. The feasibility of such transformation in an ensemble of atoms or molecules on an optical lattice is discussed below and in section 4.

Adding a site-dependent phase to the excitonic wavefunction exploits an interplay of the adiabatic and sudden time scales. Consider the n th monomer subjected to an external field $\mathcal{E}_n(t)$ which varies from 0 to some value and then back to 0 in time T . If the variation is adiabatic with respect to the evolution of the free monomer states, $T \gg \hbar/\Delta E_{e-g}$, each eigenstate $|f\rangle$ of

the monomer acquires a state-dependent phase shift [35]

$$|f_n(T)\rangle = e^{-i\phi_n^f} |f_n(0)\rangle, \quad (5)$$

where $\phi_n^f = \frac{1}{\hbar} \int_0^T E_n^f(t) dt$, $E_n^f(t)$ is the instantaneous eigenenergy and f can be e or g . Now consider the action of such phase change on the collective excitation state (2). If $T \ll \hbar/\alpha$, the change is sudden with respect to the excitation transfer between monomers and the state (2) acquires a site-dependent phase $\Phi_n = \phi_n^e - \phi_n^g$. If $\Phi_n = \Phi_0 + na\delta$, then the momentum δ is imparted onto the excitonic wavefunction. By analogy with ‘pulsed alignment of molecules’ [22], we call this transformation a ‘phase kick’ or ‘momentum kick’. Its action is also similar to that of a thin prism on a wavefront of a monochromatic laser beam.

In order to illustrate the shifting of exciton wave packets in the momentum space, we solve numerically the time-dependent Schrödinger equation with the unperturbed Hamiltonian (1), subjected to a transient site-dependent external perturbation that temporarily modulates ΔE_{e-g} . We choose the parameters $\Delta E_{e-g} = 12.14$ GHz, $\alpha = 22.83$ kHz and the lattice constant $a = 400$ nm that correspond to an array of polar molecules trapped in an optical lattice, as described in detail in section 4. The time-dependent perturbation has the form of a short pulse with the duration $T = 3 \mu\text{s}$. The phase acquired by the particles during this time is given by $\Phi_n \simeq \Phi_0 - 1.29n$, which can be achieved with a focused laser beam, as described in section 4.

The excitation at $t = 0$ is described by a Gaussian wave packet of the exciton states $|\psi_{\text{exc}}(k)\rangle$, with the central wavevector $k = 0$. Figure 1 shows that the entire wave packet acquires momentum during the external perturbation pulse (left panels). This is manifested as a phase variation in the coordinate representation, and as a shift of the central momentum in the k -representation. After the external perturbation is gone, the wave packet does not evolve in the k -representation and moves with the acquired uniform velocity in the coordinate representation.

The results presented in figure 1 and all subsequent results of this work are for a single collective excitation in an interacting many-particle system. A general experimental implementation may result in multiple excitations, leading to nonlinear exciton interactions. There are two mechanisms for exciton–exciton interactions: kinematic interactions arising from the statistical properties of excitons and dynamical interactions determined by the matrix elements of the inter-particle interactions in the Hilbert sub-space of binary excitations [33, 36]. The effects of the kinematic interactions on energy transfer in molecular crystals have never been observed so these interactions are considered to be weak, especially in the limit of a small number of excitations easily achievable in experiments [37]. For molecules on an optical lattice, the dynamical interactions are important in the presence of strong external electric fields where molecular states of different parity are strongly mixed [15, 38]. At weak parity-mixing fields considered here, the exciton–exciton interactions insignificantly mix different k states of the individual excitons, contributing weakly to localization. These effects are expected to be much smaller than the disorder-induced perturbations, discussed in sections 6 and 7.

3. Focusing of a delocalized excitation

In order to achieve full control over excitation transfer, it is desirable to find a particular phase transformation that focuses a delocalized many-body excitation onto a small part of the lattice, ideally a single lattice site. In optics, a thin lens focuses a collimated light beam by shifting the phase of the wavefront, thus converting a plane wave to a converging spherical wave. Similarly, a phase kick can serve as a time domain ‘lens’ for collective excitations: an excitation initially

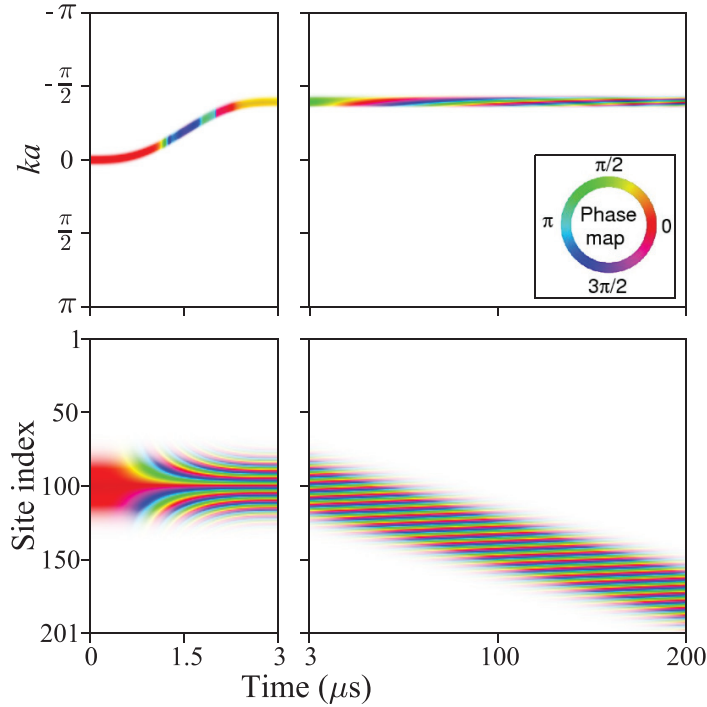


Figure 1. Example of controlled energy transfer in a 1D array of quantum monomers subjected to a linear phase transformation. The graph illustrates the evolution of the exciton wave packet centered at $k = 0$ and initially positioned at the center of the array. The phase of the wave function is shown by color. The brightness of color corresponds to the amplitude of the excitation with white color corresponding to zero amplitude. The calculation is for a 1D array of 201 monomers with $\alpha = 22.83$ kHz and $\Delta E_{e-g} = 12.14$ GHz, and the linear phase transformation $\Phi_n \simeq \Phi_0 - 1.29n$. As described in section 4, these parameters correspond to LiCs molecules trapped on an optical lattice with lattice constant $a = 400$ nm and subjected to a homogeneous dc field of 1 kV cm^{-1} directed perpendicular to the intermolecular axis. The kicking potential leading to this particular phase transformation can be provided by a $\lambda = 1064$ nm Gaussian laser beam, with the propagation direction along the array axis, focused to $5 \mu\text{m}$, with the intensity at the focus equal to 10^7 W cm^{-2} . The laser pulse is on between 0 and $3 \mu\text{s}$.

delocalized over a large number of monomers can be focused onto a small region of the array after some time. By analogy with optics, a concave or convex symmetric site-dependent phase $\Phi(n)$ applied simultaneously to all monomers may turn a broad initial distribution $C_n(t = 0)$ into a narrow one.

The dynamics of the excitation state in the lattice is determined by the time dependence of the coefficients $C_n(t)$ in equation (2). In order to find the expression for $C_n(t)$, we expand the amplitudes at $t = 0$ in a Fourier series

$$C_n(t = 0) = \sum_q \frac{e^{iqn}}{\sqrt{N}} C(q; t = 0) \quad (6)$$

and apply the propagator $e^{-iE(q)t/\hbar}$ to each q -component with $E(q)$ representing the exciton energy given by equation (3). Transforming the amplitudes $C(q)$ back to the site representation then yields

$$C_m(t) = \frac{1}{N} \sum_{n,k} C_n(t=0) e^{i[\Phi(n)+ka(m-n)-E(k)t/\hbar]}, \quad (7)$$

where $\Phi(n)$ is a site-dependent phase applied at $t=0$, as described in the previous section. Note that the phase $\Phi(n)$ does not have to be applied instantaneously. The phase $\Phi(n, t)$ can be applied continuously over an extended time interval as long as the accumulated phase gives the desired outcome $\int_0^T \Phi(n, t) dt = \Phi(n)$.

