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Disorderless Quasi-localization of Polar Gases in One-Dimensional Lattices

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One-dimensional polar gases in deep optical lattices present a severely constrained dynamics due to the interplay between dipolar interactions, energy conservation, and finite bandwidth. The appearance of dynamically bound nearest-neighbor dimers enhances the role of the $1/r^3$ dipolar tail, resulting in the absence of external disorder, in quasi-localization via dimer clustering for very low densities and moderate dipole strengths. Furthermore, even weak dipoles allow for the formation of self-bound superfluid lattice droplets with a finite doping of mobile, but confined, holons. Our results, which can be extrapolated to other power-law interactions, are directly relevant for current and future lattice experiments with magnetic atoms and polar molecules.

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Recent years have witnessed major interest in the dynamics of isolated many-body quantum systems [1–5]. This interest has been largely triggered by impressive experimental developments, especially in cold gases [6] and trapped ions [7], which realize almost perfect isolation [8–12]. Particular attention has been paid to atom dynamics in deep optical lattices, as in seminal experiments on single-particle and many-body localization in the presence of disorder [13–18]. However, in addition to energy conservation, tight-binding dynamics in deep lattices is largely determined by the finite bandwidth. This leads to the dynamical formation of (meta)stable states. A prominent example is that of a repulsively bound pair (RBP), an on-site pair of particles that, although thermodynamically unstable, remains dynamically bound if the interaction strength exceeds the lattice bandwidth [19,20]. The presence of RBPs leads, even for weak interactions, to a strong slow-down of the dynamics [21,22].

Whereas contact-interacting particles realize Hubbard models with only on-site interactions, extended Hubbard models (EHMs) with intersite interactions may be realized using particles that interact via power-law potentials. This is the case of Rydberg atoms, with strong van der Waals interaction at nearest neighbors [23,24], and of polar lattice gases with strong dipole-dipole interactions (DDI), in particular magnetic atoms and polar molecules. Intersite spin exchange has been observed using chromium [25] and KRb [26], whereas an EHM with nearest-neighbor interactions has been realized using erbium [27]. Although EHM experiments with polar molecules remain a challenge due to inelastic losses [28,29], the latter may be avoided by using fermionic molecules [30]. In addition to leading to new ground-state physics [31,32], strong dipole-induced intersite interactions, even just between nearest neighbors, lead to nonlocal RBPs [33,34] and clusters at different sites, which significantly slow down the dynamics [35].

In this Letter, we show that the formation of dynamically bound dimers leads, in the absence of disorder, to quasi-localization for surprisingly low densities and moderate dipole strengths. Moreover, superfluid self-bound lattice droplets form even for weak dipoles [36]. Our results are directly relevant for current and future experiments on magnetic atoms and polar molecules.

Model.—We consider hard-core polar bosons in a 1D lattice [37], described by the extended Bose-Hubbard Hamiltonian (EBHM):

$$\hat{H} = -J\sum_j (\hat{a}_j^\dagger \hat{a}_{j+1} + \text{H.c.}) + \frac{V}{2}\sum_{i\neq j}\frac{1}{|i-j|^3}\hat{n}_i\hat{n}_j, \quad (1)$$

with $\hat{a}_j$ ($\hat{a}_j^\dagger$) the annihilation (creation) operator for bosons at site j, $\hat{n}_j = \hat{a}_j^\dagger\hat{a}_j$, $(\hat{a}_j^\dagger)^2 = 0$, J the hopping rate, and V the DDI between nearest neighbors [38].

