Compact, flat-band based, Anderson and many-body localization in a diamond chain

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The interplay of dispersionless bands, compact localized eigenstates, disorder and interactions, in a quasi one-dimensional diamond chain results in a rich phase diagram. Localization properties of the system vary from extreme compact localization in the dispersionless limit to weak flat-band based localization in the presence of tiny disorder, to the familiar strong Anderson localization in the presence of large disorder. Furthermore, when interactions are turned on, the many-body localized phase is also realized in some parameter regimes. The phase diagram is chalked out on the basis of both single-particle properties including inverse participation ratio, return probability, wave-packet dynamics, and many-particle properties including level spacing ratio, many-particle inverse participation ratio, return probability, and imbalance parameter.

A class of Hermitian translationally invariant tight-binding networks with local symmetries, exhibiting dispersionless bands called flat bands (FBs) [1, 2] has generated considerable interest. The underlying large-scale degeneracy lies at the heart of the novel physics of these systems [3–5]. The experimental realization of these networks in ultracold atomic systems [6, 7], photonic crystal waveguides [8], and exciton-polariton condensates [9] has provided a strong foothold for theoretical advances. A fascinating property of dispersionless systems is the association of flat bands to compact localized eigenstates (CLS) which reside on a finite volume of the lattice and strictly vanish elsewhere [10, 11]. The presence of CLS has been experimentally identified in many flat band systems such as frustrated magnets, and photonic crystal waveguides [12–14]. It is only a very delicate tuning that yields flat bands, and the tiniest of perturbations would lift the degeneracy and substantially affect the states and hence bring forth interesting properties [6, 15–17].

Disorder and interactions are ubiquitous in nature, and the last decade has seen a great deal of attention devoted to the consequences of the simultaneous presence of each of these features. In flat band systems, while the role of disorder has been addressed to some extent [18–21], the effect of interactions [22] is yet to find a thorough discussion. Disorder destroys the destructive interference that sustains the CLS and couples the states to other Bloch states leading to a Fano resonance based localization [23, 24]. But, Hamiltonians with certain symmetries are known to be robust against some sorts of disorders and the existence of CLS in such disordered systems has also been reported [11]. A comprehensive understanding of the fate of CLS when interactions are turned on, is lacking and desirable. The present Letter is an attempt to fill this gap in the context of an interacting quasi one-dimensional diamond chain. We report the appearance of a rich phase diagram (Fig. 1) including compact localized, flat-band based localized, Anderson localized, and many-body localized phases, in addition to delocalized, mixed and ergodic phases.

We consider a quasi one-dimensional diamond chain (Fig. 2) which possesses only flat bands in the band structure leaving the system in the insulating phase. In the clean noninteracting limit (zero disorder and interactions), all the eigenstates of this system are compactly localized. Hence, the single particle eigenstates span the smallest possible volume and any perturbation is expected to increase their occupying volume. The FBs are separated from one another by a gap and hence small disorder perturbations couple the states in one FB, larger disorder strength leads to coupling between states in different bands. An understanding of the impact of the coupling of CLS amongst each other, which is not yet explored in detail, is one of our central objectives. Another key observation we make is that compact localization (CL) at zero disorder, flat-band based localization (FBL) at small disorder strength, and conventional...
Anderson localization (AL) at high disorder strength are all different from each other. Therefore, as disorder is increased, the localization in the system changes from the extreme CL to weak FBL to strong AL. As the interaction is switched on, the low disorder region seems to show a mixed phase, separated from the high disordered MBL phase by an intermediate disorder-assisted thermalized phase. We also report that a detailed study of the dynamics illustrating the properties of these phases, proves to be profitable.

Model: The Hamiltonian for the diamond chain is

$$\hat{H} = \hat{H}_{\text{hop}} + \hat{H}_{\text{ox}} + \hat{H}_{\text{int}},$$

where

$$\hat{H}_{\text{hop}} = -J \sum_{i=1}^{N/3} (\hat{u}_i^\dagger \hat{c}_i - \hat{c}_i^\dagger \hat{d}_i + \hat{c}_i^\dagger \hat{u}_{i+1} + \hat{c}_i \hat{d}_{i+1}) + \text{h.c.},$$

$$\hat{H}_{\text{ox}} = \sum_{i=1}^{N/3} (\zeta_i^u \hat{u}_i^\dagger \hat{c}_i + \zeta_i^c \hat{c}_i^\dagger \hat{c}_i + \zeta_i^d \hat{d}_i^\dagger \hat{d}_i),$$

$$\hat{H}_{\text{int}} = V \sum_{i=1}^{N/3} (\hat{u}_i^\dagger \hat{c}_i^\dagger \hat{c}_i \hat{d}_i + \hat{c}_i^\dagger \hat{c}_i \hat{d}_i^\dagger \hat{d}_i + \hat{c}_i \hat{u}_{i+1}^\dagger \hat{u}_{i+1} + \hat{c}_i \hat{d}_{i+1}^\dagger \hat{d}_{i+1}) + \text{h.c.}$$

