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Tunable disorder in a crystal of cold polar molecules

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We show that a two-species mixture of polar molecules trapped on an optical lattice gives rise to a system of rotational excitons in the presence of tunable impurities. The exciton-impurity interactions can be controlled by an external electric field, which can be exploited for quantum simulation of localization phenomena in disordered media. We demonstrate that an external electric field can be used to induce resonant enhancement of the exciton-impurity scattering cross sections and delocalization of excitonic states in a correlated one-dimensional disorder potential.

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I. INTRODUCTION

There is a growing interest in designing tunable many-body quantum systems, which can be used as physical simulators to access novel phenomena and to study the properties of analagous, but less controllable, many-body quantum systems [1–4]. For example, a major thrust of current research is focused on realizing lattice-spin models with ultracold molecules trapped on optical lattices [2,3,5–7]. This quantum simulation work relies on tuning interactions of ultracold molecules by external fields. While two-body interactions of ultracold molecules can be tuned by a variety of methods [8], it is much harder to achieve external field control over many-body interactions. In the present work, we demonstrate the possibility of controlling by an external field the dynamics of collective excitations (excitons) of molecules on an optical lattice.

Excitons determine the optical properties of materials, energy transfer in semiconductors and mesoscopic systems [9,10], and the reaction mechanisms in complex biological systems [11]. In molecular crystals with low excitation density, the transport properties of excitons are determined by their interaction with impurities and phonons [9] and resemble those of electrons in solids [12] or atoms in optical lattices [13]. Although the effects of phonons can be suppressed by lowering the temperature of crystals, the presence of impurities is almost unavoidable in semiconductors and organic molecular solids. Exciton-impurity interactions lead to the formation of localized exciton states [14], modifying energy transfer in crystalline materials. Therefore, it would be desirable to develop an experimentally realizable system that could be used to study exciton dynamics as a function of exciton-impurity interaction strength. Here, we show that a suitably chosen two-species mixture of ultracold polar molecules loaded on an optical lattice forms a phononless crystal, where exciton-impurity interactions can be controlled by applying an external electric field. This can be used for the controlled creation of many-body entangled states of ultracold molecules and the time-domain quantum simulation of disorder-induced localization and delocalization of quantum particles.

The present work builds on three major recent advances in atomic, molecular, and optical physics: the creation of dense ensembles of ultracold polar molecules in the rovibrational ground state by photoassociation of alkali-metal atoms [15,16]; the development of techniques for trapping ultracold atoms and molecules by optical lattices [17]; and the development of techniques for detecting and manipulating single atoms in optical lattices [18–20]. It has thus become technologically possible to create ordered ensembles of ultracold polar molecules in the rovibrational ground state trapped by an optical lattice with a lattice separation of about 400 nm [21]. By using the method of Ref. [18], molecules in specific lattice sites can be evaporated. By overlapping two optical lattices of trapped molecules or using the method of Ref. [22], it should be possible to create a mixture of molecules arranged in an arbitrary array with any spatial dimensionality.

Ultracold polar molecules in the rovibrational ground state can potentially be created by a variety of recently developed experimental methods [23], ranging from Stark deceleration of molecular beams to buffer gas cooling to photoassociation of ultracold atoms. These techniques promise to provide in a near future a wide range of ultracold molecules. Photoassociation of alkali-metal atoms to produce polar alkali-metal dimers [15,16] has so far proven to be the most effective method for the creation of ultracold molecular ensembles with high phase-space density. Therefore, we consider in this work a mixture of alkali-metal dimers LiCs and LiRb loaded on an optical lattice. We note, however, that the proposed mechanism of tuning exciton-impurity interactions can, in principle, be realized with any mixture of molecules A and B in a Σ electronic state, provided the rotational constant of molecule A is greater and the dipole moment of molecule A is smaller. The effects discussed in this work should occur at smaller electric fields, if the rotational constants of molecules A and B are closer in magnitude.