Dynamically bound dimers.—For $V/J > 7$, two particles at neighboring sites form a dynamically bound nearest-neighbor dimer (NND) [39]. We first consider that all particles are paired in NNDs, which can be prepared by superimposing a superlattice on top of the primary lattice [18]. Once the NND gas is created, the superlattice is removed, and the dimers may move via second-order hopping $J_D = 8J^2/7V$ [39]. The dimer dynamics is well approximated by a dimer EBHM:

$$\frac{\hat{H}_D}{J_D} = -\sum_l (\hat{D}_l^\dagger \hat{D}_{l+1} + \text{H.c.}) + \frac{V}{J_D}\sum_{l,L\geq 1} f(L)\hat{N}_l\hat{N}_{l+L+2}, \quad (2)$$

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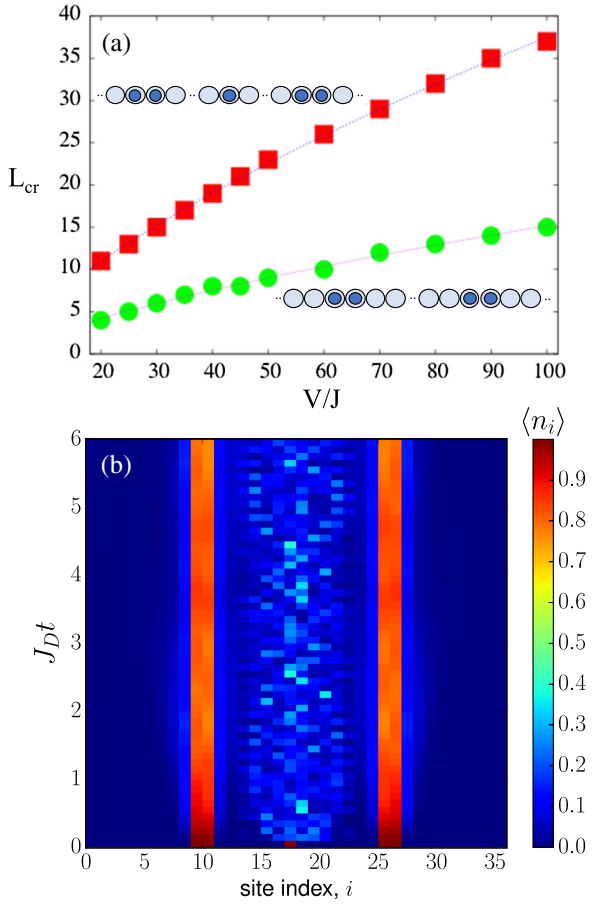

FIG. 1. (a) Squares (circles) indicate L_{cr} (see text) for two dimers with (without) a singlon in between, such that for an initial interdimer distance $L_0 < L_{cr}$ the dimers remain at a fixed distance [39]. In both cases $L_{cr} \propto (V/J)^{2/3}$ (dotted curves). (b) $\langle \hat{n}_j \rangle(t)$ evaluated by means of time-dependent density-matrix renormalization group (t-DMRG) calculations [40] using Eq. (1) for $V/J = 50$, for two dimers initially 15 sites apart and an intermediate singlon. The singlon quickly delocalizes in the interdimer space, but the dimers remain at fixed distance for $J_D t \gg 1$.

where $\hat{D}_l^\dagger = \hat{a}_l^\dagger \hat{a}_{l+1}^\dagger$ creates an NND at sites l and $l+1$, $\hat{N}_l = \hat{D}_l^\dagger \hat{D}_l$, and $f(L) = [2(L+2)^{-3} + (L+1)^{-3} + (L+3)^{-3}]$ characterizes the DDI between two dimers separated by L sites. Using $\hat{H}_D$ we determine the critical L_{cr}, such that if the initial $L_0 < L_{cr}$, then this separation remains well fixed at later times, which we quantify by imposing that the variance $\Delta L < \sqrt{L_0}$ for $J_D t = 100$ [39]. As expected from a simple inspection of $\hat{H}_D$, $L_{cr} \propto (V/J)^{2/3}$ [Fig. 1(a)].