As equation (7) shows, the focusing efficiency is determined by the phase transformation and the shape of the dispersion curve $E(k)$. Given the cosine dispersion of excitons (3), is it possible to focus a delocalized excitation onto a single lattice site? To answer this question, we assume that $C_{n=n_0}(t=0) = 1$ and apply equation (7) to calculate the coefficients $C_m(t)$ at $t = -\tau$. Using the expansion of an exponent in Bessel functions

$$e^{-ia \cos x} = \sum_n e^{i(x-\pi/2)n} J_n(a) \quad (8)$$

and the orthonormality of the Bessel functions

$$\sum_n J_n(x) J_{n-m}(x) = \delta_{m,0}, \quad (9)$$

we find that the wave packet (2) with the expansion coefficients

$$C_n^{(n_0)} = J_{n-n_0}(2\alpha\tau) e^{i\pi(n-n_0)/2} \quad (10)$$

focuses upon coherent evolution, in time τ on a single site n_0 . This shows that a phase transformation alone is, generally, not sufficient to create a collective excitation state that focuses onto a single lattice site. The best focusing must involve both the phase and amplitude modulations, which may be difficult to realize in experiments. A simpler procedure can be implemented if the phase transformations are restricted to a particular part of the exciton dispersion.

From wave optics, waves with quadratic dispersion can be focused, while those with linear dispersion propagate without changing the wave packet shape [39, 40]. It is this interplay of the quadratic (at low k) and linear (at $k \approx \pm\pi/2a$) parts of the cosine-like exciton dispersion (3) that precludes perfect focusing of a general collective excitation. In order to avoid the undesirable amplitude modulations, it may be possible to focus delocalized excitations by a phase transformation that constrains the wave packet (4) to the quadratic part of the dispersion $E(k)$. For such wave packets, adding a quadratic phase $\Phi(n) = \Phi_0(n - n_0)^2$ must lead to focusing around site n_0 . Below we illustrate the effect of the quadratic phase transformation for two types of initial states.

Firstly, consider a broad Gaussian wave packet (2) with $C_n(\tilde{\sigma}_x; t=0) = \sqrt{a/\tilde{\sigma}_x} \sqrt{\pi} \exp[-a^2(n - n_0)^2/2\tilde{\sigma}_x^2]$ where $\tilde{\sigma}_x \gg a$ is the initial width. The corresponding width in the wave vector space is given by $\sigma_k = 1/\tilde{\sigma}_x$. The application of an inhomogeneous phase $\Phi(n) = \Phi_0(n - n_0)^2$ at $t=0$ results in additional broadening of the initial state, and the total width of the wave packet in the wave vector space with the account of the phase-induced contribution becomes [39, 40]

$$\sigma_k(\tilde{\sigma}_x, \Phi_0) = \frac{1}{\tilde{\sigma}_x} \sqrt{1 + 4\Phi_0^2 \tilde{\sigma}_x^4 / a^4}. \quad (11)$$

By analogy with optics, one should expect better focusing with larger Φ_0 (the width of the wave packet in real space is $\sigma_x(\Phi_0) = 1/\sigma_k(\tilde{\sigma}_x, \Phi_0)$). However, large values of Φ_0 may take the wave packet outside the quadratic part of the dispersion, impeding the focusing. To find the optimal phase Φ_0^* that keeps the wave packet within the quadratic dispersion while focusing it, we use the condition $\Delta_k = a\sigma_k \lesssim 1$, which yields $\Phi_0^* = \pm a/2\tilde{\sigma}_x$ for the optimal focusing. At time

$$t_* \approx 1/4\alpha\Phi_0^*, \quad (12)$$

the wave packet is most focused and has a width

$$\sigma_{x,F}(\Phi_0^*) = \frac{\tilde{\sigma}_x}{\sqrt{1 + 4\Phi_0^{*2}\tilde{\sigma}_x^4/a^4}} \approx a. \quad (13)$$

For the time t_* in equation (12) to be positive, α and Φ_0^* must have the same sign. Therefore, a convex quadratic phase profile $\Phi(n)$ with $\Phi_0 > 0$ must focus collective excitations in a system with repulsive couplings between particles in different lattice sites ($\alpha > 0$), and a concave quadratic phase profile $\Phi(n)$ with $\Phi_0 < 0$ must focus excitations in a system with attractive couplings ($\alpha < 0$).

Secondly, consider a completely delocalized excitation (2) with $C_n(k; t = 0) = e^{iakn}/\sqrt{N}$ describing an eigenstate of an ideal system of N coupled monomers. If $E(k)$ in equation (7) is approximated as $E(k) = \Delta E_{e-g} - \alpha a^2 k^2$, the quadratic phase transformation $\Phi(n) = \Phi_0 n^2$ yields

$$C_m(t) = \frac{e^{-i\alpha a^2 k^2}}{N} \sqrt{\frac{i\pi}{N\Phi_0}} \sum_q e^{i[a^2(k-q)^2(\alpha t - 1/4\Phi_0) + qa(m+2\alpha ak)]} \Theta\left(-\frac{N\Phi_0}{a} < k - q < \frac{N\Phi_0}{a}\right), \quad (14)$$

where $\Theta(z) = 1$ if z is true and zero otherwise. In order to derive equation (14), we used the approximate equality

$$\int_{-M}^M dx e^{-i(ax^2+bx)} \approx \sqrt{\frac{\pi}{ia}} e^{ib^2/4a} \Theta(-2Ma < b < 2Ma), \quad (15)$$

obtained by approximating the error function of a complex argument $\text{Erf}(\sqrt{i}x)$ by the sign function, which is accurate for large argument x .

At time $t_* = 1/4\alpha\Phi_0$, the terms quadratic in q in equation (14) are canceled, and the sum over q reduces to a delta-function, if the summation limits are from $-\pi/a$ to π/a . Therefore, the choice $\Phi_0 = \pi/N$ yields $C_m(t) = \sqrt{i} e^{-iNa^2k^2/4\pi} \delta_{m,-v_k}$, where v_k is the index of the initial wave vector $k = 2\pi v_k/Na$, quantized due to the discreteness of the lattice. According to equation (14), the dimensionless width of the wave packet in the wave vector space is $\Delta_k(\Phi_0) \equiv a\sigma_k(\Phi_0) \approx 2N\Phi_0$. When $\Phi_0 = \pi/N$, the wave packet spreads over the entire Brillouin zone, including the linear parts of the exciton dispersion. Using equation (15) we find that for an arbitrary value of $\Delta_k(\Phi_0)$, the site amplitudes at the time of focusing $t_* = 1/4\alpha\Phi_0$ are

$$C_n(k; t = t_*) \approx \frac{e^{i\Delta(\Phi_0)n^2/2N}}{n} \sqrt{\frac{2i}{\pi\Delta_k(\Phi_0)}} \sin(n\Delta_k(\Phi_0)/2). \quad (16)$$

In order to keep the linear part of the dispersion spectrum unpopulated, we choose the optimal focusing phase $\Phi_0^* \sim 1/2N$, so that $\Delta_k(\Phi_0^*) \sim 1$.

