

Stability of quasicrystalline ultracold fermions to dipolar interactions

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Quasiperiodic potentials can be used to interpolate between localization and delocalization in one dimension. With the rise of optical platforms engineering dipolar interactions, a key question is the stability of quasicrystalline phases under these long-range interactions. In this work, we study repulsive ultracold dipolar fermions in a quasiperiodic optical lattice to characterize the behavior of interacting quasicrystals. We simulate the full time evolution of the typical experimental protocols used to probe quasicrystalline order and localization properties. We extract experimentally measurable dynamical observables and correlation functions to characterize the three phases observed in the noninteracting setting: localized, intermediate, and extended. We then study the stability of such phases to repulsive dipolar interactions. We find that dipolar interactions can completely alter the shape of the phase diagram by stabilizing the intermediate phase, mostly at the expense of the extended phase. Moreover, in the strongly interacting regime, a resonance-like behavior characterized by density oscillations appears. Remarkably, strong dipolar repulsions can also localize particles even in the absence of quasiperiodicity if the primary lattice is sufficiently deep. Our work shows that dipolar interactions in a quasiperiodic potential can give rise to a complex, tunable coexistence of localized and extended quantum states.

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Introduction. Since their revolutionary discovery in aluminum-manganese alloys [1], quasicrystals have been the subject of intense theoretical and experimental research due to their many exotic properties. Quasicrystals exhibit a regular structure despite lacking a canonical periodicity [2,3]. While they lack translational symmetry, they can completely tessellate a two-dimensional surface in an aperiodic fashion because they do possess unexpected rotational symmetries (fivefold, eightfold, etc.). Quasicrystals can be mathematically understood in terms of higher-dimensional periodic structures projected onto lower-dimensional slices and have thus ushered in different paradigms for crystallography [4–8], band theory in solids [9–12], and hidden dimensions [13]. Moreover, quasiperiodic structures can emulate on-site disorder, which makes them ideal platforms to study many-body localization [14–22] and its interplay with nonergodicity [23–28], integrability [29–33], and fractality [13,34–40].

In recent years, impressive advances in trapping and controlling ultracold atoms have made them an excellent platform to realize and study quasiperiodicity with extreme precision [15,41–55]. In one dimension (1D), a quasiperiodic potential can be generated by superimposing a primary optical lattice with a detuning lattice at an incommensurate frequency. Upon loading particles in such a quasiperiodic potential, it is possible to quantum simulate and study the dynamics of 1D

quasicrystals with high accuracy. A particularly interesting feature exhibited by these systems is the coexistence of localized and extended states in an intermediate phase separating the fully localized from the fully extended phase [48]. In the intermediate phase, the different states are separated by a critical energy level termed single-particle mobility edge (SPME) [48,56–60]. This coexistence manifests itself due to long-range tunneling terms that appear in the continuum description of the 1D ultracold quantum simulator. In fact, the SPME is absent in the deep lattice limit, where an effective Aubry-André model with self-duality is obtained [42,61–63]. Furthermore, a rigorous SPME does not appear in 1D systems with Anderson-type (uncorrelated) disorder [48].

While the properties of the SPME and intermediate phase have been widely explored in noninteracting systems, less attention has been given to potential interplays with interactions, in particular, long-range ones that can arise in the next generation of dipolar quantum simulators [64–67]. In fact, nowadays numerous atomic and molecular species exhibiting dipole-dipole interactions (DDIs) are available in ultracold labs, such as dysprosium ^{161}Dy [68], erbium ^{167}Er [69,70], chromium ^{53}Cr [71], potassium-rubidium ^{40}K ^{87}Rb [72], sodium-lithium ^{23}Na ^6Li [73], and sodium-potassium ^{23}Na ^{40}K [74,75]. DDIs, besides better incorporating the long-range nature of interactions in solid-state quasicrystalline materials, could potentially herald many interesting phases of matter when interfaced with quasicrystalline long-range order [76–78].

In this work, we investigate the role of DDIs in 1D ultracold fermions loaded in a quasiperiodic potential. We simulate the exact experimental protocol used in ultracold atomic setups [15,48,79,80], whereby the fermions are first loaded in a superlattice of twice the periodicity of the primary optical lattice and then are let to time evolve into the quasiperiodic

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structure quenched at time zero. By measuring the imbalance between odd and even sites and the expansion of the particle density, it is possible to classify the state of the system as being in a localized, extended, or intermediate phase. We study the stability of each phase with respect to DDIs by determining phase diagrams and by calculating observables such as pair-correlation functions.