(2)

Here $\hat{u}_i^\dagger$, $\hat{c}_i^\dagger$, and $\hat{d}_i^\dagger$ are the fermionic creation operators acting at the $u$ (up), $c$ (center) and $d$ (down) sites respectively in the $i$th unit cell, as schematically shown in Fig. 2. The unit cell consists of three sites, which repeat in the horizontal direction to bring forth the periodicity of the lattice. We denote the total number of sites by $N$, which is necessarily a multiple of 3, because of the unit cell structure. The hopping amplitude $J$ and interaction $V$ are nonzero for nearest neighbours (represented as sites connected by lines in Fig. 2) and zero otherwise. $\zeta_i^\alpha (\alpha = u, c, d)$ denotes the strength of the on-site disorder chosen from a uniform random distribution $[-\Delta, \Delta]$. The clean, noninteracting diamond chain ($\zeta_i^\alpha = 0, V = 0$), possesses three flat bands in the band structure (at $E = 0, \pm 2J$). Systems in which all bands are flat are rare, and it is only a careful tuning of the diamond chain that allows this to happen [25].

Single-particle properties: The eigenstates corresponding to the three flat bands are compactly localized within two unit cells as shown in Fig. 2. Since the CLS span two unit cells, they lack orthogonality, but they still form a complete basis for the flat band. The presence of disorder in this system has two major consequences: a detuning of the energy levels resulting in the lifting of degeneracy, and hybridization of the CLS among each other resulting in an increase in the volume spanned by states. One quantity to characterize these properties is the inverse participation ratio (IPR) defined as

$$I_k = \sum_{i=1}^{N} \sum_{\alpha = u, c, d} |\psi_k(i, \alpha)|^4$$

(3)

where the $k^{th}$ normalized single-particle eigenstate $|\psi_k\rangle = \sum_{i, \alpha} \psi_k(i, \alpha) |i, \alpha\rangle$ is written in terms of the Wannier basis $|i, \alpha\rangle$, representing the state of a single particle localized at the site $\alpha (\alpha = u, c, d)$ in the $i$th unit cell of the lattice. While $I_k = 1$ in a localized eigenstate, $I_k$ scaling as $1/N$ is characteristic of a delocalized eigenstate; intermediate behaviour is seen at criticality. The IPR averaged over all the eigenstates plotted in Fig. 3 shows a lower value at low disorder compared to high disorder indicating a crossover at $\Delta \approx 2J$ from weaker FBL to stronger AL [26]. In the low disorder region, the IPR is independent of the disorder strength as there is no energy scale to compete with the disorder strength due to the disconnect between the flat bands. The localization properties of the single-particle ground state is seen to be different from those of the excited states. Details of the ground state localization properties and complementary results from other quantities (entanglement entropy and fidelity) are shown in a longer version of this work [28].

We study non-equilibrium properties of the system by
keeping a single particle initially at a particular site i.e. $|ψ_{in}\rangle = |n_0\rangle$. Here we choose $n_0$ to be a c site, but expect similar results for the other two possibilities. We calculate the revival probability $R(t) = |⟨ψ_{in}|ψ_t⟩|^2$ of finding the particle at the initial site at time $t$. In the absence of any disorder there is a persistent oscillation in $R$ with time, as shown in Fig. 4(a). This is a consequence of the extreme compact localization of the states. As disorder is added, this oscillatory behavior is disturbed as the eigenstates hybridise with one another and a damped oscillatory behavior is observed for tiny disorder $Δ = 0.01J$ (Fig. 4(b)). The oscillation vanishes in the high disorder regime $Δ = 5.0J, 50.0J$. The saturation value $R^\infty$ of revival probability (Fig. 4(c)) turns out to be independent of system size $N$ and shows two distinct localized phases: a low-disorder $FBL$ phase where $R^\infty$ is independent of $Δ$, and a high-disorder $AL$ phase where $R^\infty$ increases with $Δ$. A strong correspondence between dynamics and statics is evident from the similarities between Fig. 4(c) and Fig. 3(a). In Fig. 4(d), we have shown the on-site occupancy of a single particle in the long time limit. As can be seen, for $Δ = 0$, the wavefunction is extremely localized within a very few sites reflecting the underlying compact localization. Turning on a tiny disorder $Δ = 0.01J$ makes the distribution extended in space with an exponential tail. Increasing the disorder further to $Δ = 5.0J, 50.0J$ shrinks the distribution with a more sharply defined exponential tail. This establishes the hierarchy $CL > AL > FBL$ in terms of the strength of localization.