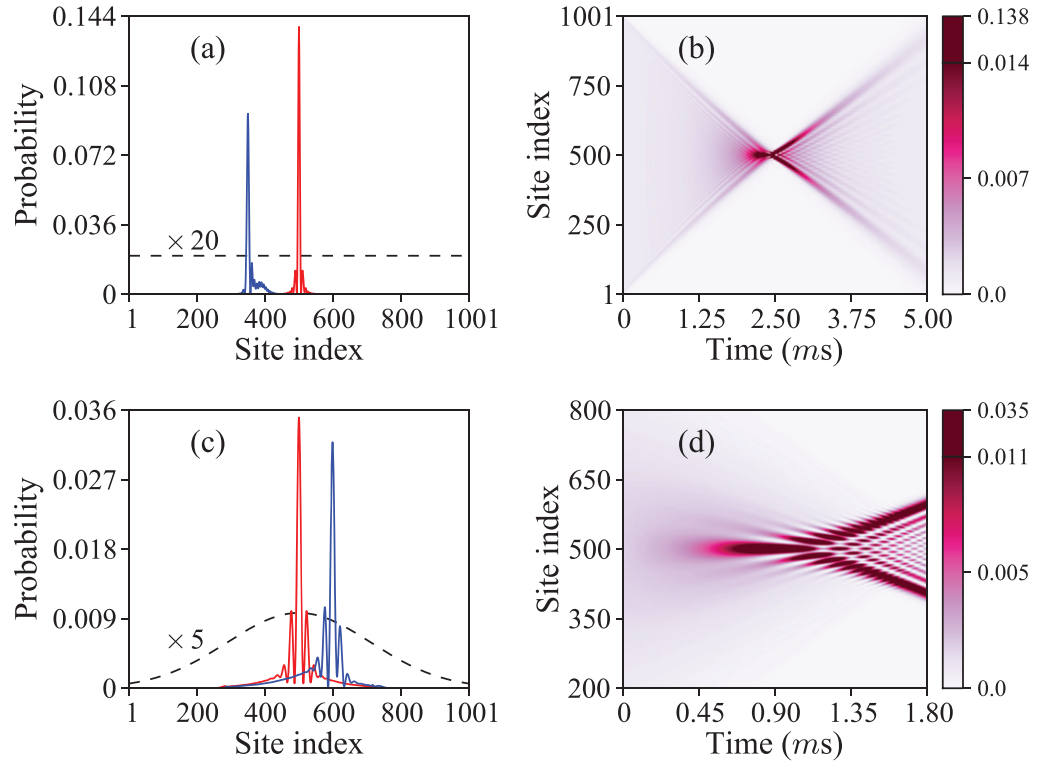


Figure 2. Focusing of a completely delocalized collective excitation (panels (a) and (b)) and a broad Gaussian wave packet of Frenkel excitons (panels (c) and (d)) in a 1D array using the quadratic phase transformations at $t = 0$ as described in text. In panels (b) and (d), the excitation probability distribution is displayed by color. The dashed lines show the initial distribution magnified by 20 and 5 respectively in (a) and (c). The solid curves in panels (a) and (c) correspond to two different phase transformations focusing the same wave packet onto different parts of the array. The calculations are performed with the same parameters α , a and ΔE_{e-g} as in figure 1. The results are computed with all couplings accounted for.

Equations (13) and (16) are valid for a many-body system with nearest neighbor interactions only. In most physical systems, the energy dispersion is modified by long-range couplings. In order to confirm that the above predictions are also valid for systems with long-range interactions and illustrate the focusing of delocalized excitations, we compute the time evolution of the wave packets by solving the wave equation numerically for a system with long-range dipole–dipole interactions. Figure 2 illustrates the focusing dynamics of a completely delocalized excitation (panels (a) and (b)) and a broad Gaussian wave packet (panels (c) and (d)) in a system with all (first neighbor, second neighbor, etc) couplings explicitly included in the calculation. The results show that the collective excitations can be focused to a few lattice sites. The role of the long-range coupling will be explicitly discussed in section 6.

The focusing scheme demonstrated above can be generalized to systems of higher dimensionality. To illustrate this, we repeated the calculations presented in figures 2(c) and (d) for a delocalized excitation placed in a square two-dimensional (2D) lattice with an external

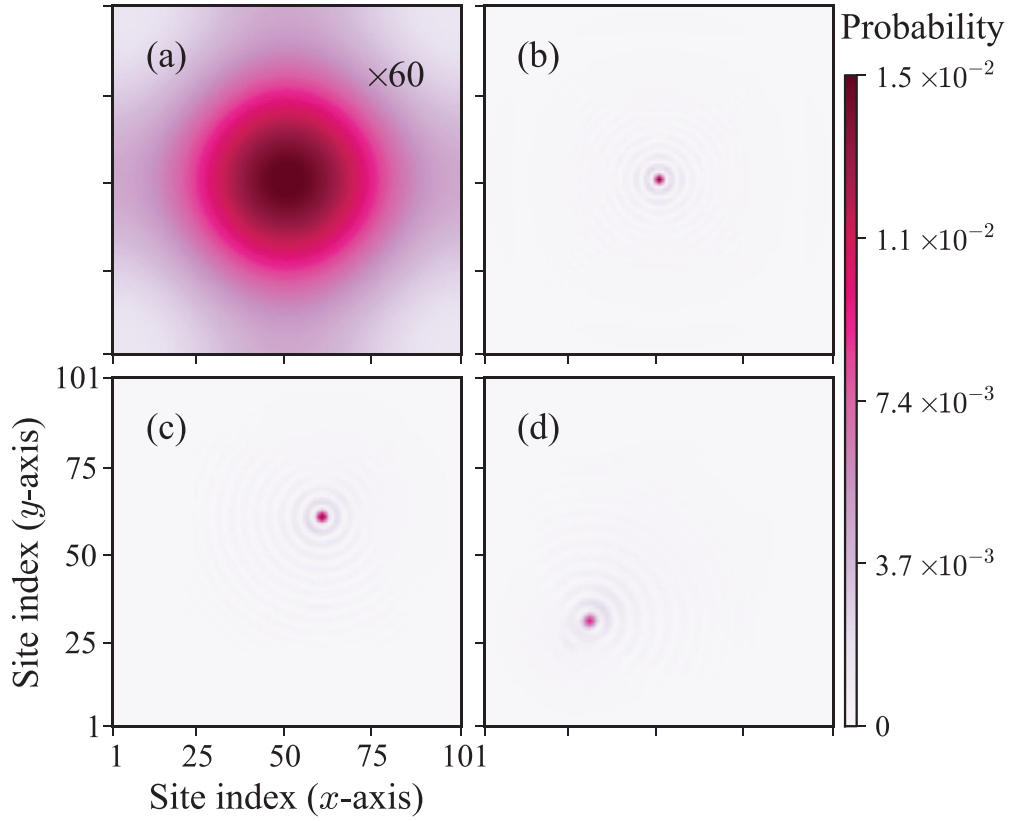


Figure 3. Focusing of a delocalized excitation in a 2D array shown at $t = 0$ in panel (a) onto different parts of the lattice (panels (b)–(d)). For better visualization, the probability distribution in panel (a) is magnified by a factor of 60. The calculations are performed with the same parameters α , a , and ΔE_{e-g} as in figure 1 and the quadratic phase transformation at $t = 0$.

potential that modulates the phase as a function of both x and y . Figure 3 shows the focusing of an initially broad wave packet onto different parts of a 2D lattice induced by the quadratic phase transformation $\Phi(x, y) = \Phi_0[(n_x - n_{x_0})^2 + (n_y - n_{y_0})^2]$, where n_x and n_y are the lattice site indices along the x and y directions. The calculations include all long-range couplings as in figure 2. The comparison of figures 2(c) and (d) and 3 illustrates that the focusing efficiency in 2D is greater. The results also demonstrate that the delocalized excitations can be effectively focused on different parts of the lattice simply by varying the reference site (n_{x_0}, n_{y_0}) in the phase transformation.

4. Controlled excitations of ultracold atoms and molecules

The techniques proposed in sections 2 and 3 can be realized with ultracold atoms or molecules trapped in an optical lattice with one particle per lattice site [41–44]. There are three general requirements that must be satisfied:

- (i) The time required for a phase transformation must be shorter than the spontaneous decay time of the excited state.

- (ii) The overall coherence of the system must be preserved on the time scale of the excitonic evolution in the entire array, set by $K\hbar/\alpha$, where K is the number of monomers participating in the dynamics of the collective excitation.
- (iii) The lattice constant must be large enough to allow considerable variation of the external perturbation from site to site.