We find that DDIs tend to stabilize the intermediate phase, mostly to the detriment of the extended phase. Examining the correlation functions, this stabilization results from a decreased correlation between far away particles that can be attributed to interference between the long-range tails of the DDIs. At strong DDIs, the same mechanism not only strengthens the imbalance in the localized phase but also induces a different kind of localization in regimes where the noninteracting system would only host extended states. Surprisingly, we find that this localization persists also when the detuning lattice is zero, i.e., for a fully periodic optical lattice. By combining the effect of quasiperiodicity and DDIs-induced bound clusters, we bring forth an explanation for the pathway from disorder-free localization, to delocalization, to eventual relocalization. Our study illustrates the potential for long-range interacting systems to induce different types of localization phenomena in conjunction with quasicrystalline structures.

Model. We consider the dynamics of a system of N ultracold fermions placed in a 1D-dimensional quasiperiodic optical lattice. The fermions are described by creation/annihilation field operators $\hat{\Psi}(x)^{(\dagger)}$ obeying canonical anticommutation relations and their single-particle Hamiltonian is given by

$$\mathcal{H} = \int dx \hat{\Psi}^\dagger(x) \left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right] \hat{\Psi}(x). \quad (1)$$

The quasiperiodic lattice $V(x)$ is realized by interfering a detuning laser of amplitude V_d , wave vector k_d , and phase ϕ , with a primary laser of amplitude V_p and wave vector k_p ,

$$V(x) = \frac{V_p}{2E_r} \cos(2k_p x) + \frac{V_d}{2E_r} \cos(2k_d x + \phi), \quad (2)$$

with E_r the recoil energy of the primary lattice (unit of energy). For the potential parameters, we choose values compatible with experimental realizations of this system [48,81]. We also add hard wall boundaries [82–85] to obtain a finite system containing 64 sites in the primary lattice. While this spatial extent is smaller than in typical experiments, it is more than enough to capture the hallmarks of each phase.

The fermions interact with one another through the interaction Hamiltonian

$$\mathcal{H}_{\text{int}} = \frac{1}{2} \int dx \int dx' \hat{\Psi}^\dagger(x) \hat{\Psi}^\dagger(x') W(x, x') \hat{\Psi}(x') \hat{\Psi}(x), \quad (3)$$

where

$$W(x, x') = \frac{W \bar{L}^3}{E_R(|x - x'|^3 + \alpha)} \quad (4)$$

is a dipolar repulsion with interaction strength W and regularization factor $\alpha = 0.01$ (phenomenologically accounting for Pauli pressure), and $\bar{L}$ is the distance between two neighboring minima in the primary lattice (unit of length).

Experimental protocol and observables. To probe the properties of the system, we follow the protocol employed in previous experiments [15,48]. We first build a superlattice with half the primary lattice wave vector and load particles into its center. At time zero, we then quench the primary and detuning lattices to their respective values and let the system time evolve. We monitor the real time evolution and extract dynamical observables from the many-body wave function $|\Psi(t)\rangle$ of the system. To characterize the localization properties of the system, we calculate two dynamical quantities: *imbalance* $\mathcal{I}(t)$ and *edge density* $\mathcal{D}(t)$. The imbalance is defined as the instantaneous normalized density difference between the odd and even sites in the superlattice:

$$\mathcal{I}(t) \equiv \frac{\mathcal{N}_e(t) - \mathcal{N}_o(t)}{\mathcal{N}_e(t) + \mathcal{N}_o(t)}, \quad (5)$$

where $\mathcal{N}_{e/o}(t) \equiv \int_{e/o} dx \rho(x, t)$, $\rho(x, t) = \langle \Psi(t) | \hat{\Psi}^\dagger(x) \hat{\Psi}(x) | \Psi(t) \rangle$, and e and o indicate the spatial points belonging to the even and odd superlattice sites, respectively. The edge density is defined as the ratio of particles outside the central range populated at time zero:

$$\mathcal{D}(t) \equiv 1 - \mathcal{N}_c/N, \quad (6)$$

with $\mathcal{N}_c = \int_c dx \rho(x, t)$ and c referring to the initially populated central region (e.g., for $N = 4$, $c = [-4.5, 3.5]$). These two observables in the long-time limit help us to determine the many-body phase of the system. A finite imbalance $\mathcal{I}$ indicates the persistence of the initial charge density wave pattern imposed by the superlattice and is a proxy for the presence of localized states. A finite (and growing) value of the edge density $\mathcal{D}$ reveals instead the presence of extended states. Therefore, in the localized phase $\mathcal{I} > 0$ and $\mathcal{D} = 0$, while in the extended phase $\mathcal{I} = 0$ and $\mathcal{D} > 0$. Localized and extended states can also coexist at different energies in an intermediate phase, where both values of $\mathcal{I}$ and $\mathcal{D}$ are nonzero, and an SPME is present. While the SPME should occur at arbitrarily small nonzero $\mathcal{I}$ and $\mathcal{D}$, numerical simulations introduce small imprecisions. Thus, small but finite thresholds $t_{\mathcal{I}}$ and $t_{\mathcal{D}}$ for the imbalance and the edge density, respectively, have to be introduced. Throughout our analysis, we will empirically set them to be $t_{\mathcal{I}} = 0.1$ and $t_{\mathcal{D}} = 0.03$ [86].

Besides exploring how interactions impact the phase diagram and the boundaries between different phases, we also probe the correlations within each phase. For simplicity, we focus here on the behavior of the diagonal of the reduced two-body density matrix (2-RDM), defined as

$$\rho^{(2)}(x, x'; t) = \langle \Psi(t) | \hat{\Psi}^\dagger(x) \hat{\Psi}^\dagger(x') \hat{\Psi}(x') \hat{\Psi}(x) | \Psi(t) \rangle, \quad (7)$$

where $|\Psi(t)\rangle$ is the time-evolved many-body state of the system. The diagonal of the 2-RDM is equivalent to the pair-correlation function and describes the conditional probability of finding a fermion at position x , when another fermion is located at x' ; i.e., it quantifies how a fermion is surrounded by other fermions. Thus, it encodes the entire information about pairwise interactions among particles and is a proxy for the (unnormalized) pairwise correlations of the system.

Methods. To simulate the full many-body interacting system, we employ the multiconfigurational time-dependent Hartree (MCTDH) method for indistinguishable particles

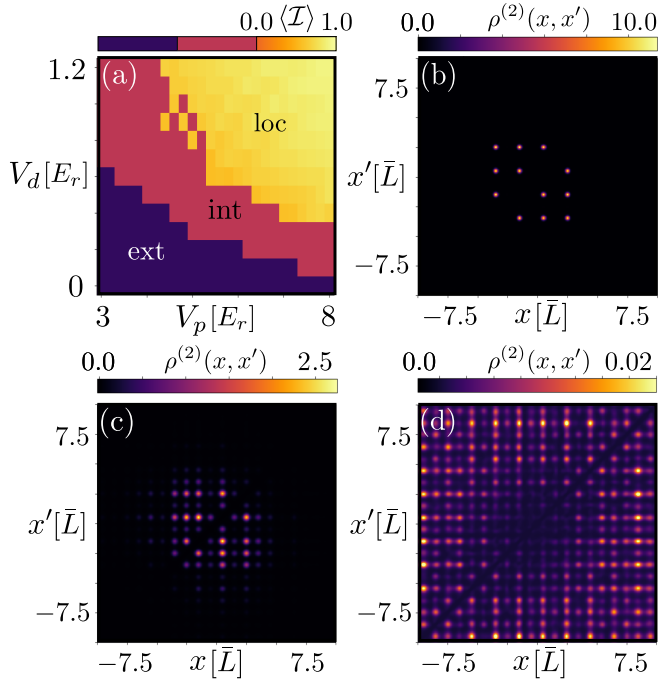


FIG. 1. Behavior of the noninteracting system: (a) Phase diagram for $N = 4$ fermions with $M = 9$ orbitals in a 1D quasiperiodic potential. For the localized phase, the time-averaged imbalance $\langle \mathcal{I} \rangle$ is plotted in a continuous color scheme. 2-RDM at $t = 20\tilde{t} = 3.7$ ms for (b) localized phase ($V_p = 16.0E_r$, $V_d = 2.4E_r$), (c) intermediate phase ($V_p = 5.0E_r$, $V_d = 0.4E_r$), and (d) extended phase ($V_p = 3.0E_r$, $V_d = 0E_r$).

