Many-Body Localization in Dipolar Systems

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In this Letter, we investigate dilute dipolar systems as a platform for realizing MBL phases and studying the associated localization phase transition. Our work is motivated by recent experimental advances that make it possible to produce and probe isolated, strongly interacting ensembles of disordered particles, as found in systems ranging from trapped ions [30] and Rydberg atoms [31,32] to ultracold polar molecules [33,34] and spin defects in solid-state systems [35–38]. The presence of strong interactions in these systems underlies their potential for exploring physics beyond that of single-particle Anderson localization [1]. However, the power-law decay of those interactions immediately raises the following question: Can localization persist in the presence of such long-range interactions? Indeed, Anderson observed in his seminal paper that long-ranged hopping, \( t \sim 1/\rho^\alpha \), delocalizes any putatively localized single-particle states for \( \alpha \leq d \), with \( d \) the dimension of space. In what follows, we consider the generalization of Anderson’s criterion to the interacting power-law regime and produce a necessary condition for localization with such interactions [6–9]. To support these considerations, we carry out an extensive numerical analysis of power-law interacting systems in \( d = 1 \) spatial dimensions. With this criterion in hand, we analyze the feasibility of observing MBL states in two complementary ultracold polar molecule proposals, wherein the power laws, interaction scales, and dimensionality may be tuned. Finally, we generalize our analysis to solid-state systems where localization can be studied in the quantum dynamics of magnetic spin impurities.

FIG. 1 (color online). (a) Schematic of four-spin resonance structure. Each pair of (red) spins at separation \( R_1 \) forms a pseudospin (blue) with the level structure shown below. (b) A pseudospin at the origin resonates with another pseudospin in a shell \( R_2 < r < 2R_2 \).

\[ H = \sum_i \epsilon_i S_i^z - \sum_{ij} \frac{t_{ij}}{|r_{ij}|^\alpha} (S_i^+ S_j^- + \text{H.c.}) + \sum_{ij} \frac{V_{ij}}{|r_{ij}|^\beta} S_i^z S_j^z, \]

where \( \epsilon_i \) is a site-dependent disorder field of bandwidth \( W \), while \( \alpha \) and \( \beta \) are the exponents governing the power-law decay of spin flip-flops and spin interactions, respectively [39]; we assume \( \beta \leq \alpha \), consistent with all physical
realizations of which we are aware. Clearly, the analysis applies to general long-range interacting two-level systems with a conserved charge.

We identify resonant pairs of spins as those for which $|\epsilon_i - \epsilon_j| \lesssim t_{ij}/|r_{ij}|^\alpha$; the expected number of resonant spins at a distance $R_1 < |r_{ij}| < 2R_1$ from a central spin is

$$N_1(R_1) \sim \left(\frac{\rho N_1}{R_1^d} \right) \frac{t/R_1^d}{W},$$  

(2)

where $\rho$ is the density of spins. If $N_1(R_1)$ diverges as $R_1 \rightarrow \infty$, that is, if $d > \alpha$, then any spin resonates with arbitrarily distant spins and localization is impossible; this is precisely Anderson’s criterion for single-particle localization. In the critical case, $d = \alpha$, a detailed renormalization group treatment confirms subdiffusive but delocalized behavior for the noninteracting case [1,40,41].

As shown in Fig. 1(a), the two strongly hybridized central levels of a resonant pair define a new pseudospin degree of freedom (blue arrows) with local splittings $\delta \sim t/R_1^d$. Pseudospins can exchange energy through the interaction $V$ since the operators $S_i^+$ have spin-flip matrix elements between the two pseudospin states [6–9]. Two pseudospins separated by $R_2$ resonate if $|\delta_1 - \delta_2| > V(R_2) > |\delta_1 - \delta_2|$ [42]. The number of such resonances available in a shell from distance $R_2$ to $2R_2$ around a fixed pseudospin [Fig. 1(b)] is

$$N_2(R_1, R_2) \sim |n_1(R_1)R_2^\beta| \frac{V/R_2^\beta}{t/R_1^d},$$  

(3)