Optical lattices offer long coherence times (>1 s) and large lattice constants (>400 nm) [45]. The lifetime of the collective excitations depends on the internal states of the particles used in the experiment and the momentum distribution of the excitonic states in the wave packet (4).

For ultracold alkali metal atoms in an optical lattice, an optical excitation may generate collective states (2), as discussed in [30, 31]. The lifetime of these excited states is limited by the spontaneous emission of the electronically excited atoms and is in the range of 10–30 ns. However, the collective excited states can be protected from spontaneous emission if the wave vector range populated by excitons in the wave packet (4) is outside of the so-called light cone, so that $k > \Delta E_{e-g}/\hbar c$.¹ In an ideal infinite system these states have infinitely long radiative lifetimes, as there is no free-space photon they can emit, assuming the conservation of both energy and momentum [30–33]. In finite and/or disordered systems, the emission of photons may occur at the array boundaries or due to perturbations breaking the translational symmetry. In this case, the time scale for spontaneous decay must depend on the size of the system (i.e. the probability of the excitation to reach the array boundary) and the disorder potential breaking the translational symmetry.

Once collective excited states are created, the phase-kicking technique introduced in section 2, if implemented on a time scale faster than the radiative lifetime of a single atom, can be used to shift the excited states in the wave vector space away from the light cone (cf figure 1) and thus protect the excited states from fast spontaneous decay. This phase transformation can be induced by a pulse of an off-resonant laser field $\mathcal{E}_{ac}$, detuned from the $e \leftrightarrow g$ resonance by the value $\delta\omega$, leading to the ac Stark shift (see e.g. [39])

$$\Delta E_{ac} = \mathcal{E}_{ac}^2 \frac{V_{eg}^2}{4\delta\omega}, \quad (17)$$

where V_{eg} is the matrix element of the dipole-induced transition. By choosing $V_{eg} = 1$ au, $\delta\omega = 3V_{eg}$, and the laser intensity $I = 5 \times 10^{10} \text{ W cm}^{-2}$, we obtain that the shift $\phi = \Delta E_{ac} \times T_{\text{pulse}} = \pi$ can be achieved in less than 1 ns. Another phase transformation can bring the excited state back to the light cone region, where it can be observed via fast spontaneous emission. The experiments with ultracold atoms have demonstrated the lattice filling factor reaching 99% [41–43]. The phase transformations proposed here can be used to stabilize excitonic states in ultracold atomic ensembles against spontaneous emission for multiple interesting applications [29, 46].

The spontaneous decay problem can be completely avoided by using rotational excitations in an ensemble of ultracold polar molecules trapped in an optical lattice. The rotational states are labeled by the quantum number of the rotational angular momentum J and the projection M_J of J on the space-fixed quantization axis Z . We choose the rotational ground state $|J = 0, M_J = 0\rangle$

¹ The number of k -states in the bright and dark regions depends on the relation between the wavelength of the excitation $\lambda_0 = 2\pi\hbar/\Delta E_{e-g}$ and the lattice constant, with bright states appearing at $k < k_* = 2\pi/\lambda_0$, and dark states at $k_* < k < \pi/a$. For Frenkel excitons originating from electronic transitions in solid-state crystals, $\lambda_0 \gg a$ and $k_* \approx 0$. For atoms trapped in optical lattices, the typical values of $\lambda_0 \sim 2a$, and the dark region may be narrow.

as $|g\rangle$ and the rotational excited state $|J = 1, M_J = 0\rangle$ as $|e\rangle$. The state $|J = 1, M_J = 0\rangle$ is degenerate with the states $|J = 1, M_J = \pm 1\rangle$. This degeneracy can be lifted by applying a homogeneous dc electric field, making the $|g\rangle$ and $|e\rangle$ states an isolated two-level system. The molecules in different lattice sites are coupled by the dipole–dipole interaction $V_{dd}(n - m)$. The magnitude of the coupling constant $\alpha(n - m) = \langle e_n, g_m | V_{dd}(n - m) | g_n, e_m \rangle$ between molecules with the dipole moment 1 Debye separated by 500 nm is on the order of 1 kHz [38]. Due to the low value of ΔE_{e-g} , the spontaneous emission time of rotationally excited molecules exceeds 1 s.

For molecules on an optical lattice, one can implement the phase kicks by modifying the molecular energy levels with pulsed ac or dc electric fields. The rotational energy levels for $^1\Sigma$ molecules in a combination of weak ac and dc electric fields are given by [47]

$$E_{J,M_J} \approx BJ(J+1) + \frac{\mu^2 \mathcal{E}_{dc}^2}{2B} G(J, M_J) - \frac{\alpha_{\perp} \mathcal{E}_{ac}^2}{4} + \frac{(\alpha_{\parallel} - \alpha_{\perp}) \mathcal{E}_{ac}^2}{4} F(J, M_J), \quad (18)$$

where B is the rotational constant, $G(0, 0) = -1/3$, $G(1, 0) = 1/5$, $F(0, 0) = -1/3$, $F(1, 0) = -3/5$, $\mathcal{E}_{ac}$ is the envelope of the quickly oscillating ac field, $\alpha_{\parallel}$ and $\alpha_{\perp}$ are the parallel and perpendicular polarizabilities and μ is the permanent dipole moment of the molecule.

The momentum shift of the exciton wave packets can be achieved by applying a time-varying dc electric field $\mathcal{E}(t) = \mathcal{E}_* + \mathcal{E}(n) \sin^2(\pi t/T)$, where $\mathcal{E}(n)$ is linear with respect to n . Assuming that $\mathcal{E}(n) = (n - n_0)A$ and $\mathcal{E}(n) \ll \mathcal{E}_*$, and using equations (5) and (18), gives $\delta = 4A\mathcal{E}_*\mu^2 T/15\hbar Ba$. We have confirmed this result by a numerical computation showing that for LiCs molecules in an electric field of $\mathcal{E}_* = 1 \text{ kV cm}^{-1}$, an electric field pulse with $A = 7.434 \times 10^{-4} \text{ kV cm}^{-1}$ and $T = 1 \mu\text{s}$ results in a kick of $\delta = \pi/2a$, bringing an excitonic wave packet from the $k = 0$ region to the middle of the dispersion zone.

An alternative strategy is to use a pulse of an off-resonance laser field, as for atoms. The phase transformations can be induced by a Gaussian laser beam with the intensity profile

$$I(r, z) = \frac{I_0}{1 + \frac{z^2}{z_R^2}} \exp \left[-\frac{2r^2}{w_0^2 \left(1 + \frac{z^2}{z_R^2}\right)} \right], \quad (19)$$

where I_0 is the light intensity at the beam center, r is the radial distance from the center axis of the beam, z is the axial distance from the beam center, $z_R = \pi w_0^2/\lambda$ is Rayleigh range, w_0 is the beam waist and λ is the wavelength. With the 1D molecular array arranged along the z -axis, the laser field intensity can be made to vary nearly linearly along the array

$$I(r = na, z = 0; t) \approx [I_c + nI_1] \sin^2(\pi t/T) \quad (0 < t < T), \quad (20)$$

where I_c is the intensity at the center of the wave packet. This can be achieved if $z_0 = z_R/\sqrt{3}$ and $\sigma_x^{(2D)}a \lesssim 0.5z_R$, where z_0 is the distance between the center of the wave packet and the beam center, and $\sigma_x^{(2D)}$ is the width (in the coordinate representation) of the 2D wave packet. Using equations (5), (18) and (19), we estimate the momentum kick by such a pulse as $\delta = -\sqrt{3}T I_0(\alpha_{\parallel} - \alpha_{\perp})/80z_R$. The results presented in figure 1 were obtained for a 1D array of LiCs molecules on an optical lattice with $a = 400 \text{ nm}$ and the external perturbation given by the laser field pulse (20) with parameters I_c and I_1 derived from equation (19) with $z_0 = 45 \mu\text{m}$ and $z_R = 73.8 \mu\text{m}$. The numerical results deviate from the analytical prediction for δ by less than 7%.