Dimer clusters strongly slow down the dynamics, as illustrated [Fig. 2(a)] by the Shannon entropy $S(t) = -\sum_{\{n_j\}} |c(\{n_j\}, t)|^2 \log |c(\{n_j\}, t)|^2$, obtained from the state of the system $|\psi(t)\rangle = \sum_{\{n_j\}} c(\{n_j\}, t)|\{n_j\}\rangle$, with $|\{n_j\}\rangle$ Fock states characterized by occupations $n_j = 0, 1$. For $J_D t \ll 1$, $S(t)$ remains very low [41], since dimers move via second-order hopping. For $J_D t \gtrsim 1$, the dimer cluster quickly unravels for $L_0 > L_{cr}$, reaching a maximal entropy $S_{max} \simeq 2 \ln N_s$ [42]. For $L_0 < L_{cr}$, a stable dimer cluster is formed. $S(t)$ increases much slower, and only for $J_D t \gg 1$ due to the center-of-mass motion of the dimer cluster, up to $S_{max} \simeq \ln N_s$ [42].

For sufficiently large densities, clusters of more than two dimers form, strongly constraining entropy growth due to center-of-mass motion. This is illustrated in Fig. 2(b), where we depict for $V/J = 40$, the inhomogeneity parameter $\eta(t) = \sum_j |\langle \hat{n}_j \rangle - N/L|^2$ ($\eta \simeq 0$ indicates homogenization), obtained using the exact evolution of $\hat{H}_D$ for $N_D = 2$, 3, and 4 dimers initially separated by three empty sites in a lattice with $5(N_D + 1)$ sites (particle filling $\simeq 0.3$ in all cases). The homogenization time increases by 1 order of magnitude with every dimer added to the cluster. Polar dimers have hence a much stronger effect than nonpolar RBPs [43]. Whereas for the latter the larger mass of the pairs just leads to a slow-down, dimer hopping is out competed by the dipolar tail even at large distances, leading

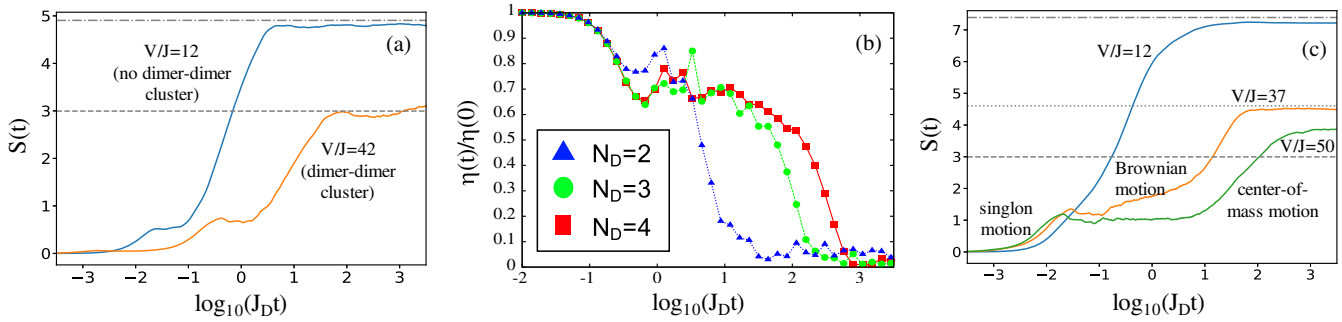

FIG. 2. (a) Shannon entropy $S(t)$, evaluated using exact evolution of Eq. (1) for 25 sites and periodic boundary conditions for two dimers initially 5 sites apart, for $V/J = 12$ (blue) and 42 (orange). Horizontal lines indicate S_{max} for unbound (dashed-dotted) and bound (dashed) dimer clusters [42]. (b) Inhomogeneity $\eta(t)/\eta(0)$ as a function of $J_D t$ evaluated using exact evolution of Eq. (2) for $V/J = 40$ for $N_D = 2$ (triangles), 3 (circles), and 4 (squares) dimers, initially with 3 sites between each dimer in a lattice with $5(N_D + 1)$ sites and periodic boundary conditions (particle filling $\simeq 0.3$). (c) Same as (a) but for two dimers initially 7 sites apart and a singlon in between for $V/J = 12$ (blue), 37 (orange), and 50 (green). Horizontal lines indicate S_{max} for dimers with an unbound relative distance (dashed-dotted), for dimers at a fixed distance with a singlon freely moving between them (dotted), and when the dimer-dimer and the dimer-singlon distance are fixed (dashed) [42].

to quasi-localization via clustering even for dilute gases and moderate dipoles [44].