where $n_1 = \rho N_1$ is the density of pseudospins. As before, if $N_2$ diverges as $R_2 \rightarrow \infty$, large-scale pseudospin resonances induce delocalization [6–9]. There are two limits. The simplest case occurs when one holds the pair size $R_1$ fixed as $R_2$ diverges; this “small pairs” condition yields a localization criterion $d < \beta$. The second case requires optimizing $R_1$ as $R_2$ grows in order to saturate the probability of pseudospin resonance. More precisely, one should replace $(V/R_{2i}^\beta)/(t/R_1^d) \rightarrow \min[1, (V/R_{2i}^\beta)/(t/R_1^d)]$ in Eq. (3). The optimum arises for $R_1 \sim R_{2i}^\beta$, yielding a more stringent “extended pairs” condition, $d < \alpha \beta/(\alpha + \beta)$.

It is clear that one can continue iterating the construction of pair resonances. However, the resulting criteria for MBL saturate after the third level [42,43],

$$N_3(R_1, R_2, R_3) \sim |n_1(R_1)N_2(R_2)R_3^\beta| \frac{V/R_3^\beta}{V/R_2^\beta},$$  

(4)

where $n_2 = n_1N_2$ is the density of pseudo-pseudospins. There are three limits as $R_3$ diverges. Holding $R_1, R_2$ fixed reproduces the small-pairs criterion. Holding $R_1$ fixed but optimizing $R_2 \sim R_3$ [to saturate the probability of resonance in Eq. (4)] yields a new, “iterated pairs” criterion $d < \beta/2$. Finally, optimizing both $R_1 \sim R_{2i}^\beta$ and $R_2 \sim R_3$ reproduces the extended pairs criterion.

The above results hold for generic anisotropic distributions of $t_{ij}, V_{ij}$ (first two columns of Table I). In certain cases, which we term “multipole,” the effective matrix elements that arise in the four-spin construction cancel at leading order. To be precise, this cancellation occurs when the derivatives of the interaction scale as the interaction divided by the distance separating the spins. This can be understood within a multipole expansion (for $R_1 < R_2$), which amounts to replacing $V/R_{2i}^\beta \rightarrow V/R_{3j}^\beta/R_{3j}^{\beta+2}$ for $N_2$ and analogously for subsequent iterations (last column of Table I).

A few comments are in order. (1) In the anisotropic and unmixed ($\alpha = \beta$) cases, the iterated pairs criterion $d < \beta/2$ is always most stringent, a result first derived in Refs. [8,9]. (2) In the multipole case, for $\alpha < \beta + 4$, the extended-pairs criterion is most stringent, while for $\alpha > \beta + 4$, the iterated-pairs criterion dominates. (3) The case of an Anderson insulator with Coulomb interactions corresponds to the $\alpha \rightarrow \infty$ limit of the multipole case, giving an upper critical dimension of $d_c = 1.5$.

The case of interacting dipoles with $\alpha = \beta = 3$ also gives $d_c = 1.5$. Interestingly, the orientation dependence of the dipolar interaction is sufficiently isotropic to enable a multipole expansion. Thus, in experiments that can realize $\alpha = 6, \beta = 3$ (as will be discussed later), $d_c \approx 2.3$ [42].

Ultimately, all of the resonance arguments described above rely upon the analysis of finite subsets of spins. While providing useful insights, such arguments must be viewed as heuristic. To supplement, we have performed extensive exact diagonalization studies of Eq. (1) in $d = 1$ for $\alpha = \beta = 1, 3/2, 2, 3$. We consider periodic systems up to size $L = 14$ at the filling fraction $\nu = 1/2$. The random fields are drawn from a uniform distribution of width $W$, the interaction $V_{ij} = V = 2$, and the hopping $t_{ij} = t = 1$. The presence of a many-body localized phase may be detected by the finite-size flow of the dynamic polarization $D$, a measure of spin transport across the 1D system at infinite temperature [11]. We perturb each eigenstate with a small (long-wavelength) inhomogeneous spin modulation of the form $\hat{F} = \sum_j S_j^z e^{i2\pi j/k}$ and measure the relaxation of this inhomogeneous polarization at infinite time. For each disorder realization $\eta$ and eigenstate $k$, the dynamic polarization is given by

$$D_\eta^k = 1 - \frac{\langle |\hat{F}^\dagger| k \rangle \langle k | \hat{F}^\dagger \rangle}{\langle k | \hat{F}^\dagger \hat{F} | k \rangle}. \quad (5)$$