The Gaussian intensity profile (19) can be used also to implement the quadratic phase transformations needed for focusing of collective excitations. To achieve this, a 2D molecular

array must be arranged in the $z = 0$ plane, with the x -axis defined to be along the polarization direction of a linearly polarized field. If the dimension of the molecular array is smaller than one third of the beam waist, the Gaussian intensity profile in equation (19) can be approximated by

$$I(r = na, z = 0; t) \approx I_0 \left[1 - \frac{2(n_x^2 + n_y^2)a^2}{w_0^2} \right]. \quad (21)$$

This is a concave quadratic intensity profile which can be used to focus a wave packet in a system with negative couplings α (see section 3).

5. Control of energy transfer in dipolar systems

Dipolar interactions play a central role in the study of long-range interaction effects using ultracold systems [48]. While, in general, the coupling constant α in equation (1) can be determined by a variety of interactions, the dominant contribution to α for atoms and molecules on an optical lattice is determined by the matrix elements of the dipole–dipole interaction. It is therefore particularly relevant to discuss the specifics of energy transfer in systems with dipolar interactions.

The dipolar interactions are long-range and anisotropic. This long-range character manifests itself in the modification of the exciton dispersion (3). While equation (3) is valid for a system with nearest neighbor couplings only, higher-order couplings in the case of $\alpha(n - m) \propto 1/|n - m|^3$ modify the exciton dispersion leading to a cosine-like, but non-analytic dispersion relation, both in 1D and 2D. To investigate the effect of this non-analyticity in dispersion curve, we have performed a series of calculations with the long-range couplings neglected after a certain lattice site separation $n - m$ for the 1D system. The results become converged (to within 0.2%) when each molecule is directly coupled with 20 nearest molecules. While the calculations with only the nearest neighbor couplings are in good agreement with the analytical predictions given by equations (12) and (13), the full calculations reveal that long-range couplings somewhat decrease the focusing efficiency. The long-range couplings also decrease the focusing time, by up to a factor of 2. The dynamics of collective excitations leads to interference oscillation patterns clearly visible in panels (a) and (c) of figure 2. These oscillations are much less pronounced when all but nearest neighbor couplings are omitted. The numerical results of figures 1–3 are particularly important because they demonstrate that the phase transformations introduced in the present work are effective for systems with dipolar interactions.

The anisotropy of the dipolar interactions can be exploited for controlling energy transfer in dipolar systems by varying the *orientation* of a dressing external dc electric field. For example, for polar molecules on an optical lattice, the matrix elements $\alpha(n - m) = \langle e_n, g_m | V_{dd}(n - m) | g_n, e_m \rangle$ depend not only on the choice of the states $|g\rangle$ and $|e\rangle$, but also on the magnitude and orientation of an external dc electric field [15, 38]. Since the value of α determines the exciton dispersion (3), the exciton properties can be controlled by varying the angle θ between the intermolecular axis and the applied dc field. This is illustrated in figure 4.

The calculations presented in figure 4 are for a 1D array of LiCs molecules in a lattice with $a = 400$ nm. As before, $|g\rangle$ is the absolute ground state of the molecule and $|e\rangle$ is the rotationally excited state that adiabatically correlates with the rotational state $|J = 1, M_J = 0\rangle$ in the limit of vanishing electric field. The upper panel of figure 4 shows that the angle θ between the electric

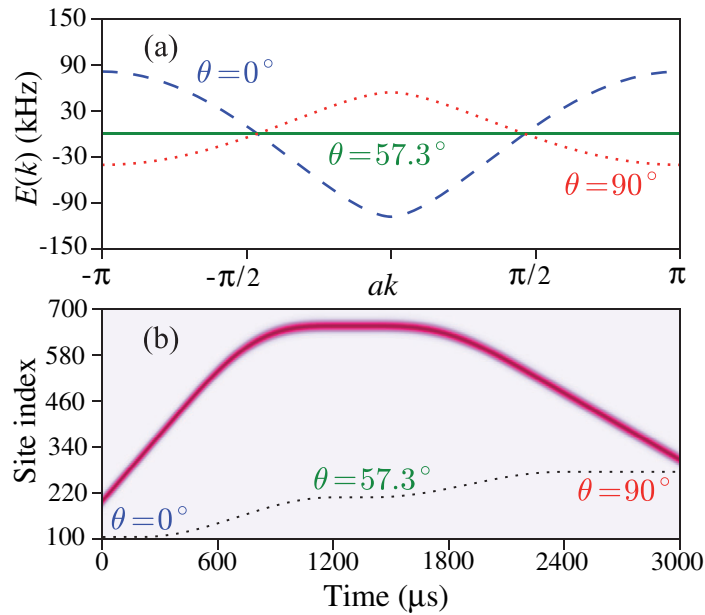


Figure 4. Control of excitation transfer in a 1D many-body system with dipolar interactions by varying the direction of an external electric field. (a) Exciton dispersion curves for a 1D ensemble of diatomic molecules on an optical lattice for different angles θ between the direction of the external dc electric field and the axis of the molecular array. In 1D, the coupling $\alpha \propto (1/3 - \cos^2 \theta)$. (b) Propagation of a wave packet centered at $ak = -\pi/3$ controlled by tuning the electric field direction. Thin dotted line depicts the corresponding angle variations with time. The brightness of color corresponds to the probability of the excitation.

field vector and the molecular array axis determines the sign and magnitude of α , and therefore the shape of the dispersion curve. This enables control over the sign and magnitude of the group velocity of an excitonic wave packet containing contributions with $k \neq 0$. Dynamically tuning θ , one can propagate a localized excitation to different parts of the lattice, as shown in figure 4(b).

In a 2D lattice, the intermolecular interactions depend on an additional azimuthal angle ϕ that describes the rotation of the electric field axis around the axis perpendicular to the lattice. The numerical calculations presented in figure 5 show that the energy flow in two dimensions can be controlled by varying both θ and ϕ . In addition to the phase transformation discussed earlier, this allows for a dynamical energy transfer in quantum many-body systems with anisotropic interparticle interactions.

6. Energy transfer in the presence of vacancies

While experiments with ultracold atoms have produced states with one atom per lattice site with 99% fidelity [41–43], the latest experiments with molecules yield lattice-site populations about 10% [44]. Multiple experiments are currently underway to trap polar molecules on an optical lattice with close to the full population of the lattice. However, lattice vacancies may be unavoidable in the best experiments. In this section, we examine the effect of vacancies on the possibility of focusing collective excitations to a desired region of the lattice by the phase