[87–90], implemented in the MCTDH-X software [91–95]. With it, we solve the many-body Schrödinger equation directly for the continuum system consisting of kinetic energy, interparticle interactions, and optical lattice. MCTDH-X has been widely used to study ground-state and dynamical properties of long-range interacting systems [96–108]. MCTDH-X relies on a time-dependent variational optimization procedure, in which the many-body wave function is decomposed into an adaptive basis set of M time-dependent single-particle functions called *orbitals*. Due to the Pauli exclusion principle, to correctly describe a set of N fermions, we require $M \geq N + 1$ orbitals [109]. For strongly interacting systems, a larger number of orbitals might be required to capture many-body correlation effects. In this work, we have verified that including orbitals beyond $M = N + 4$ leads to a negligible population for the timescales probed by our dynamics [81].

Results for noninteracting fermions. We begin by describing the dynamics for noninteracting particles. Figure 1(a) shows the noninteracting phase diagrams for $N = 4$ fermions with $M = 9$ orbitals, constructed by calculating the imbalance and expansion observables as the depth of the primary and detuning lattices is varied. We use parameter ranges compatible with experimental regimes, i.e., $V_p \in [3E_r, 8E_r]$ and $V_d \in [0, 1.2E_r]$. The imbalance is calculated by averaging over the last 50 time steps at the end of each time evolution, with maximal simulation times reaching ≈ 45 ms. The edge density is typically calculated at a target time $\tilde{t}$, well before the particles can reach the boundaries of the system. Typical target times are $\tilde{t} = 1.8$ ms to $\tilde{t} = 7.2$ ms [110]. From Fig. 1(a),

we can clearly distinguish the three expected phases, which have the same structure observed in prior studies [48,60]. At low values of V_d , the system is always in the extended phase (purple region). Increasing the value of V_d at low to moderate values of V_p pushes the system into an intermediate region, where extended and localized states coexist (magenta region). Further increasing V_d or V_p eventually localizes all the states (yellow region).

The three phases of the quasicrystal system can also be distinguished by the dynamics of their many-body correlations encoded in the 2-RDM, shown for selected times in Figs. 1(b)–1(d) (see the Supplemental Material for more time snapshots [81]). The 2-RDM in the localized phase [Fig. 1(b)] does not change at all with time and merely shows the expected exchange hole at $x = x'$ with strong many-body correlation between the sites of the initial superlattice. On the contrary, the extended phase [Fig. 1(d)] exhibits a rapid spread of correlations at very short times already. Between the two extremes of localization and expansion lies the intermediate phase [Fig. 1(c)]. The correlation pattern here reveals an almost immediate exchange correlation between neighboring sites within the populated area of the initial superlattice, and a relatively small spread to sites outside of it. However, the intensity of the 2-RDM is not uniform: Correlations between sites in the initial superlattice structure still dominate throughout the time evolution even for longer times [81]. These results indicate that the intermediate phase is characterized by two types of correlations showcasing the coexistence of localized and extended states. Localized states mediate static, short-range correlations between the initially populated sites, while extended states mediate long-range correlations spanning many sites in the quasiperiodic lattice.

Results for interacting fermions. We now address how the DDIs impact the various quasicrystalline phases. The protocol studied is analogous to the one used in the noninteracting case. For simplicity, in our simulations, we turn off the interactions during the initial loading procedure. In an experiment, dipolar fermions could be directly loaded in their starting position by employing optical tweezers or letting them relax into the superlattice with a very large depth. We again compute imbalance $\mathcal{I}$ and edge density $\mathcal{D}$ to obtain measures of localization and expansion properties, and collect them as a function of lattice depths and interaction strength. We also calculate densities, correlations, and energies [81] to better describe the behavior of each phase.

Figure 2 shows how the noninteracting phase diagram changes when interactions are progressively increased [panels (a)–(c)]. At small interaction values, the intermediate phase only grows slightly, while the imbalance in the localized phase decreases. As the interactions become stronger, though, the phase diagram changes drastically and in a nonmonotonic fashion. For $W = 0.2E_r$, the intermediate phase grows sizably at the expense of most of the localized phase and part of the extended phase. Therefore, DDIs *stabilize* the coexistence of extended and localized states in the intermediate phase. At even stronger interactions, $W = 2.0E_r$, the intermediate phase dominates the probed parameter region. Note that in Fig. 2(c), V_p is plotted to larger values up to $12E_r$. The purely extended region is instead reduced to a tiny pool around $V_p = 3E_r$ and $V_d = 0E_r$.