**Many-body properties:** In the following we study the transport properties of interacting spinless fermions in the disordered diamond lattice. We employ level-spacing ratio and spectrum averaged many-particle inverse participation ratio to capture the interaction-induced ($V \neq 0$) phase transitions in this disordered model. Level-spacing ratio is defined as

$$r = \frac{1}{D-1} \sum_{k=1}^{D-1} \frac{\min(s_k, s_{k+1})}{\max(s_k, s_{k+1})}$$

where energy level-spacing $s_k = E_{k+1} - E_k$ and the energy spectra $(E_1, E_2, E_3, ..., E_D)$ of the interacting Hamiltonian are obtained via exact diagonalization. Here the dimension of the particle-number constrained many-body Hilbert space is $D = (N/np^\nu)$ where $np$ and $N$ are the number of fermions and lattice sites respectively. In the thermal phase, $r \approx 0.528$ whereas in the $MBL$ phase $r \approx 0.386$. The level-spacing ratio $r$ as a function of disorder strength $Δ$ for increasing interaction strength $V$ is shown in Fig. 5(a) for $N = 18$ and $ν = 1/6$, where the filling fraction $ν = N/np$. As can be seen from the plots in Fig. 5(a), for all values of interaction $V$, the system exhibits many-body localization ($MBL$) for $Δ > 10.0J$ as the level-spacing ratio $r$ is 0.386. For intermediate disorder $Δ \approx 2J$ and interaction $V \approx J$, the many-body system starts delocalizing as indicated by $r$ approaching 0.53. As the filling fraction $ν$ increases, the system becomes thermal as shown in the inset of Fig. 5(a). We have also verified that the system becomes thermalized as the system size is increased while keeping $ν$ fixed. The many-body system shows a mixed phase in the low disorder regime ($Δ << J$) where $r$ is neither 0.528 nor 0.386. However, in this regime, when the interaction $V \approx Δ$ the amount of delocalization increases in the system with $r$ displaying a peak (see the longer version for details [28]).

![Figure 4](image1.png)

![Figure 5](image2.png)
The many-particle inverse participation ratio (MIPR) of a normalized eigenstate $|\Psi\rangle$ is defined as:

$$\text{MIPR} = \sum_{n=1}^{D} |C_n|^4$$

where the coefficients come from an expansion: $|\Psi\rangle = \sum_{n=1}^{D} C_n |n\rangle$ in terms of the $N_p$ particle basis $|n\rangle$. For an extremely localized eigenstate $\text{MIPR} = 1$ whereas for a perfect delocalized eigenstate $\text{MIPR} = 1/D$. The spectrum-averaged MIPR as a function of $\Delta$ for increasing interaction $V$ are shown in Fig. 5(b) for system size $N = 18$ and filling $\nu = 1/6$. When interaction is of the order of hopping $V \approx J$, the study of MIPR reveals (Fig. 5(b)) three sharply defined phases: a localized phase (MBL) for large disorder $\Delta \approx 10.0 J$, a delocalized phase (Ergodic) for moderate disorder $\Delta \approx J$ and a mixed phase (Mixed) for low disorder $\Delta < J$ which are schematically shown in the phase diagram in Fig. [1].

In the low disorder and low interaction regime, we observe an increase in the amount of delocalization in the mixed phase at $V \approx \Delta$, which is highlighted in yellow in Fig. [1]. With increase in filling fraction and system size, the dips of MIPR plots become deeper indicating more delocalization. A detailed analysis leading up to these conclusions and more, can be found in the longer version of this work [28].