II. ROTATIONAL EXCITONS IN AN OPTICAL LATTICE OF POLAR MOLECULES

We consider an optical lattice of $^1\Sigma$ polar molecules, such as LiCs, with one molecule in the rovibrational ground state per lattice site (see Fig. 1 for a schematic illustration of the system). We assume that the tunneling of molecules to different lattice sites is entirely suppressed, which can be achieved

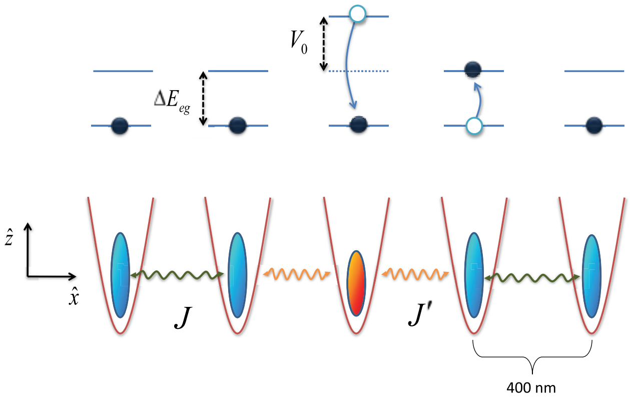

FIG. 1. (Color online) Schematic illustration of a crystal with tunable impurities. Molecules are confined by the periodic potential of an optical lattice and coupled by the dipole-dipole interaction, which allows the exchange of a rotational excitation between molecules in different lattice sites. An impurity is a molecule with a different dipole moment and different rotational energy splitting. For certain combinations of molecules, the energy defect V_0 can be tuned by an external electric field from zero to a large magnitude, thereby modifying the energy transfer in the crystal.

by applying laser fields of sufficient power [17]. The lattice sites are separated by 400 nm so the interaction between the molecules is entirely determined by the long-range dipole-dipole interaction potential. We consider the lowest excited states of the molecular crystal. In the absence of the dipole-dipole interactions, these would be the rotational excitations of the individual molecules. However, the interactions between the molecules lead to collective modes known as Frenkel excitons [9].

The excitonic states are the eigenstates of the following Hamiltonian:

$$\hat{H} = \sum_{n=1}^{N_{\rm mol}} \left(B_e \hat{N}_n^2 - \mathbf{d}_n \cdot \mathbf{E}\right) + \frac{1}{2} \sum_{n=1}^{N_{\rm mol}} \sum_{m \neq n}^{N_{\rm mol}} \hat{V}_{\rm dd}(\mathbf{r}_n - \mathbf{r}_m), \quad (1)$$

where $\mathbf{r}_n$ is the position of the nth lattice site, B_e is the rotational constant and $\mathbf{d}_n$ is the electric dipole operator of the individual molecules, $\mathbf{E}$ is a static electric field, $\hat{V}_{\rm dd}$ is the dipole-dipole interaction between molecules in different lattice sites, and $N_{\rm mol}$ is the total number of molecules. In the absence of an electric field, the rotational ground state of a ${}^1\Sigma$ diatomic molecule is characterized by the rotational angular momentum $N = 0$. The first excited rotational state $N = 1$ is triply degenerate. The $N = 0 \to N = 1$ excitation of molecules therefore leads to three excitonic states, which we denote α, β, and γ. In the presence of an electric field, the rotational state $N = 1$ splits into two Stark energy levels corresponding to the projections $M = 0$ and $M = \pm 1$ of $\hat{N}$ on the electric field axis.