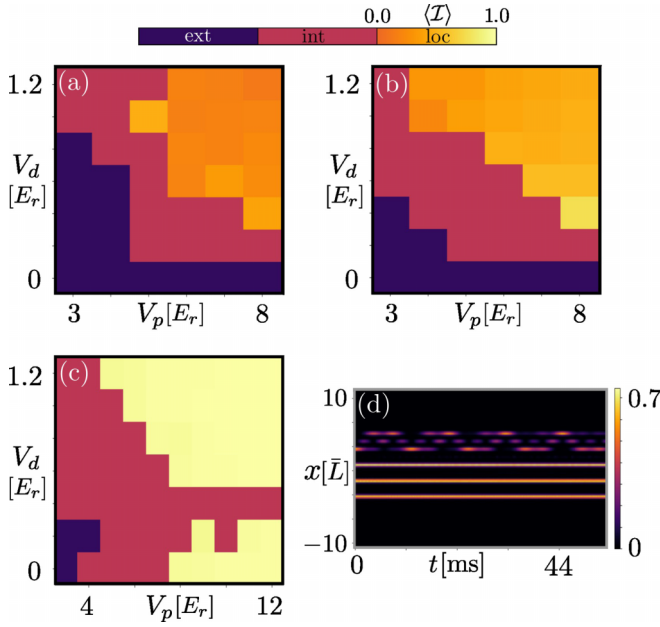


FIG. 2. Phase diagram for increasing DDIs strength W : (a) $W = 0.02E_r$, (b) $W = 0.2E_r$, and (c) $W = 2.0E_r$. For the localized phase, the time-averaged imbalance parameter $\langle \mathcal{I} \rangle$ is plotted as a continuous color scheme. Panel (d) depicts the density dynamics of the resonance lobe at $V_p = 6E_r$ and $V_d = 0.4E_r$.

Most strikingly, however, a different localized region emerges at low values of V_d . Note that this region was initially part of the extended phase in the noninteracting case. The localized phases at low and high V_d are divided by a strip of intermediate phase that persists for very large values of V_p (as large as $V_p = 16.0E_r$ —not shown in the phase diagram), reminiscent of the Arnold tongues found in parametrically driven systems [97,111,112]. In this lobe, the particles undergo density oscillations around their initial pinned configuration, indicating a potential resonance between DDIs and quasiperiodic potential [see Figs. 2(d) and 3(b)–3(d)]. While both regions above and below the intermediate phase lobe show strong localization, their behavior is different. Above the lobe

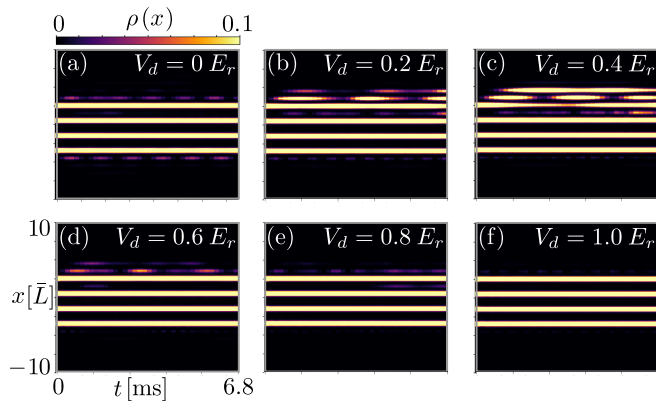


FIG. 3. Two types of localization at strong interactions. Density dynamics at $V_p = 8E_r$ and $W = 2.0E_r$ for increasing values of V_d between 0 and $1.0E_r$, illustrating how correlated disorder impacts the DSBS. The scale is zoomed in to increase resolution.

