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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:

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

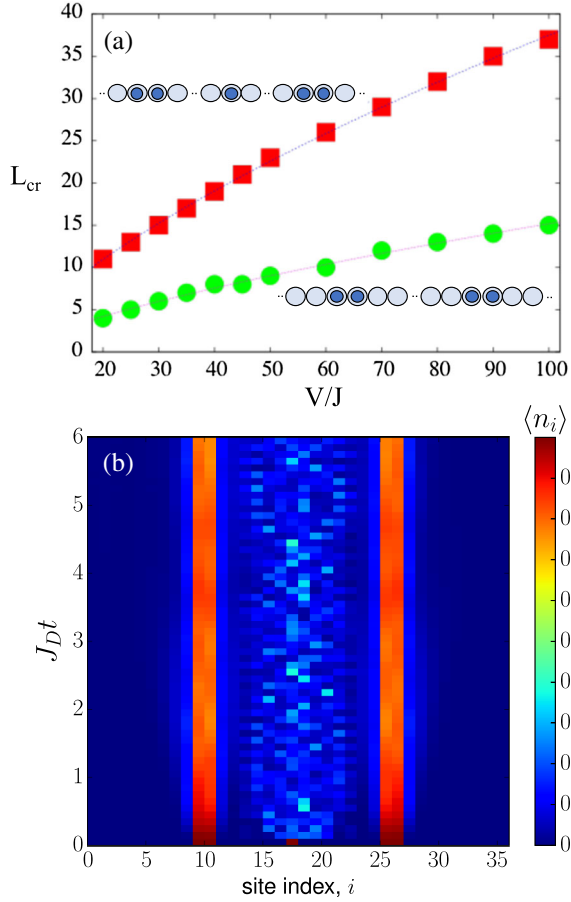


FIG. 1. (a) Squares (circles) indicate  $L_{cr}$  (see text) for two dimers with (without) a singlon in between, such that for an initial interdimer distance  $L_0 < L_{cr}$  the dimers remain at a fixed distance [39]. In both cases  $L_{cr} \propto (V/J)^{2/3}$  (dotted curves). (b)  $\langle \hat{n}_j \rangle(t)$  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