Hamiltonian (1) can be written as [9]

$$\hat{H} = \Delta E_{eg} \sum_n \hat{B}^\dagger_{n,M} \hat{B}_{n,M} + \frac{1}{2} \sum_{n,m\neq n} J^{M,M}_{n,m} \hat{B}^\dagger_{n,M} \hat{B}_{m,M}$$
$$+ \frac{1}{2} \sum_{M,\, M' \neq M} \sum_{n,m\neq n} J^{M,M'}_{n,m} \hat{B}^\dagger_{n,M} \hat{B}_{m,M'}. \quad (2)$$

The exciton creation operators are defined by $\hat{B}^\dagger_{n,M}|g\rangle_n = |e,M\rangle_n$, where $|g\rangle$ and $|e,M\rangle$ denote the ground and excited field-dressed rotational states. For clarity, we label these states by the quantum number of the rotational angular momentum of the corresponding field-free states: $|N = 0\rangle_n$ for $|g\rangle_n$ and $|N = 1, M\rangle_n$ for $|e,M\rangle_n$. The excitation transfer between molecules at lattice sites $\mathbf{r}_n$ and $\mathbf{r}_m$ is described by the coupling constant $J^{M,M'}_{n,m} = \langle e,M|_n \langle g|_m \hat{V}_{\rm dd} |g\rangle_n |e',M'\rangle_m$. In Eq. (2), we have neglected the gas–condensed-matter shift in the diagonal terms since it is much smaller than ΔE_{eg}. If $\mathbf{E}$ is perpendicular to the intermolecular axis $\mathbf{R} = \mathbf{r}_n - \mathbf{r}_m$, then the dipole-dipole interaction between molecules n and m couples two-molecule states with $\Delta(M_n + M_m) = 0, \pm 2$, and if $\mathbf{E}$ is parallel to $\mathbf{R}$, the selection rule is $\Delta(M_n + M_m) = 0$.

By using $\hat{B}^\dagger_{n,M} = \frac{1}{\sqrt{N_{\rm mol}}} \sum_{\mathbf{k}} \hat{B}^\dagger_{\mathbf{k},M} e^{-i\mathbf{k}\cdot\mathbf{r}_n}$, where $\mathbf{k}$ is the exciton wave vector, Hamiltonian (2) can be rewritten as

$$\hat{H} = \sum_{\mathbf{k}} \sum_{M,M'} [\Delta E_{eg} \delta_{M,M'} + L_{M,M'}(\mathbf{k})] \hat{B}^\dagger_{\mathbf{k},M} \hat{B}_{\mathbf{k},M'}, \quad (3)$$

with $L_{M,M'}(\mathbf{k}) = \sum_n J^{M,M'}_{n,0} e^{i\mathbf{k}\cdot\mathbf{r}_n}$.

Hamiltonian (3) is diagonalized by the unitary transformation $\hat{B}^\dagger_{\mathbf{k},M} = \sum_\mu \alpha_{M,\mu} \hat{A}^\dagger_{\mathbf{k},\mu}$ [9]. The resulting Hamiltonian is $\hat{H} = \sum_{\mathbf{k},\mu} E_\mu(\mathbf{k}) \hat{A}^\dagger_{\mathbf{k},\mu} \hat{A}_{\mathbf{k},\mu}$, where $\mu = \alpha,\beta,\gamma$ labels the dispersion relations associated with the eigenstates. When $\mathbf{E}$ is parallel to the molecular array, the eigenstates of Hamiltonian (3) are $|\alpha_{\mathbf{k}}\rangle = |\Psi_{\mathbf{k},M=1}\rangle$, $|\beta_{\mathbf{k}}\rangle = |\Psi_{\mathbf{k},M=-1}\rangle$, and $|\gamma_{\mathbf{k}}\rangle = |\Psi_{\mathbf{k},M=0}\rangle$, where $|\Psi_{\mathbf{k},M}\rangle$ are the eigenstates of Hamiltonian (2) with all off-diagonal matrix elements $J^{M,M'}_{n,m}$ in the third sum set to zero. If the electric field $\mathbf{E}$ is perpendicular to the molecular array, the eigenstates are $|\alpha_{\mathbf{k}}\rangle = \frac{1}{\sqrt{2}}[|\Psi_{\mathbf{k},M=1}\rangle - |\Psi_{\mathbf{k},M=-1}\rangle]$, $|\beta_{\mathbf{k}}\rangle = \frac{1}{\sqrt{2}}[|\Psi_{\mathbf{k},M=1}\rangle + |\Psi_{\mathbf{k},M=-1}\rangle]$, and $|\gamma_{\mathbf{k}}\rangle = |\Psi_{\mathbf{k},M=0}\rangle$.