We then define $D$ as the infinite temperature disorder average of $D_\eta^k$. As $L \rightarrow \infty$, in the ergodic phase, one expects $D \rightarrow 1$.

<table>
<thead>
<tr>
<th>Unmixed $\alpha = \beta$ [8,9]</th>
<th>Anisotropic $\beta &lt; \alpha$</th>
<th>Multipole $\beta &lt; \alpha$</th>
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<tr>
<td>Hopping</td>
<td>$d &lt; \alpha$</td>
<td>$d &lt; \alpha$</td>
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<tr>
<td>Small pairs</td>
<td>$d &lt; \beta$</td>
<td>$d &lt; \beta$</td>
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<tr>
<td>Extended pairs</td>
<td>$d &lt; \beta/2$</td>
<td>$d &lt; \alpha \beta/(\alpha + \beta)$</td>
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<td>Iterated pairs</td>
<td>$d &lt; \beta/2$</td>
<td>$d &lt; \beta/2$</td>
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α = β = 1

FIG. 2 (color online). Finite-size scaling of the long-time dynamic polarization for Eq. (1) in d = 1 (with units t = 1, V = 2) with (a) α = β = 1, (b) α = β = 3/2, (c) α = β = 2, and (d) α = β = 3. The lack of flow reversal in (a) suggests delocalization at all disorders. The sharpening of the crossover as a function of increasing system size in (d) suggests the existence of a phase transition at approximately $W_c \approx 10$ into an MBL phase. The flow at intermediate power laws (b) is inconclusive.

since the initial inhomogeneity relaxes away; in the MBL phase, one expects $D \to 0$ since there is no transport.

The results are shown in Fig. 2. For all exponents, we find that the finite-size flow of $D$ is consistent with delocalization at weak disorder. At strong disorder, for $α = 2, 3$, there are signs of flow reversal, consistent with a transition into a MBL phase, while for $α = 1$, the flow remains toward delocalization for all disorder strengths. Owing to the small sizes accessible to exact diagonalization, flow reversal does not prove the existence of a transition; however, for $α = 3$, the combination of relatively clear flow and the previous theoretical argument suggests the existence of a MBL phase. The strong disorder flow at intermediate exponents $α = 3/2$ is inconclusive. Accordingly, for $d = 1$, we numerically bound the critical power law with $1 < α_c < 3$, noting that the extended-pairs criterion gives $α_c = 2$. The difficulty of investigating a MBL transition in small-size numerics emphasizes the importance of controlled experiments.

Experimental realizations.—Next, we analyze two classes of experimentally accessible systems in which MBL phases may be realized. First, we consider an array of polar molecules confined to a one-dimensional tube geometry (via an optical lattice) as depicted in Figs. 3(a) and 3(b) [33]. The optical lattice is strongly confining along the $y$ and $z$ axes, but molecules can tunnel with nearest-neighbor hopping strength $t$ along the tube in the $\hat{x}$ direction ($α \to \infty$). The molecules are prepared in their rovibrational ground state and are subject to a static electric field $E$ perpendicular to the tube direction. The applied electric field weakly aligns the molecules along the field direction, inducing a finite dipole moment $d$ and a long-range electric dipole-dipole interaction between the molecules $V \sim d^2/R^3$ ($β = 3$). By ensuring that the dipolar interaction strength is much weaker than the rotational splitting $B$ [Fig. 3(d)], all molecules remain in the rovibrational ground state. Finally, an optical speckle field may be superimposed on top of the underlying lattice, introducing on-site potential disorder with strength $W$ controlled by the laser intensity [Fig. 3(b)] [44].