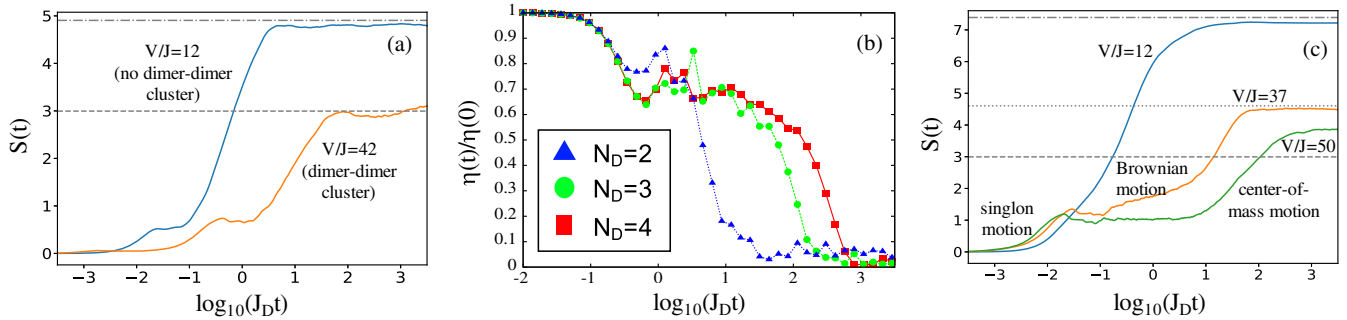


FIG. 2. (a) Shannon entropy  $S(t)$ , evaluated using exact evolution of Eq. (1) for 25 sites and periodic boundary conditions for two dimers initially 5 sites apart, for  $V/J = 12$  (blue) and 42 (orange). Horizontal lines indicate  $S_{max}$  for unbound (dashed-dotted) and bound (dashed) dimer clusters [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,  $|\dots 1101\dots\rangle \rightarrow |\dots 1011\dots\rangle$ , 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  $L_{\text{cr}}$ , 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  $\rho \gtrsim \rho_{\text{cr}} \simeq 1/\sqrt{L_{\text{cr}}}$ . 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  $V/J = 50$ ,  $\rho_{\text{cr}} \simeq 0.2$ ) into quasi-localization via massive dimer clustering. This estimation is conservative [48]. For lower  $\rho$ , smaller dimer clusters already constrain severely the dynamics. The required  $|V|/J$  values are achievable with current state-of-the-art technology. For  $^{164}\text{Dy}$  in an UV lattice with 180 nm spacing and depth of 23 recoil energies,  $|V|/J \simeq 30$ , with  $J/\hbar \simeq 93 \text{ s}^{-1}$ . The dimer-hopping time is  $1/J_D \simeq 280 \text{ ms}$ .

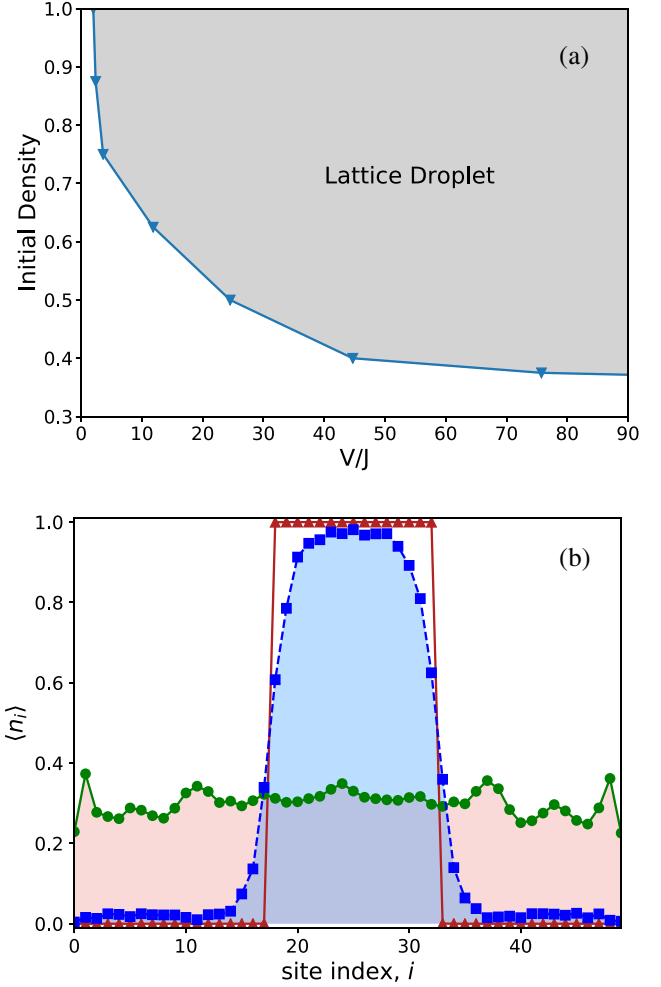


FIG. 3. (a)  $(V/J)_{\text{cr}}(\rho)$  for self-bound droplets obtained using exact evolution of Eq. (1) for 16 sites. The particles are initially in the ground state (with  $V = 0$ ) of a box trap in the central 8 sites. We determine  $F(V/J, \rho) = \xi(t_f)/\xi(0)$ , where  $\xi(t) = \rho_c(t) - \rho_{\text{av}}$ , with  $\rho_{\text{av}}$  the density for an homogeneous lattice gas,  $\rho_c(t)$  the central density, and  $t_f = 100t_D$ , with  $t_D$  the homogenization time for  $V = 0$ . We determine  $(V/J)_{\text{cr}}$  as that for which  $F[(V/J)_{\text{cr}}, \rho] = 0.1$ . (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  $(V/J)_{\text{cr}}(\rho)$  such that the cloud remains self-bound [Fig. 3(a)]. These self-bound