The dispersion curves $E_\mu(\mathbf{k})$ of the three exciton branches are shown in Fig. 2 for a one-dimensional (1D) array of LiCs molecules ($d_0 = 5.529$ Debye, $2B_e = 11.7998$ GHz [24]) with lattice constant $a = 400$ nm in the presence of an electric field parallel and perpendicular to the array. Analogous dispersion curves can be obtained in two and three dimensions and for other directions of the electric field. The energy bands shown in Fig. 2 are centered at the isolated molecule transitions and describe the effect of intermolecular interactions on the energy spectrum of the crystal. Exciton γ corresponds to the $|N = 0\rangle \to |N = 1, M = 0\rangle$ excitation. The calculated excitonic bandwidths are of the order of 100 kHz. We verified that the broadening of the excitonic line due to the variation of the dipole-dipole interaction caused by the vibrations of the molecules about their equilibrium positions is less than 5% of its bandwidth for experimentally realizable trapping frequencies $\omega_{\rm trap} \geqslant 100$ kHz.

When the electric field is perpendicular to the molecular array, excitons γ and β have negative effective mass (i.e., their energy decreases with increasing wave vector), while the

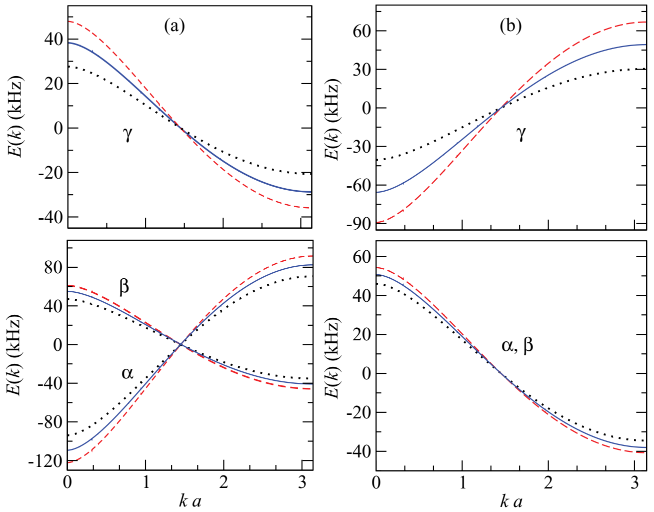

FIG. 2. (Color online) Stark effect on rotational excitons, showing the exciton energy $E(k)$ calculated for three lowest excitations in a 1D array of 10^5 LiCs molecules ($d_0 = 5.529$ Debye, $2B_e = 11.8$ GHz [24]) separated by 400 nm as functions of the exciton wave number k. Exciton states α, β, and γ centered at the isolated molecule transition energies ΔE_{eg} are shown in the presence of an electric field perpendicular to the array (a) and parallel to the array (b). The electric field magnitudes are 2 kV/cm (dashed lines), 3.2 kV/cm (solid lines), and 5 kV/cm (dotted lines). At these electric fields, exciton γ is separated from excitons α and β by an energy much larger than the exciton bandwidths.

effective mass of exciton α is positive. Figure 2 demonstrates that the effective mass and, consequently, the group velocity of the excitons can be changed by varying the strength and the direction of the external electric field. We also note that, unlike electronic excitons in molecular crystals, rotational excitons have a very long radiative lifetime exceeding seconds. In the following, we focus on the exciton state labeled by γ in Fig. 2(a).