The magnitude of the electric field tunes the strength of the dipolar interaction $V \sim d^2$. In the limit $E \to 0$, the interaction strength $V \to 0$, and the resulting nearest-neighbor Hamiltonian can be fermionized. This noninteracting model is completely Anderson localized in the presence of any disorder. With the addition of local interactions, the existence of a MBL phase has been established both theoretically and numerically [4,5,10–12]. According to the criterion in Table I, the MBL phase ought to also survive the introduction of long-range dipolar interactions. To confirm this expectation and further establish an experimentally relevant phase diagram, we perform exact diagonalization for molecular filling fractions $ν = 1/2, 1/3, 1/4$ up to system sizes of $L = 16, 18, 20$, respectively [Fig. 4(a)]. As depicted in Fig. 4(b), we obtain the MBL phase diagram as a function of interaction strength, filling fraction, and speckle intensity [44].

Next, we consider disordered arrays of interacting molecules with a fixed center-of-mass position and focus on the dynamics of rotational excitations [Fig. 3(c)]. In the deep lattice limit, the orbital motion of the molecules is pinned, and the residual rotational degree of freedom is governed by an effective Hamiltonian, $H_m = BJ^2 - dE$ [45]. A combination of electric and magnetic fields allows us to...
isolate an effective two-level system: $|\downarrow\rangle = |J = 0, m_j = 0\rangle$ and $|\uparrow\rangle = |J = 1, m_j = 1\rangle$ [Fig. 3(d)] [46]. The rotors interact via electric dipole-dipole interactions with the Hamiltonian, $H_{dd} = \frac{1}{2} \sum_{ij} \mathbf{d}_i \cdot (1 - 3 \hat{r}_{ij} \hat{r}_{ij}) \mathbf{d}_j / r_{ij}^3$, where $\mathbf{d}$ is the dipole moment operator. Projecting $H_{dd}$ onto the two-level subspace $\{|\downarrow\rangle, |\uparrow\rangle\}$ and keeping only secular terms yields the Hamiltonian of Eq. (1) with effective on-site fields given by $e_i = \sum_{j \neq i} (d_i \cdot d_j / r_{ij}^3)$ and $d_{x,a} = 1/2((|d|^2|1\rangle + |0\rangle|d|^2|0\rangle)$. Assuming Poissonian (uncorrelated) dilution, the fields $e_i$ become random variables with standard deviation $W \sim (\langle d_i \cdot d_i \rangle a_0^3) / \sqrt{v(1 - v)}$, where $a_0$ is the lattice spacing [42]. We expect the weak correlations of the random fields to leave the previous numerical phase diagrams in $d = 1$ qualitatively unchanged [Fig. 2(d)].

This dipolar spin model becomes particularly intriguing as one varies the dimensionality of the system since the “extended-pairs” criterion predicts $d_{c} = 3/2$ for $\alpha = 1$. Compared to the simple Anderson criterion, which predicts $d_{c} = 3$, this already allows one to investigate the validity of the resonant pair counting arguments for optical lattice pancakes where $d = 2$.

An additional feature of such systems is the ability to tune the spin-flip power law. The large rotational constant $B$ enables restriction to the Hilbert space spanned by $|J = 1, m = -1\rangle$ and $|J = 1, m = 1\rangle$. In this case, the dipolar flip-flop process is effectively eliminated at first order; the system instead hops two units of $J$: via a second-order process of the form [see Fig. 3(e)] $H' = \sum_{ij} \hat{r}_{ij}^3 [(d_+^\dagger)^2 (d_+^2) + (d_-^2)^2 (d_-^\dagger)^2]$, while the interaction remains formally unchanged. With the effective hopping power law increased to $\alpha = 6$ and the interaction remaining as $\beta = 3$, one finds that (in $d = 2$) all criteria for the consistency of localization are now satisfied, including both the extended-pairs criterion, which predicts $d_{c} \approx 2.3$, and the iterated-pairs criterion with $d_{c} = 2.5$.