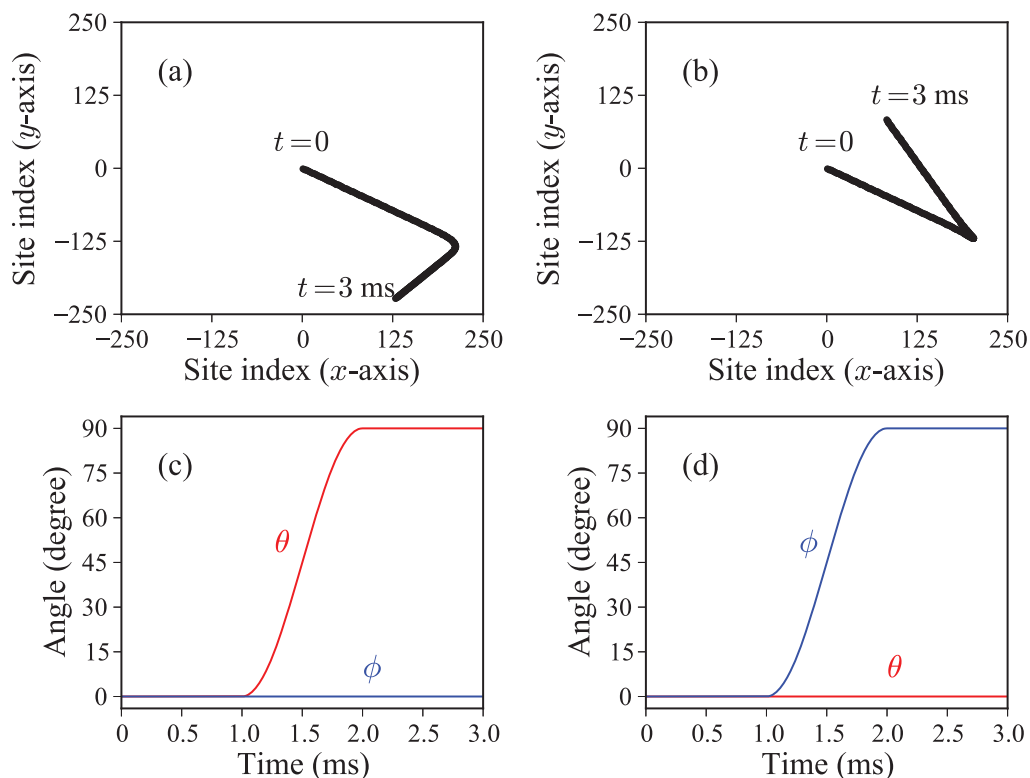


Figure 5. Control of excitation transfer in a 2D many-body system with dipolar interactions by varying the direction of an external electric field. Panels (a) and (b) show the trajectories of the center of an exciton wave packet in a 2D lattice during the time from 0 to 3 ms; panels (c) and (d) represent the changing of the dressing dc field orientation (θ , ϕ) associated with (a) and (b) respectively. The initial wavepacket is a 2D Gaussian distribution centered around $ak_x = ak_y = \pi/2$ and has a width of ~ 60 lattice sites in coordinate space. The magnitude of the dc field is fixed to 6 kV cm^{-1} while its direction is changing. The calculations are done for a 2D array of LiCs molecules in a lattice with $a = 400 \text{ nm}$.

transformations discussed in section 3. For concreteness, we perform calculations for the system described in section 4, namely a 2D array of LiCs molecules on a square optical lattice with $a = 400 \text{ nm}$.

To explore the effect of vacancy-induced interactions, we performed simulations for different vacancy numbers using the same parameters for molecule–field and inter-molecular interactions as in the calculations presented in figure 3(b). For each vacancy concentration, we carried out 48 calculations with random distributions of empty lattice sites. The quadratic phase transformations are applied, as described in section 3, in order to focus the collective excitation at time t_* to the molecule in the middle of the 2D array.

Vacancies disturb the translational symmetry of the system and produce an effective disorder potential that tends to localize collective excitations [49]. Because the natural time evolution of the wave packet in a disorder potential may lead to enhancement of the probability in certain regions of the lattice, it is necessary to distinguish the effect of the vacancy-induced localization and the effect of the focusing phase transformation. To quantify these two effects,

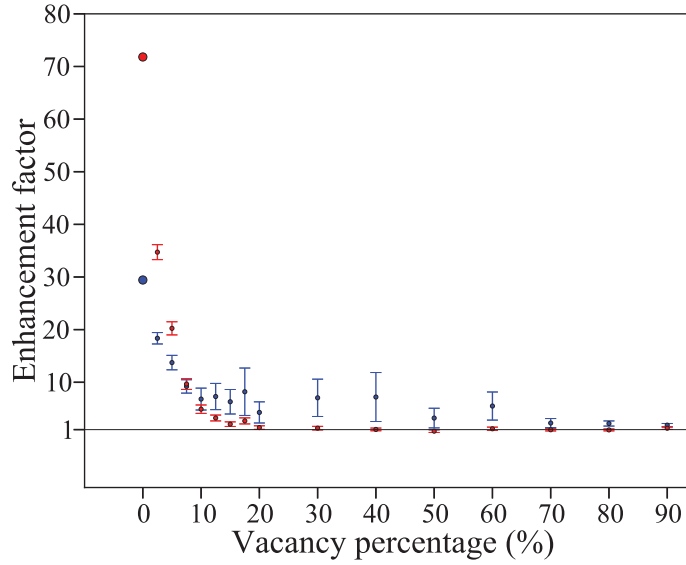


Figure 6. Enhancement factors η (red symbols) and χ (blue symbols) as functions of vacancy percentage in a 2D lattices. See text for the definitions of η and χ . The error bars are for 95% of confidence interval.

we define two factors: the enhancement of the probability at the target molecule with respect to the initial value

$$\eta = \frac{p'(t = t_*)}{p(t = 0)}, \quad (22)$$

and the ratio of the probability to find the excitation on the target molecule with (p') and without (p) the focusing phase transformation

$$\chi = \frac{p'(t = t_*)}{p(t = t_*)}. \quad (23)$$

The time t_* is the focusing time found numerically for the corresponding vacancy-free system. The quantity η illustrates the actual enhancement of the probability to focus a collective excitation, while the quantity χ illustrates the effect of the focusing phase transformation. Figure 6 presents the values of η and χ as functions of the vacancy concentration. It illustrates two important observations. First, the disorder potential with vacancy concentrations $> 20\%$ renders the phase transformation ineffective. In the presence of strong disorder, the dynamics of the system is entirely determined by the disorder potential and the energy transfer becomes highly inefficient (however, see section 7). On the other hand, vacancy concentrations of less than 10% appear to have little effect on the efficacy of the focusing phase transformation.

Our calculations indicate that the focusing time may be somewhat modified by the disorder potential, even if the concentration of vacancies is less than 10% . Figure 7 depicts the excitation wave functions at the time of the maximal enhancement on the target molecule, chosen as molecule (71, 71). Figure 7 shows that despite the presence of multiple vacancies, the focusing transformation enhances the probability to find the excitation on the target molecule by 16 times.

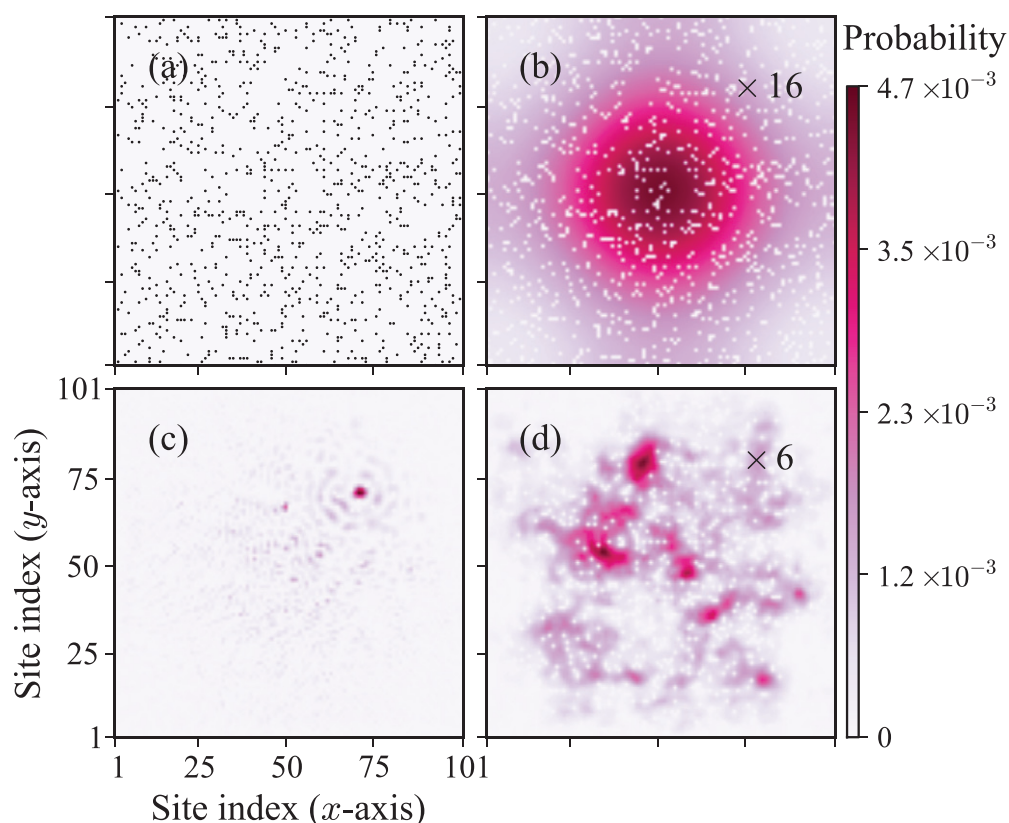


Figure 7. Time snapshots of a collective excitation in a 2D array with a vacancy concentration of 10%: (a) the distribution of the vacant sites; (b) the initial probability distribution of the excited state; (c) the probability distribution of the excitation at the focusing time when the focusing scheme is applied. The focusing time is found numerically as the time when the probability at the target molecule (71, 71) reaches maximum for a given phase transformation. (d) The probability distribution of the wave function at the focusing time when the focusing scheme is not applied. The calculations are performed with the same parameters as in figure 3. The probabilities in (b) and (d) are magnified by 16 and 6 respectively.