III. TUNABLE IMPURITIES

If a small number of LiCs molecules are replaced with molecules of a different kind, such as LiRb ($d_0 = 4.165$ Debye, $2B_e = 13.2$ GHz [24]), the translational symmetry of the lattice is disturbed, as in a solid crystal with impurities (see Fig. 1). Let ΔE_{eg} be the rotational excitation energy in host molecules, $\Delta E_{eg} + V_0$ the energy of the same transition in impurities, and $\Delta J_{n,m}$ the difference between impurity-host and host-host coupling constants for molecules at sites n and m. Consider first the lattice with a single impurity at site $n = 0$, which is described by the Hamiltonian [25]

$$\hat{H} = \hat{H}_0 + V_0 \hat{B}_0^\dagger \hat{B}_0 + \sum_{n\neq 0} \Delta J_{n,0}(\hat{B}_n^\dagger \hat{B}_0 + \hat{B}_n \hat{B}_0^\dagger), \qquad (4)$$

where $\hat{H}_0$ is the free-exciton Hamiltonian and $\hat{B}_n^\dagger$ and $\hat{B}_n$ are the operators creating and annihilating the rotational excitation in site n. The exciton-impurity interaction can thus be described as a sum of a delta-function potential with strength V_0 and a perturbation due to the difference in the dipole moments of host and impurity molecules. The exciton-impurity interaction leads to the appearance of bound exciton states [25,26].

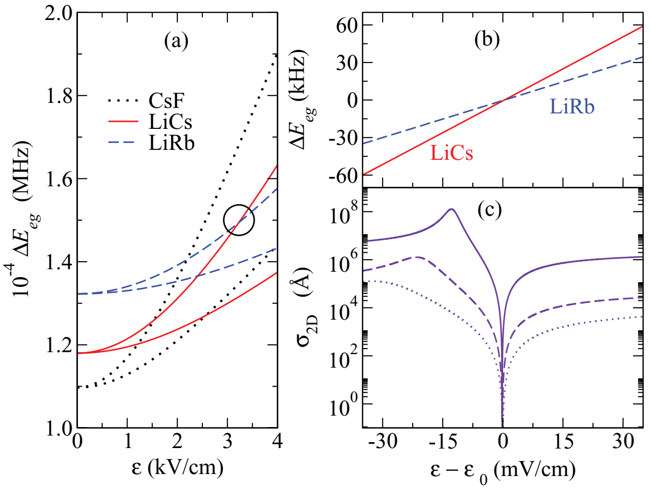

FIG. 3. (Color online) Excitation energies of noninteracting molecules in an electric field. (a) The excitation energies ΔE_{eg} for transitions $|N = 0, M = 0\rangle \to |N = 1, M\rangle$ with $M = 0$ (upper curve) and $M = \pm 1$ (lower curve) vs electric field for three polar molecules. (b) An expanded view of the encircled area in panel (a). (c) The exciton-impurity two-dimensional scattering cross sections for exciton γ in Fig. 2(a) with $|\mathbf{k}|a = 4 \times 10^{-5}$ (solid line), $|\mathbf{k}|a = 4 \times 10^{-3}$ (dashed line), and $|\mathbf{k}|a = 4 \times 10^{-2}$ (dotted line). The calculations are for an array of LiCs molecules with one LiRb impurity. The lattice constant is $a = 400$ nm and $\mathcal{E}_0 = 3228.663$ V/cm.