Finally, solid-state implementations can be considered using spin defects in semiconductors. For example, nitrogen-vacancy (NV) defects in diamond [35–38] are spin-1 magnetic impurities described by the Hamiltonian $H_{NV} = D_0 S_z^2 + \mu_e B S_z$, where $D_0$ is a large crystal field splitting. In the presence of an applied magnetic field, one can restrict the NV dynamics to a two-level subspace and recover the Hamiltonian of Eq. (1).

**Experimental feasibility.**—There are several probes available for detecting many-body localization in quantum optical systems: (1) observing arrested decay of a long-wavelength spin-number modulation, (2) generalized single-site spin-echo protocols that exhibit anomalously slow dephasing [14,15,17–19], and (3) direct measurements of real-space correlation functions. The simplest approach is to directly observe a lack of diffusion. In a typical ergodic system, an initial long-wavelength inhomogeneous spin polarization decays as $\sim e^{-D_k t}$, where $D_k$ is the diffusion constant. For a many-body localized phase, $D_k = 0$. In any experiment, coupling to an external bath is unavoidable and produces characteristic decoherence time scales; $T_1$-type depolarization provides a uniform $k$-independent contribution to the overall decay. In the presence of weak Markovian $T_2$ dephasing, extrinsic energy fluctuations induce diffusion, with $D_k \sim a_0^2 / T_2$ (neglecting backaction onto the bath). Since $T_2 \lesssim T_1$, the figure of merit in such experiments is a separation of scale between $D_k$ and the expected ergodic diffusion, $D_e \sim a_0^2 / T_{a0}$, where $T_{a0}$ represents the lattice scale hopping time. Alternatively, one can also measure the decay of an initially polarized region; for a Gaussian spot of initial size $\ell$ (larger than any correlation length), the modulation at the origin decays as $\sim (e^2 + D_k t) - D_e t / 2 e^{-T_1}$. Here, one hopes to extract the subexponential diffusive behavior, which can, in principle, be achieved by varying the spot size.

In the molecular case, the most direct experimental realization of our proposals would be in diatomic alkali systems [34,47–51]. Both the orbital and rotational cases can be carried out with currently available technology; indeed, the loading of $^{40}$K$^+$/Rb molecules into 1D [33] and 3D [47] lattices, as well as dipolar spin exchange [46], has already been demonstrated. For a typical polar molecule with saturated dipole moment $\sim 3$ Debye, the interaction strength at 532 nm (optical lattice spacing) corresponds to approximately 100 kHz, yielding $T_{a0} \approx 10 \mu$s. Meanwhile, dephasing times of up to $T_2 \sim 100$ ms [46] and ground-state lifetimes of up to $T_1 \approx 25$ s have been observed [47].

In the case of NVs, recent advances in implantation and annealing have enabled dense defect ensembles with average spacing $\sim 2–3$ nm [52]. The magnetic dipolar interaction at such distances is given by $T_{a0} \sim 1 \mu$s, significantly smaller than the typical room-temperature coherence times $T_1, T_2 \sim 10$ ms of isolated NVs (working at cryogenic temperatures can lead to further improvements [53]). To observe many-body localization in such a system will require the ability to reduce the effective dimensionality; this can be achieved by fabricating quasi-1D diamond nanopillars [54] or by controlled implantation in 2D layers [55,56].

In summary, by constructing hierarchical spin resonances, we have analyzed upper critical dimensions for many-body localization in the presence of power laws (Table I). Our
arguments suggest that MBL is accessible to AMO-type experiments involving dipolar spins in two dimensions or hopping polar molecules in three or fewer dimensions. Our work opens a number of intriguing directions: (1) generalizations to other dipolar platforms such as Rydberg atoms, trapped ions, and other spin qubits and (2) working near the upper critical dimensions to probe the nature of the MBL transition.

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