Brownian motion.—Singlons (unpaired particles) radically change the dynamics. For weak-enough dipoles a singlon and a dimer can approach at one site of distance, and may resonantly swap positions, $|\ldots 1101\ldots\rangle \to |\ldots 1011\ldots\rangle$, where 0 (1) denotes an empty (occupied) site. These swaps result in dimer recoils, which induce a Brownian-like dimer motion for $Jt > 1$. In Fig. 2(c) we depict $S(t)$ for $V/J = 12$, 37, and 50 for a singlon initially between two dimers separated by 7 sites [45]. For $Jt \lesssim 1$, $S(t)$ grows due to singlon motion between dimers. For $1/J \lesssim t \lesssim 1/J_D$, Brownian motion results in an increase of $S(t)$, visible for $V/J = 37$, which is sped up by dimer hopping for $J_D t \gtrsim 1$. Being based on dimer-singlon swaps, Brownian motion is absent in a dimer gas without singlons [Fig. 2(a)], and for large V/J, [e.g., $V/J = 50$ in Fig. 2(c)] for which singlons and dimers cannot approach at one site of distance.

Singlon-gluing.—Large-enough V/J results in a dramatic singlon-induced enhancement of the interdimer binding. Because of the DDI, a singlon between two NNDs experiences a boxlike potential [39], freely moving up to a distance r_B from the dimers, with $V/r_B^3 \sim J$, fully delocalizing in a time $\sim 1/J$ over the box length $L - 2r_B$ [Fig. 1(b)]. Because of the singlon-dimer interaction, the change in singlon energy constrains the dimer motion even more strongly than the interdimer interaction. This mechanism resembles that discussed, for nonpolar gases, in Refs. [46,47], and also for polar gases in Ref. [35], in which the interplay between slow and fast particles (here dimers and singlons) was shown to result in quasi many-body localization. However, the surprisingly strong role of the DDI tail, crucial here, was overlooked in Ref. [35]. By solving a system of two dimers with an intermediate singlon [39], we confirm that $L_{\rm cr}$, which remains $\propto (V/J)^{2/3}$, is strongly enlarged [Fig. 1(a)]. For $V/J = 50$, two dimers initially $L_0 = 15$ sites apart remain at fixed distance for $J_D t \gg 1$ [Fig. 1(b)], despite the tiny interdimer DDI $Vf(L_0) \simeq 0.02J$.

Singlon-gluing crucially affects the dynamics of even dilute gases for moderate dipoles. A lattice gas at filling $\rho \ll 1$ is formed mainly by singlons, with a small dimer density $\rho_D \simeq \rho^2$ [48]. Hence, for a sufficiently large V/J that precludes Brownian motion, singlon-gluing leads to dimer clustering for $\rho \gtrsim \rho_{\rm cr} \simeq 1/\sqrt{L_{\rm cr}}$. As in the dimer gas without singlons, larger clusters of more than two dimers prevent the center-of-mass motion that results in the long-time entropy growth of Fig. 2(c). Hence even moderate DDI results for very low densities (for $V/J = 50$, $\rho_{\rm cr} \simeq 0.2$) into quasi-localization via massive dimer clustering. This estimation is conservative [48]. For lower ρ, smaller dimer clusters already constrain severely the dynamics. The required $|V|/J$ values are achievable with current state-of-the-art technology. For ^{164}Dy in an UV lattice with 180 nm spacing and depth of 23 recoil energies, $|V|/J \simeq 30$, with $J/\hbar \simeq 93\ {\rm s}^{-1}$. The dimer-hopping time is $1/J_D \simeq 280$ ms.