7. Focusing in the presence of strong disorder

Although the focusing method demonstrated in sections 3 and 6 appears to be robust in the presence of a disorder potential induced by a small concentration of vacancies, it is important for practical applications to also consider controlled energy transfer in quantum arrays under a strong disorder potential. To consider focusing in a strongly disordered system, we employ an analogy with the ‘transfer matrix’ methods for focusing of a collimated light beam in opaque medium [50–59].

In optics, a collimated laser beam passing through an opaque medium results in a random pattern of speckles arising from random scattering of light inside the medium [60]. Likewise, the random distribution of empty sites in an optical lattice with molecules scatters the exciton wavepackets, resulting in a completely random excited state. However, in optics, the randomness

of the scattering centers inside the opaque medium can be compensated for by shaping the incident wavefront with a spatial light modulator such that the contributions from various parts of the medium can add constructively upon exit from the medium, producing a focus. We suggest that the same can be achieved with a many-body system on a lattice by separating the entire lattice into multiple blocks and applying proper phase transformations to those individual blocks.

The initial state for an ensemble of molecules on a lattice with multiple vacancies can be written as

$$|\psi(t=0)\rangle = \sum_i c_i(t=0)|i\rangle, \quad (24)$$

where

$$|i\rangle = |e_i\rangle \prod_{j \neq i} |g_j\rangle \quad (25)$$

and the indexes i and j run over all occupied sites. After a long evolution time T , the probability amplitude for the excitation to reside on a particular target molecule is given by

$$c_o(T) = \sum_i U_{o,i}(T)c_i(t=0) \equiv \sum_i c_{oi}(T), \quad (26)$$

where $U_{o,i}(t) = \langle o | \exp[-iH_{\text{exc}}t] | i \rangle$ is a matrix element of the time evolution operator. In a disordered system, the transfer coefficients $U_{o,i}$ are not *a priori* known and depend on the disorder potential. The phasors $c_{oi}(T)$ have quasi-random amplitudes and phases. While the amplitude of each phasor cannot be controlled experimentally, their phases are controllable via the phases of the coefficients c_i at $t=0$, which can be tuned using the phase-kicking transformations introduced above. To achieve the highest probability at the target molecule, it is necessary to ensure that the contribution $c_{oi} = U_{o,i}(T)c_i(t=0)$ from every site i has the same phase so that they add up constructively.

In a practical implementation, it may be difficult to control the phase of each molecule in each individual site. It may be more desirable to work with blocks of several lattice sites. Assuming that the entire array of molecules can be divided into M blocks, each containing many molecules, and that the blocks can be perturbed individually, the excitation probability amplitude at the target molecule at time T is

$$c_o(T) = \sum_{\gamma=1}^M c_{\gamma}(T), \quad (27)$$

where

$$c_{\gamma}(T) \equiv |c_{\gamma}| e^{i\phi_{\gamma}} = \sum_{i \in \gamma} U_{o,i}(T)c_i(t=0). \quad (28)$$

This equation implies that the contributions from different blocks can be made to interfere constructively by adding a phase $\exp(-i\phi_{\gamma})$ to each occupied site in block γ . For M blocks in the array and quasi-random evolution matrix, simply setting all the phases equal must lead to $\sim M$ -fold increase of the excitation probability at the target molecule, as compared to a sum of M quasi-random phasors in equation (27) [50].

Similarly to optics, the phases $-\phi_{\gamma}$ which must be added in each block, can be found experimentally provided that the same (or similar) realization of disorder persists in a series of

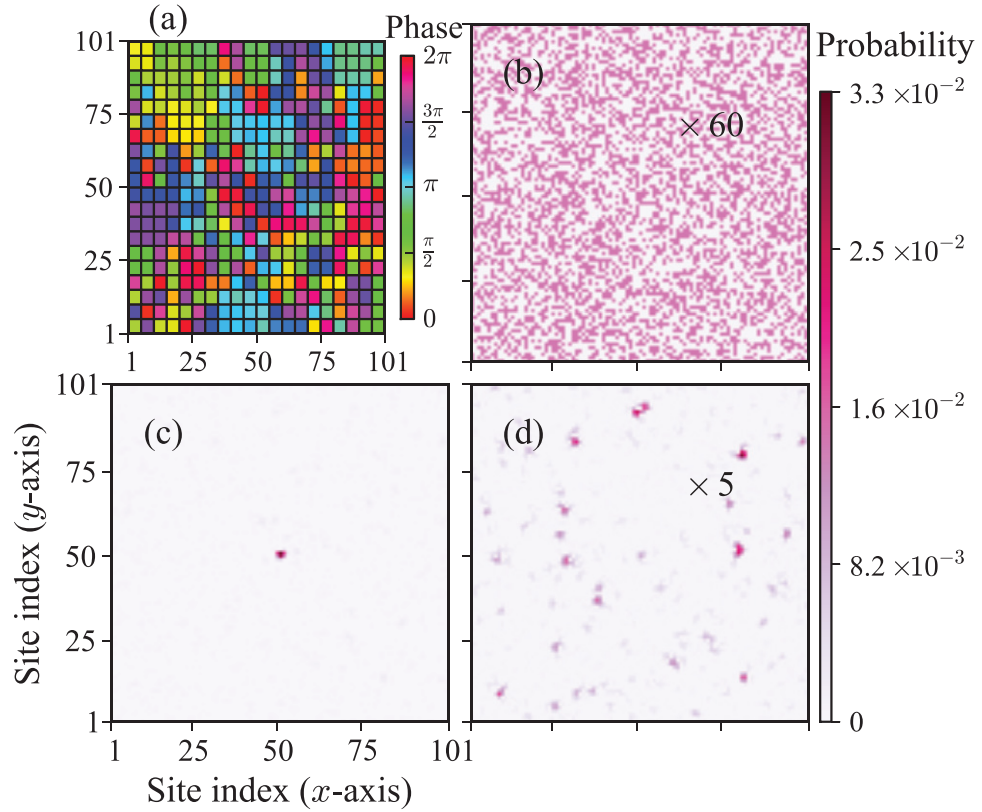


Figure 8. Focusing of a collective excitation in a strongly disordered system with 60% of lattice sites unoccupied. Panel (a) shows different phases applied to different blocks of the lattice before the time evolution. (b) The initial probability distribution of the excited state. (c) The probability distribution of the excited state at the focusing time $T = 3$ ms with the phase transformation depicted in panel (a) before the time evolution. (d) The probability distribution of the excited state at the focusing time $T = 3$ ms with no phase transformation applied. The calculations are performed with the same parameters as in figure 3. The probabilities in (b) and (d) are magnified by 60 and 5, respectively.

trials. A straightforward optimization would scan through the strengths of phase kicks applied to different blocks. In each experiment one would measure the excitation probability at the target molecule $|c_o(T)|^2$, e.g. via resonance fluorescence from the target molecule at the end of the experiment. More sophisticated optimization techniques, aimed at fast focusing multi-frequency light in optical systems, are currently under rapid development [51–59].