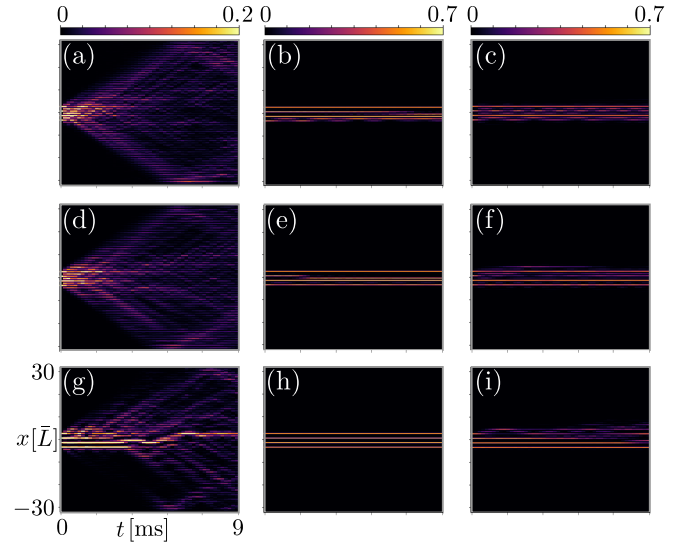


FIG. 4. Dynamics of dipolar fermions with increasing DDIs strength W in a quasiperiodic lattice. The interaction strength is (a)–(c) $W = 0.02E_r$, (d)–(f) $W = 0.2E_r$, and (g)–(i) $W = 2.0E_r$. The potential depths are (a), (d), (g) $V_p = 3.0E_r$ and $V_d = 0.0E_r$ (extended phase), (b), (e), (h) $V_p = 8.0E_r$ and $V_d = 1.2E_r$ (localized phase), (c) $V_p = 7.0E_r$ and $V_d = 0.2E_r$, (f) $V_p = 6.0E_r$ and $V_d = 0.4E_r$, and (i) $V_p = 5.0E_r$ and $V_d = 0.6E_r$ (intermediate phase). The axes in panel (g) apply to all panels.

[high V_d , Figs. 3(e) and 3(f)], the particles do not move at all from their initial configuration. Below the lobe [low V_d , Fig. 3(a)], the particle density periodically leaks back and forth from the initial boundaries while retaining a strong localization inside them, indicating a dynamically self-bound state (DSBS). Such states were recently discovered in bosonic lattice models with attractive DDIs [113–117]. Here, we reveal that DSBS can also exist for fermionic gases with repulsive DDIs and away from the lattice limit $V_d \rightarrow \infty$.

A more systematic calculation of the density dynamics, shown in Fig. 4, allows us to better discuss the behavior in each phase. The dynamics in the extended phase, localized phase, and intermediate phase is pictured, respectively, in the left, middle, and right columns. The rows show the dynamics for increasing interaction strength. In the extended phase [Figs. 4(a), 4(d), and 4(g)], the DDIs have initially little effect on the density, which maintains its linear spread in time consistent with the Lieb-Robinson bounds [118]. At strong interactions, however, the long-range repulsive tail in the DDIs hinders the spread of correlations [119], resulting in both a delayed expansion and a more chaotic density spread [Fig. 4(g)]. In the localized phase [Figs. 4(b), 4(e), and 4(h)], very small oscillations can be seen at one edge of the density profile for small and intermediate interaction strengths. At strong interactions, however, this behavior is suppressed. This stabilization of localization is also observed in the intermediate phase [Figs. 4(c), 4(f), and 4(i)]. At low DDIs, the density in the intermediate phase maintains a strong imbalance toward the initial superlattice configuration (due to localized states) while expanding toward outer lattice sites (due to extended states). However, stronger DDIs increase the imbalance while simultaneously reducing the expansion. This behavior is again