Next we discuss the non-equilibrium dynamics of the return probability and imbalance parameter, which are of direct interest to experimentalists. We choose the initial state as an experimentally relevant, density-wave type of state: $|\Psi_i\rangle = \prod_{i=1}^{N/3} \psi_i |0\rangle$, which is a product state with the filling fraction of fermions $\nu = 1/6$ with $N = 18$. The return probability is defined as

$$R(t) = |\langle \Psi_i | \Psi_t \rangle|^2.$$ (6)

In a perfectly delocalized phase, the long-time limit of the return probability $R^{\infty} = 1/D$ while in a perfectly localized phase $R^{\infty} = 1$. In the absence of any disorder the dynamics of $R$ shows persistent oscillations in the many-body configuration space, as shown in Fig. [6(a)] for $V = 1.0 J$. This type of non-ergodic behavior in the interacting but disorder-free chain hints that the interaction does not entirely break the degeneracy. The dynamics of $R$ in the presence of disorder is shown in Fig. [6(b)]. For $\Delta = 0.01 J$, the oscillation becomes damped whereas for $\Delta = 3.0 J$ and 50.0 J the oscillatory behavior is absent. We also study the imbalance parameter, which is given by:

$$I_b(t) = \frac{\sum_{i=1}^{N/3} (-1)^i n_i^c - n_i^u - n_i^d}{\sum_{i=1}^{N/3} n_i^c + n_i^u + n_i^d},$$ (7)

where $n_{i}^{\alpha}$ is the occupancy of fermions at the site $\alpha$ of the $i^{th}$ unit cell where $\alpha \in \{u, c, d\}$. In the thermal phase $I_b = -2/3$ and in the MBL phase $I_b = 1$. Similar to $R$, $I_b$ also shows (Fig. [6(c)]) damped oscillatory behaviour in the presence of low disorder. For large disorder $\Delta > J$, the recurrence is absent entirely, and no oscillations are seen. For intermediate disorder strength of the order of $\Delta = 3.0 J$, the saturation value of $I_b$ is low indicating delocalization. The MBL phase in the high disorder regime $\Delta = 50.0 J$ is signalled by a very high saturation value of $I_b$. We plot the the saturation value $I_b^{\infty}$ vs $\Delta$ for different interaction $V$ in Fig. [6(d)] that shows signatures of the three phases: MBL for $\Delta \gg J$, delocalization for $\Delta \approx J$ and the mixed phase for $\Delta \ll J$. In the low disorder region, the dips observed in $I_b^{\infty}$ indicates an increment in the amount of delocalization in the mixed phase when $V \approx \Delta$. Thus we see that the many-particle properties complement the single-particle properties to jointly signal the phase diagram in Fig. [1].

**Summary:** In this Letter, we investigate the effect of disorder and interaction on the flat band states in a quasi one-dimensional diamond chain. We obtain a rich phase diagram illustrating the localization and delocalization properties of the system in the presence of disorder and interaction. A detailed study of single-particle and many-particle static and dynamic properties provides complementary insights, in addition to chalking out the phase diagram. The system possesses three distinct phases of localization: CL at no disorder, FBL at low disorder and AL at high disorder with the strength of localiza-
tion $CL > AL > FBL$. We explore the dynamics of the states in these phases in detail. A persisting oscillatory recurrence is a signature of compact localization of the eigenstates. Disorder detunes and hybridizes states and for low disorder, a damped oscillatory recurrence is observed while for high disorder, the oscillatory recurrence is completely absent.

In the simultaneous presence of interaction and disorder, an $MBL$ phase at high disorder, a thermal phase at intermediate disorder and a mixed phase at low disorder, are obtained. A delocalized region is spotted within the mixed phase in the low disorder region when the interaction strength is of the order of disorder. For the intermediate and higher ranges of disorder-strength, one always obtains the thermal and $MBL$ phases in the thermodynamic limit. Nonequilibrium dynamics reveals more distinctive features in the various many-body phases. The non-interacting many-particle system in the absence of disorder exhibits a persistent oscillatory recurrence in the configuration space. This persistent behavior can sustain even when interactions are turned on. In the presence of both disorder and interactions, the persistent oscillatory recurrence changes to a damped oscillatory recurrence in the mixed phase at small disorder and vanishes in the thermal and $MBL$ phases at intermediate and high disorder strengths respectively. Furthermore, the saturation values of the dynamical quantities also help distinguish the mixed, thermal and $MBL$ phases. We believe that our results can be tested with standard ultra-cold atom based set-ups in ongoing experiments. We envisage that this work will generate more interest in flat-band based systems and trigger multi-disciplinary interactions.

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