For a proof-of-principle calculation, we consider a 2D lattice of size 101×101 with 60% of sites vacant and each non-vacant site occupied by a single LiCs molecule. Due to time reversibility of the time evolution operator $U(T)$,

$$|c_\gamma| \exp(-i\phi_\gamma) = \left[\sum_{j=1}^n U_{o,j}^\gamma(T) c_j^\gamma(0) \right]^* = \left[\sum_{j=1}^n U_{j,o}^\gamma(-T) c_j^\gamma(0) \right]^*. \quad (29)$$

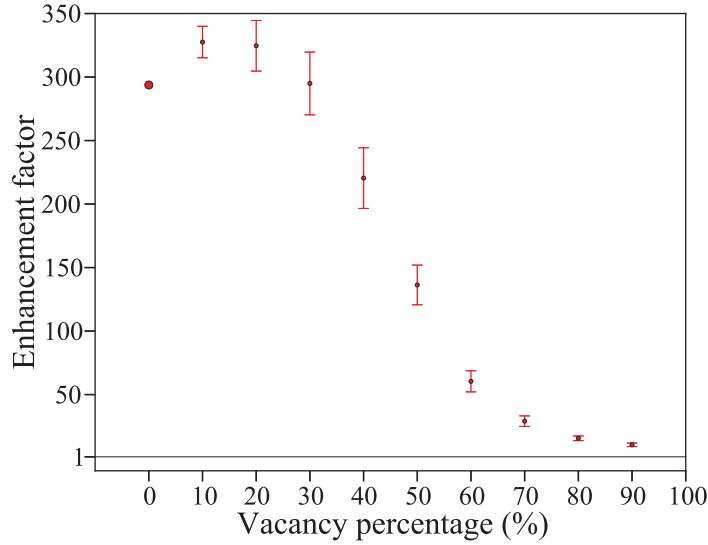


Figure 9. Efficiency of focusing collective excitations in strongly disordered 2D lattices. The molecular array is divided into 400 blocks as shown in figure 8(a). The focusing time t_* is arbitrarily set to 4 ms. For each realization of disorder, we use equation (31) with $T = t_*$ to find the phase mask applied to different blocks. Shown are the enhancement factors η (red symbols) defined in equation (22), as a function of the vacancy percentage. The error bars are for 95% confidence interval.

The matrix element $U_{j,o}^\gamma(-T)$ can be calculated by performing a backward time propagation starting from a local excitation at site ‘ o ’ and calculating the coefficient $c_j(t)$ at time $-T$. Alternatively, one can propagate the evolution equations forward in time, finding $c_j(T)$: since the Hamiltonian (1) is real, its eigenfunctions are real, and the evolution matrix U is symmetric, $U_{o,j} = U_{j,o}$. Thus we find

$$c_j(T) = \sum_i U_{j,i}^\gamma(T) c_i(0) = U_{j,o}^\gamma(T), \quad (30)$$

since $c_o(0) = 1$ and all other coefficients are zero. For a completely delocalized initial state, we assume that all coefficients in equation (24) are equal, so that the phases ϕ_γ required for block γ are

$$|c_\gamma| \exp(-i\phi_\gamma) = \left[\sum_j c_j(T) \right]^*, \quad (31)$$

where the index j runs over all occupied sites in block γ . Figure 8 shows that this choice of phases leads to effective focusing of the collective excitation in a strongly disordered system.

To illustrate the efficiency of the focusing method described above, we have carried out a series of calculations with different vacancy concentrations. For each vacancy concentration, we performed 48 calculations with random distributions of empty lattice sites. The phase transformations are calculated individually for each random distribution of vacancy sites as described above. The results are shown in figure 9. As can be seen, the transformations proposed above are effective for vacancy concentration $< 70\%$. At higher concentrations of vacancies,

the excited states become strongly localized and immobile. The focusing efficiency at vacancy concentrations 10 and 20% appears to be higher than that in the absence of vacancies, which we attribute to the effect of the boundaries.

8. Conclusion

We have proposed a general method for controlling the time evolution of quantum energy transfer in ordered 1D and 2D arrays of coupled monomers. Any elementary excitation in an aggregate of coupled monomers can be represented as a coherent superposition of Frenkel exciton states. We propose shaping the exciton wave packets using non-adiabatic perturbations that temporarily modulate the energy levels of the monomers leading to monomer-dependent linear phase transformation and a displacement of the wave packets in the wave vector representation. This, combined with the possibility of focusing a collective excitation on a particular part of the lattice by a quadratic phase transformation and with the directed propagation of collective excitations, allows for control of energy transfer in the lattice. An experimental observation of the excitations described here can be achieved by measuring site-selective populations of the molecular or atomic states by applying a gradient of an electric field and detecting resonant transitions from Stark-shifted levels [34].

We have presented numerical calculations for an ensemble of polar molecules trapped on an optical lattice that demonstrate the feasibility of both momentum-shifting and focusing of collective excitations by applying external laser fields, with parameters that can be easily achieved in the laboratory. We have also investigated the effect of disorder potential arising from incomplete population of the lattice. Our results show that the phase transformations leading to focusing of collective excitations on different regions of a 2D lattice remain effective in the presence of vacancies with concentrations not exceeding 10%. For systems with larger concentrations of vacancies and affected by strong disorder potentials, we propose an alternative procedure based on engineering constructive interference of the wave function contributions arising from different parts of the lattice.

The momentum-shifting technique proposed here can be used to protect collective excitations of ultracold atoms from spontaneous emission. The spontaneous decay processes, which in the case of an ordered many-body system must satisfy both the energy and wave vector conservation rules, can be restricted by shifting the exciton wave packets to a region of the dispersion curve, where the wave vector conservation cannot be satisfied. If performed faster than the spontaneous emission time, such phase transformations should create collective excitations with much longer lifetimes, which opens a variety of new applications for ultracold atoms on an optical lattice.

As was proposed by multiple authors [61–66], molecular wavepackets can be used to encode quantum information. Similarly, collective excitations can be used for quantum memory [18]. Control over excitation transfer is needed for creating networks of quantum processors where information is transmitted over large distances with photons and stored in arrays of quantum monomers via one of the quantum memory protocols [67]. Momentum kicking can be used for wave packet transport within a single array. Focusing excitonic wave packets would enable local storage of information, while directed propagation combined with controlled interactions of multiple excitons [15] or excitons with lattice impurities [68] may be used to implement logic gates. Controlled energy transfer in molecular arrays may also be used for the study of controlled chemical interactions for a class of reactions stimulated by

energy excitation of the reactants. Directing energy to a particular lattice site containing two or more reagents can be used to induce a chemical interaction [69], an inelastic collision or predissociation [70] with the complete temporal and spatial control over the reaction process.

Finally, the present work may prove to be important for simulations of open quantum systems. We have recently shown [38, 71] that the rotational excitations of ultracold molecules in an optical lattice can, by a suitable choice of the trapping laser fields, be effectively coupled to lattice phonons. The exciton–phonon couplings can be tuned from zero to the regime of strong interactions [38, 71]. The possibility of shaping (accelerating, decelerating and focusing) collective excitations as described in the present work combined with the possibility of coupling these excitations to the phonon bath opens an exciting prospect of detailed study of controlled energy transfer in the presence of a controllable environment. Of particular interest would be to study the effect of the transition from a weakly coupled Markovian bath to a strongly coupled non-Markovian environment on energy transfer with specific initial parameters.

We note that the effect of site-dependent phase transformations on quantum transport was independently considered in [72] from the point of view of time-reversal symmetry breaking. The authors of [72] propose an experimental realization based on ions in a linear Paul trap. Their method relies on the possibility of tuning time-dependent phases, leading to new effects. This paper and [72] should be considered complementary.

Acknowledgments

This work was supported by NSERC of Canada and the Peter Wall Institute for Advanced Studies.

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