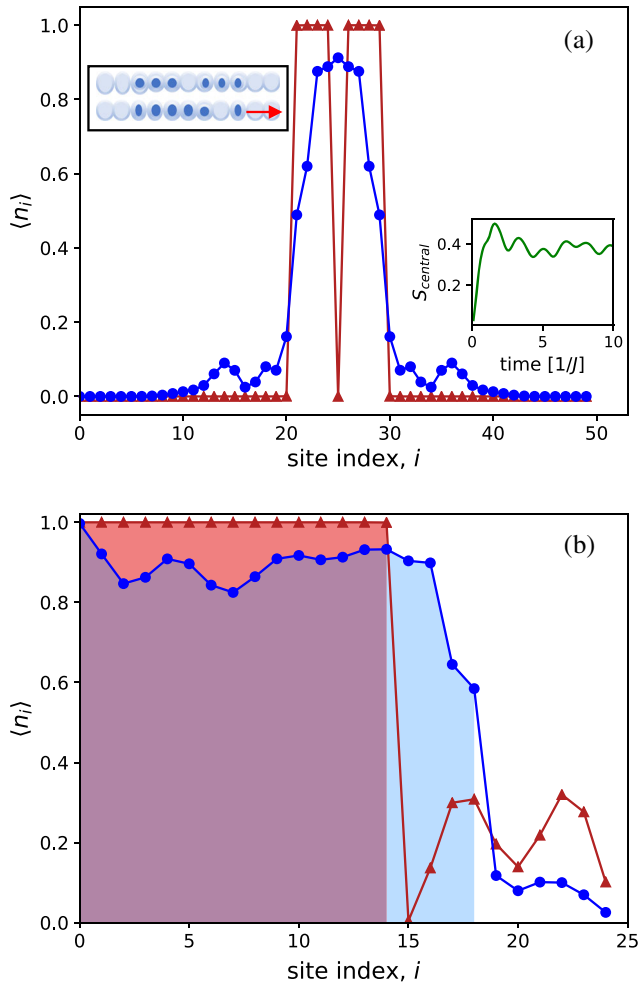


FIG. 4. (a) Droplet with a holon initially at the center (red triangles) after  $Jt = 6$  (blue circles), for  $V/J = 30$ . Partial holon evaporation results in particle ejection (left inset), but is inefficient, as shown by the particle-hole entropy averaged over the 5 central sites (right inset). (b) 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  $^{166}\text{Er}$  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,  $L_{\text{cr}}$  is only slightly modified compared to 1D. The critical lattice filling for dimer localization via clustering scales, however, as  $\rho_{\text{cr}} \simeq 1/L_{\text{cr}}$ , and hence for moderate  $V/J \sim 30$ ,  $\rho_{\text{cr}} \lesssim 0.1$ . 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  $\rho_D \simeq \rho_{\text{cr}}^2$  [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.
- [40] M. L. Wall and L. D. Carr, *New J. Phys.* **14**, 125015 (2012).
- [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,  $D \simeq N_s$ .
- [43] D. Petrosyan, B. Schmidt, J. R. Anglin, and M. Fleischhauer, *Phys. Rev. A* **76**, 033606 (2007).
- [44] Note that dimers remain at a fixed distance for all initial separations  $L < L_{\text{cr}}$ . 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.
- [46] T. Grover and M. P. A. Fisher, *J. Stat. Mech.* (2014) P10010.
- [47] M. Schiulaz, A. Silva, and M. Müller, *Phys. Rev. B* **91**, 184202 (2015).
- [48] We consider neither nearest-neighbor clusters of  $n > 2$  particles, which occur with density  $\rho^n$ , 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  $\theta$  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  $\alpha$ , the critical interdimer distance for dimer clustering scales as  $L_{\text{cr}} \propto (V/J)^{2/\alpha}$ .
- [53] This must be compared to clusters of nonpolar RBPs resulting from quantum distillation [43] which occur at a unit filling of pairs.