We propose to modify V_0 by shifting the rotational levels of host and impurity molecules simultaneously using a static electric field. Figure 3(a) shows the excitation energies ΔE_{eg} for the rotational transition $N = 0 \to 1$ of CsF, LiCs, and LiRb molecules as functions of the electric field and demonstrates that the excitation energies for these combinations of molecules become the same at certain values of the electric field. The interaction of polar molecules with the electric field allows for the possibility to explore the dependence of the exciton-impurity scattering cross section not only on the exciton wave vector k but also on the scattering strength V_0, which is not possible in conventional solids. The results of Fig. 3(a) are obtained using the spectroscopically determined values of the rotational constants and the permanent dipole moments of the molecules borrowed from the literature [24]. The magnitudes of the rotational constants and the dipole moments determine the value of the electric field at which the energy differences of the molecules depicted in Fig. 3(b) become equal. The crossing of the energy differences shown in Fig. 3(b) should occur for any combination of molecules A and B, provided the rotational constant of molecule A is greater and the dipole moment of molecule A is smaller. Molecules with a larger difference of the dipole moments and a smaller difference of the rotational constants must exhibit the crossing of the energy differences at smaller electric fields.

The cross sections for exciton-impurity scattering in two-dimensional (2D) and three-dimensional (3D) crystals as functions of V_0 can be obtained by solving the Lipmann-Schwinger equation. Using the effective mass approximation, we obtain

$$\sigma_{2\mathrm{D}}(k,V_0) = \frac{4\pi^2/k}{\pi^2 + \ln^2\left[\frac{E_b^{(2\mathrm{D})}(\Delta - T_k)}{T_k\left(\Delta - E_b^{(2\mathrm{D})}\right)}\right]}, \tag{5a}$$

$$\sigma_{3\mathrm{D}}(k,V_0) = \frac{2\pi\hbar^2/|m_*|}{T_k + E_b^{(3\mathrm{D})}}, \tag{5b}$$

where $T_k = \hbar^2|\mathbf{k}|^2/2|m_*|$ is the kinetic energy of the exciton with effective mass m_*, Δ is the exciton bandwidth and E_b is the energy of a bound state produced by V_0 and given by $E_b^{(2\mathrm{D})} = \Delta/[\exp(4\Delta/\pi V_0) - 1]$ and $E_b^{(3\mathrm{D})} = (2/\pi - V_0/\Delta)^2\Delta$. Equations (5) show that the exciton-impurity scattering cross sections can be tuned by varying the electric field. In particular, resonant enhancement of the scattering cross section occurs for values of V_0 that support a shallow bound state for values of $V_0 < 0.2\Delta$ in two dimensions and $V_0 \sim 2\Delta/\pi$ in three dimensions [see Fig. 3(c)]. These resonances are analogous to Feshbach resonances in atomic collisions, commonly used to tune the scattering properties of ultracold atoms [27]. In one dimension, shallow bound states appear only for vanishingly small V_0 and resonances may not be observable. As a result of the negative effective mass of the exciton, the bound state that leads to resonance is produced by a repulsive potential with $V_0 > 0$. Equations (5) are derived in the approximation $\Delta J_{n,0} = 0$. Including $\Delta J_{n,0}$ in the calculation leads to a shift of the positions of the resonance [25] and the resonant enhancement of the scattering cross section at a slightly different value of V_0.

Figure 3(c) shows that the elastic mean free path of excitons, $l \sim 1/\sigma n$ (where n is the concentration of the impurities), can be dynamically tuned by several orders of magnitude by varying the applied electric field. According to the Ioffe-Regel criterion [28], this should allow for a possibility to transfer the system dynamically from the regime of weak localization ($l \gg \lambda$) to the regime of strong localization ($l \sim \lambda$) of excitons with the wavelength $\lambda = 2\pi/k$.