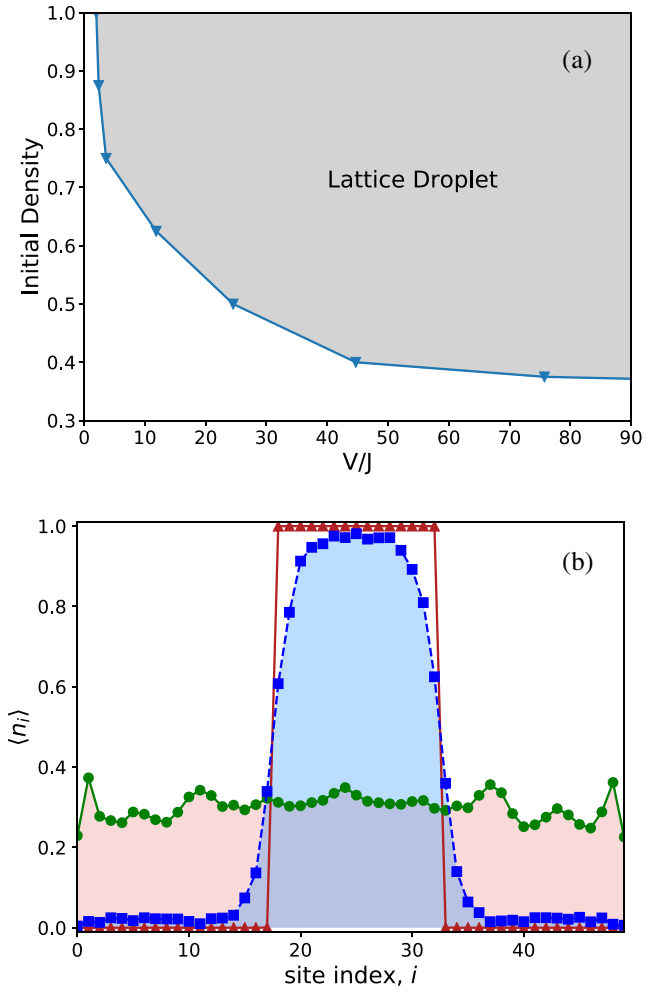

FIG. 3. (a) $(V/J)_{\rm cr}(\rho)$ for self-bound droplets obtained using exact evolution of Eq. (1) for 16 sites. The particles are initially in the ground state (with $V = 0$) of a box trap in the central 8 sites. We determine $F(V/J, \rho) = \xi(t_f)/\xi(0)$, where $\xi(t) = \rho_c(t) - \rho_{\rm av}$, with $\rho_{\rm av}$ the density for an homogeneous lattice gas, $\rho_c(t)$ the central density, and $t_f = 100 t_D$, with t_D the homogenization time for $V = 0$. We determine $(V/J)_{\rm cr}$ as that for which $F[(V/J)_{\rm cr}, \rho] = 0.1$. (b) Density distribution, obtained using t-DMRG simulations of Eq. (1) [40], for a gas initially confined with $\rho = 1$ (red triangles) $Jt = 30$ after release, for $V/J = 1$ (unbound, green circles) and $V/J = 2.5$ (droplet, blue squares).

Dimer clustering may then be probed in a few seconds, well within experimental lifetimes.

Lattice droplets.—Even much weaker DDI may dramatically impact the dynamics. We consider a hard-core gas at filling $\rho \leq 1$ initially prepared, with $V = 0$ (using the magic-angle orientation between dipole moment and lattice axis), in the ground state of a boxlike potential [49–51]. At time $t = 0$ the box trap is released and the dipole orientation is changed such that $V > 0$. In contrast to nonpolar experiments [21,22], where stable or partially stable on-site RBPs still allowed for an overall (slowed-down) expansion, in the polar case there is a critical $(V/J)_{\rm cr}(\rho)$ such that the cloud remains self-bound [Fig. 3(a)]. These self-bound