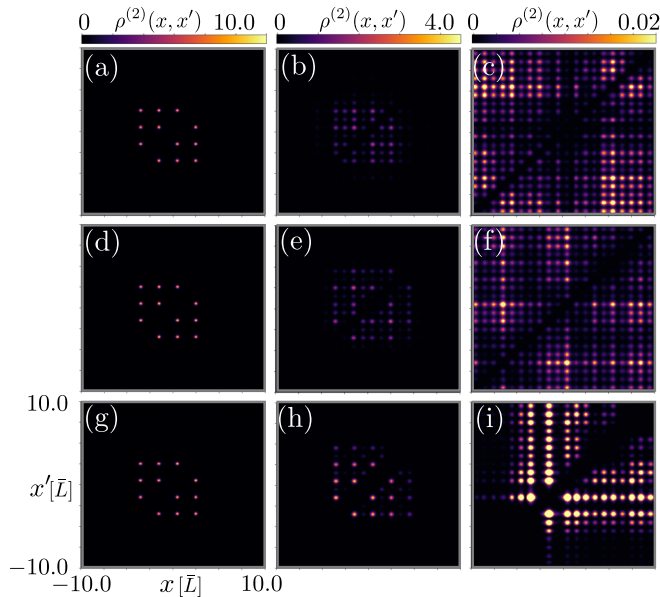


FIG. 5. 2-RDM in the dynamics of fermions with DDIs. The snapshots are taken at $t = 20\bar{t} \approx 3.6$ ms and for increasing DDIs: (a)–(c) $W = 0.02E_r$, (d)–(f) $W = 0.2E_r$, and (g)–(i) $W = 2.0E_r$. The parameters are (a), (d), (g) $V_p = 16.0E_r$ and $V_d = 2.4E_r$ (localized phase), (b), (e), (h) $V_p = 5.0E_r$ and $V_d = 0.4E_r$ (intermediate phase), and (c), (f), (i) $V_p = 3.0E_r$ and $V_d = 0E_r$ (extended phase). The axes in panel (g) apply to all panels.

consistent with a less effective spread of correlations in dipolar systems due to the interference between the repulsive tails in the interactions. Furthermore, it is an indication that DDIs can be used to control the value of the SPME similarly to what was shown for contact interactions [120].

The increase in localization due to DDIs interference is also observed in the 2-RDM. This is shown in Fig. 5 for the three different phases and at three increasing values of W . The behavior for weak DDIs [$W = 0.02E_r$, Figs. 5(a)–5(c)] is similar to that already observed in the noninteracting case. However, when DDIs are increased [$W = 0.2E_r$ in Figs. 5(d)–5(f) and $W = 2.0E_r$ in Figs. 5(g)–5(i)], the correlation spread becomes progressively stiffer for all phases. This leads to a complete freeze of correlations in the localized phase [Fig. 5(g)], while in the intermediate phase correlations are able to spread only partially [121]. Even for the extended phase, the pinning effect is visible, with correlations spreading more easily toward the right than the left. This observation agrees with the uneven density spread observed in Fig. 4(g).

Discussion. There are several mechanisms at play that explain the overall shape of the phase diagram at strong DDIs. The localized state appearing at large V_p (lattice limit) in the clean limit $V_d \rightarrow 0$ is a DSBS stabilized by DDIs, as evinced by the small density oscillations at the boundaries suggesting dynamical self-confinement [see Fig. 3(a)]. The $1/r^3$ tails of the DDIs cause an interference that locks particles within a

certain distance, as demonstrated in similar bosonic systems [113–117], and is likely connected with Hilbert space fragmentation [122–124]. Away from the clean limit ($V_d \neq 0$, but $V_d \ll V_p$), correlated disorder can be regarded as a perturbation on top of the DSBS. In this setting, it is known that the DDIs give rise to effective correlated hopping at a distance, i.e., between the edges of the localized clusters [125–131], which explains the resonant like behavior at the edges at their progressive delocalization [Figs. 3(b)–3(d)]. Increasing the disorder further eventually pushes the system again into localization [Fig. 3(f)]. In this limit, the system approaches an Aubry-André model, whose localized phase is known to be stable against DDIs [132–134].

On the other hand, as V_p is decreased, the lattice becomes shallower, increasing the effective particle hopping. In the clean limit ($V_d \rightarrow 0$), this progressively reduces the critical distance under which particles can be confined by the DDIs [113], and full localization is lost. With correlated disorder ($V_d \gg 0$), the loss of localization is analogous to what happens in the noninteracting case [cf. Fig. 1(a)]. However, the repulsive nature of the DDIs—unhindered by the DSBS resonances in shallow lattices—provides more mobility, resulting in an enlarged intermediate phase.

Repulsive composite objects have been shown to be stable with respect to on-site interactions in a structured environment such as a simple optical lattice [135–139]. Our study propels these notions to a full many-body horizon by combining quasiperiodicity and dipolar interactions in a realistic quantum simulator setting [105,106]. Our scheme, inspired by experiments in 1D geometries, could be readily extended to higher-dimensional setups, where a richer landscape of quasicrystalline phases with different rotational symmetries can be engineered [50,52,140]. Moreover, clean system localization can appear when other mechanisms induce effective disorder, such as an external linear field [141–146], slow interaction dynamics [147], or both [148]. Given that the system presented in our work interpolates between the clean and the quasiperiodic case, it should help shed light on commonalities across a multitude of exotic localization phenomena that combine long-range interactions and correlated disorder.

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Data availability. The data that support the findings of this article are not publicly available upon publication because it is not technically feasible and/or the cost of preparing, depositing, and hosting the data would be prohibitive within the terms of this research project. The data are available from the authors upon reasonable request.

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