Consider now a lattice with multiple impurities. It is well known that quantum particles in the presence of a random distribution of scattering centers undergo coherent localization [14]. In the system proposed here, the localization of excitons can be tuned by an electric field. As an example, we consider localization of excitons in a 1D array of LiCs separated by 400 nm, with a random homogeneous distribution of LiRb impurities (see Fig. 4). The Hamiltonian describing an exciton in the presence of N_i substitutional impurities at positions $\mathbf{i}_n$ can be written as $\hat{H} = \hat{H}_0 + \hat{W} + \hat{V}$, with the corresponding matrix elements in the basis of free-exciton states $|\gamma_{\mathbf{k}}\rangle$ given by

$$\langle \hat{H}_0 \rangle_{\mathbf{q},\mathbf{k}} = E(\mathbf{k})\delta_{\mathbf{k},\mathbf{q}}, \tag{6a}$$

$$\langle \hat{W} \rangle_{\mathbf{q},\mathbf{k}} = \frac{2\Delta J(a)}{N_{\mathrm{mol}}}[\cos(\mathbf{q}\cdot\mathbf{a}) + \cos(\mathbf{k}\cdot\mathbf{a})]\sum_{\mathbf{i}_n=1}^{N_i} e^{i(\mathbf{q}-\mathbf{k})\cdot\mathbf{i}_n}, \tag{6b}$$

$$\langle \hat{V} \rangle_{\mathbf{q},\mathbf{k}} = \frac{V_0}{N_{\mathrm{mol}}}\sum_{\mathbf{i}_n=1}^{N_i} e^{i(\mathbf{q}-\mathbf{k})\cdot\mathbf{i}_n}, \tag{6c}$$

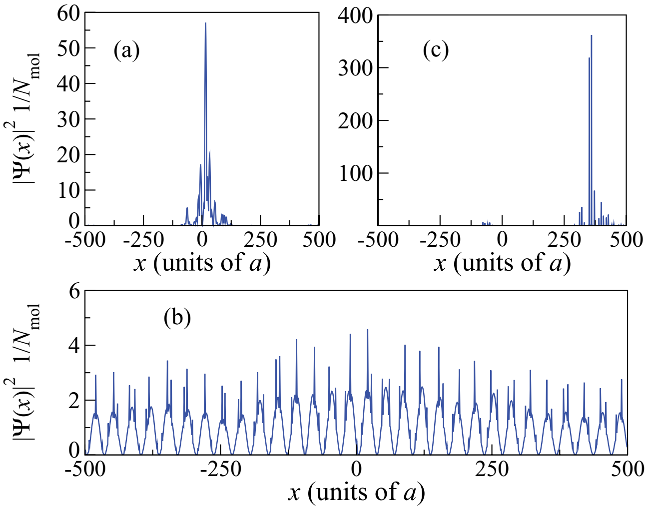

FIG. 4. (Color online) Probability density $|\Psi(x)|^2$ describing an exciton near the top of the energy spectrum for a 1D array of 1000 LiCs molecules with 10% homogeneously and randomly distributed LiRb impurities. Panels correspond to different values of V_0: (a) $V_0 = 0$, (b) $V_0/h = 22$ kHz, and (c) $V_0/h = 100$ kHz. The difference of the dipole moments of LiCs and LiRb molecules leads to the value $\Delta J = -6.89$ kHz.

where $E(\mathbf{k})$ is the energy of the exciton, $\mathbf{k}$ and $\mathbf{q}$ denote exciton wave vectors, and $\Delta J(a) = \Delta J_{n,n-1}$. We consider nearest-neighbour coupling between impurities and host molecules. If the impurities are distributed randomly, the terms $\hat{V}$ and $\hat{W}$ correspond to diagonal and off-diagonal disorder, respectively.

When an external electric field is such that $V_0 = 0$, exciton-impurity scattering occurs only due to the difference in dipole moments between host and impurity molecules. Figure 4 shows the probability density of a particular eigenstate of Hamiltonian (6) near the top of the energy spectrum, for different values of V_0. Due to the negative effective mass of free-exciton states, high-energy eigenstates are dominated by free-exciton states with $\mathbf{k} \approx 0$. These eigenstates are localized [Fig. 4(a)]. Delocalization of these states can be achieved by applying an electric field so that $V_0 \approx -4\Delta J(a)$ [see Fig. 4(b) and Eqs. (6)]. In this case, for a given $\mathbf{k}$, the matrix elements $\langle \hat{V} \rangle_{\mathbf{q},\mathbf{k}}$ and $\langle \hat{W} \rangle_{\mathbf{q},\mathbf{k}}$ cancel for $\mathbf{q} \approx \mathbf{k}$, which suppresses the coupling between the corresponding free-exciton states. Localized eigenstates with different energies become delocalized at different values of V_0. The wave packets are localized for values of V_0 that do not balance the effect of $\Delta J(a)$ [Fig. 4(c)].