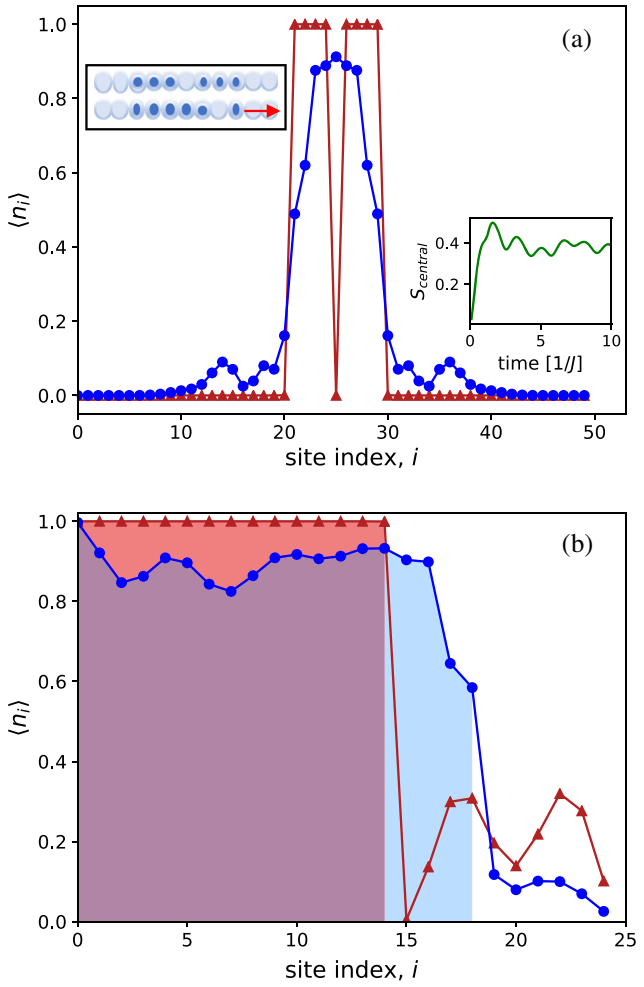

FIG. 4. (a) Droplet with a holon initially at the center (red triangles) after $Jt = 6$ (blue circles), for $V/J = 30$. Partial holon evaporation results in particle ejection (left inset), but is inefficient, as shown by the particle-hole entropy averaged over the 5 central sites (right inset). (b) Initial droplet with $\rho = 1$ and two singlons outside (red triangles) after $Jt = 55$ (blue circles). The shadowed region is that of the droplet. Note singlon aggregation at the droplet edge. Figures obtained by t-DMRG calculations using Hamiltonian (1) [40].

lattice droplets present a finite final average $\rho' < 1$ [Fig. 3(b)]; i.e., holons (empty sites) remain mobile but confined within a droplet. As a result, lattice droplets remain superfluid. For $\rho = 1$, droplets occur already for $V/J \simeq 2.5$. For current ^{166}Er experiments [27], with a lattice spacing of 266 nm and a typical lattice depth of 20 recoil energies, $V/J \simeq 2.7$, with a hopping time $1/J = 6.5$ ms.

For large-enough V/J, holons remain confined in the droplet due to the potential exerted by the droplet boundaries via the DDI tail. For $V/J \lesssim 8$ [Fig. 4(a)], this mechanism is insufficient, since only NN DDI are relevant. A holon, initially inside a droplet with $\rho = 1$, expands by resonant hops up to the edges. At that point, the last particle may escape without breaking any NN bond [left inset of Fig. 4(a)]. This holon evaporation becomes drastically inefficient for growing droplet sizes, since the holon quickly spreads uniformly within the droplet [right inset of Fig. 4(a)]. Therefore, holons remain confined within the droplet. The converse also occurs: a singlon may stick to the droplet edge, pushing a holon inside [Fig. 4(b)]. Mobile holons inside the droplet may be revealed using quantum gas microscopy.

Conclusions.—Polar gases in 1D lattices present a severely constrained dynamics. Dynamically bound dimers dramatically enhance the role of the dipolar tail, leading to quasi-localization in absence of disorder via dimer clustering even for low densities and moderate dipole moments. Moreover, polar gases may form, even for weak dipoles, self-bound superfluid lattice droplets. Our results hint at inherent difficulties in particle-hole entropy removal in polar lattice gases. Our work is directly relevant for current lanthanide experiments and future experiments with polar molecules, and may be easily extrapolated to other power-law interactions, $V/|i-j|^{\alpha}$ [52].