The eigenstates of quantum particles in a 1D disordered potential must be exponentially localized [14]. However, in the presence of specific correlations in the disordered potential, some localized states may undergo delocalization. For example, it follows from the results of Ref. [29] that the correlation between diagonal and off-diagonal disorder corresponding to substitutional disorder with one kind of impurity in a 1D molecular lattice with nearest neighbor interactions leads to delocalization of one eigenstate. Figure 4(b) illustrates the delocalization of excitons in a 1D disordered system caused by this type of correlation between diagonal and off-diagonal disorder. Unlike in crystals with fixed disorder, where disorder correlations lead to delocalization of one (or a small number) of states, tunable disorder can be used to induce delocalization of any state in the exciton energy spectrum, as long as V_0 can be tuned to the value balancing the wave-vector-dependent off-diagonal disorder contribution.

IV. APPLICATIONS

The system proposed here offers three unique features: (i) long-lived excitons that are stable against spontaneous decay and whose effective mass can be controlled by an external electric field; (ii) dynamically tunable impurities; and (iii) the possibility of arranging impurities and host molecules in various configurations and dimensions. This opens up possibilities for quantum simulation of fundamental physical phenomena:

Exciton-impurity scattering leads to localization of excitons in crystalline solids [14]. In particular, large cross sections for exciton-impurity scattering lead to Anderson localization. The exciton-impurity interactions in the system proposed here can be tuned from resonantly enhanced to entirely suppressed scattering, which can be used to study the dynamics of exciton localization, including the time scales for the formation of localized and delocalized states and their dependence on exciton bandwidth and exciton-impurity interaction strength. In addition, the system proposed here is ideally suited for the study of the effects of correlations in the disordered potentials. The presence of short- and long-range correlations in the disordered potentials may result in the appearance of a discrete [30,31] or even continuous [32,33] set of delocalized states in low-dimensional crystals. Measurements of exciton localization in a crystal with tunable impurities can be used for time-domain quantum simulation of disorder-induced localization and delocalization of quantum particles.

Controlled spatial distributions of impurities and molecular crystals with specific arrangements of crystal particles in one, two, or three dimensions may be used to study the effects of dimensionality and finite size on energy transfer in mesoscopic materials [10]. The localized states displayed in Fig. 4 are many-body entangled states of the molecules in an optical lattice. The possibility to tune exciton-impurity interactions can thus be exploited for the controlled creation of many-body entangled states of ultracold molecules, necessary for the experimental realization of quantum computation with molecular ensembles [34].

The negative effective mass of the excitons may be used for studies of negative refraction of microwave fields. In addition, the ability to tune dynamically the effective mass of an exciton from a positive to a negative value may open interesting possibilities for studies of Anderson localization [14] and the creation of localized excitons with zero effective mass. The latter correspond to many-body entangled states of noninteracting molecules.

Finally, a mixture of ultracold molecules with impurities forming a sublattice may be used to study the formation of wave-vector space crystals of excitons. The eigenstates of such a two-species lattice correspond to a discrete distribution in $\mathbf{k}$ space. Tuning the impurities by a sinusoidally varying electric field could then be used to induce resonant transitions between different k states. In particular, it could be interesting to couple reversibly the low-k optically active, but slow (small group velocity) states with optically inactive, but fast (larger group velocity) states from the middle of the Brillouin zone. This would lead to the creation of excitonic wave packets, which can be slowed down or accelerated by an external electric field.

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