Our results may be extrapolated to higher dimensions. Whereas singlon-gluing just occurs in one dimension, since it requires singlon confinement between dimers, clusterization due to dimer-dimer DDI and self-bound lattice droplets occurs also in higher dimensions. For square lattices, L_{cr} is only slightly modified compared to 1D. The critical lattice filling for dimer localization via clustering scales, however, as $\rho_{cr} \simeq 1/L_{cr}$, and hence for moderate $V/J \sim 30$, $\rho_{cr} \lesssim 0.1$. Moreover, in contrast to 1D, when removing the overall confinement, but keeping the lattice on, singlons evaporate leaving an immobile dimer cluster behind despite the extremely dilute dimer density $\rho_D \simeq \rho_{cr}^2$ [53].

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[36] For Fermi gases the droplets would remain metallic.

[37] The hard-core condition assumes strong on-site interactions, such that maximally one boson is allowed per site.

[38] Our results should not change qualitatively for single-component fermions.

[39] See Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevLett.124.010404 for the details on the evaluation of the stability of NN dimers, the dimer-dimer states, and the dimer-singlon-dimer model.

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[41] The nature of the short-time plateaux of Fig. 2(a) is different for $V/J = 12$ and for $V/J = 42$. For $V/J = 12$, the atoms within the dimers are not fully rigidly bound at nearest neighbors, but rather have small probability to separate to next-nearest neighbors. This slight spreading explains the entropy growth for $t \sim 1/J$. This initial growth is followed by a plateau, because any further entropy growth demands the dimer motion, which occurs at $t \sim 1/J_D \gg 1/J$. This entropy growth then proceeds unhindered since no dimer cluster forms. For $V/J = 42$ the dimers are rigidly formed by nearest-neighbor atoms, and hence entropy growth at the $1/J$ timescale is prevented. The small entropy growth at $t \sim 1/J_D$ is due to the slightly undefined relative interdimer distance having a finite variance $\Delta L \ll L_0$. That growth of $S(t)$ is followed by a plateau, since further entropy growth demands the motion of the whole dimer-dimer cluster, which occurs in a longer timescale.

[42] $S_{\max}$ may be determined from the dimension of the energetically available Hilbert manifold D, as $S_{\max} = \log(D)$. For the case of two freely moving dimers, $D \simeq N_s^2$, whereas for bound dimers at a rigid fixed distance, $D \simeq N_s$. Similarly for two dimers with a singlon in between, $D \simeq N_s^3$ if the dimers and the singlon move freely. For bound dimers at a fixed distance L with a freely moving singlon in between, $D \simeq N_s L$. Finally, if the singlon position is pinned at the center of the two dimers, $D \simeq N_s$.

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[44] Note that dimers remain at a fixed distance for all initial separations $L < L_{\rm cr}$. As a result, multidimer clusterization does not require an initial dimer crystal, i.e., the distance between neighboring dimers in the cluster may be in general unequal.

[45] Because of periodic boundary conditions, a single singlon, which may present different winding numbers around the periodic system, will lead to Brownian motion of the NNDs, mimicking the behavior expected for NNDs in a singlon bath.

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[48] We consider neither nearest-neighbor clusters of $n > 2$ particles, which occur with density ρ^n, nor the formation of dimers beyond nearest neighbors. For sufficiently large V/J these dimers may become stable as well. Their presence, however, would result in an even stronger localization of the lattice gas.

[49] More general confinements, e.g., harmonic traps or finite-temperature effects do not modify our conclusions.
[50] The hard core condition may be easily imposed by setting a large value for the scattering length using Feshbach resonances.
[51] V depends as $(1-3\cos^2\theta)$, with θ the angle between the dipole moment and the lattice axis. Hence, in one dimension $|V|$ can be changed all the way from its maximal value to zero. The latter occurs at the so-called magic angle, $\theta_M = \arccos(1/\sqrt{3})$.
[52] For a power α, the critical interdimer distance for dimer clustering scales as $L_{\mathrm{cr}} \propto (V/J)^{2/\alpha}$.
[53] This must be compared to clusters of nonpolar RBPs resulting from quantum distillation [43] which occur at a unit filling of pairs.