Phase diagram for the Harper model of the honeycomb lattice

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Received 18 March 2018, revised 10 August 2018
Accepted for publication 14 August 2018
Published 31 August 2018

Abstract

The Harper equation arising out of a tight-binding model of electrons on a honeycomb lattice subject to a uniform magnetic field perpendicular to the plane is studied. Contrasting and complementary approaches involving von Neumann entropy, fidelity, fidelity susceptibility, and multifractal analysis are employed to characterize the phase diagram. Remarkably even in the absence of the quasi-periodic on-site potential term, the Hamiltonian allows for a metal-insulator transition. The phase diagram consists of three phases: two metallic phases and an insulating phase. A variant model where next nearest neighbor hopping is included, exhibits a mobility edge and does not allow for a simple single phase diagram characterizing all the eigenstates.

Keywords: graphene, honeycomb lattice, Harper equation, metal-insulator transition, multifractal analysis, von Neumann entropy

(Some figures may appear in colour only in the online journal)

1. Introduction

The localization of electronic states in a random medium due to quantum interference effects is known as Anderson localization [1]. A consequence of this phenomenon is insulating behaviour in a one-dimensional (1D) lattice of non-interacting electrons subject to a random potential [2]. It is also the driving mechanism behind the metal-insulator transition (MIT) in disordered materials in 3D [2–4]. However, for quasi-periodic systems such as the Aubry–Andre–Harper model (AAH) it is well known that a metal-insulator phase transition is exhibited even in 1D [5, 6].

The AAH model is obtained from a 1D tight-binding Hamiltonian and is given by

\[ H = -t_1 \sum_{i} \left\{ \psi_{i+1} \psi_{i} + \psi_{i} \psi_{i-1} + V_i \psi_i \right\} - \mu \sum_{i} \cos[2\pi s_i] \psi_i^\dagger \psi_i + \text{h.c.} \]

where \( t_1 \) and \( V_i \) are the hopping terms, the on-site potential term and the wave function at the \( i \)-th site, respectively. For the choice \( t_1 = 1 \) and \( V_i = \lambda \cos(2\pi \phi_i + \theta) \) the above equation is derivable from the 2D square lattice nearest-neighbor hopping model in the presence of a uniform magnetic field [7]. For irrational values of \( \phi \), the potential term \( V_i \) is quasi-periodic and exhibits a localization-delocalization transition at \( \lambda = 2 \) [6]. Below this value all the eigenstates are extended, while they are all localized for \( \lambda > 2 \). The wave-functions at \( \lambda = 2 \) are critical, exhibiting features such as multi-fractality.

Generalisations of the above model are called the extended Harper model. Two of the widely studied examples include the effective 1D Hamiltonian derived from the next-nearest-neighbor (NNN) hopping on a square lattice in the presence of magnetic field and has the form [8]

\[ H = -t \sum_{s} \left\{ \left\{ 1 + \lambda \cos[\frac{2\pi}{s} (s + \frac{1}{2}) \phi] \right\} \psi_{s+1} \psi_{s} + \text{h.c.} \right\} + \mu \sum_{s} \cos[2\pi s \phi] \psi_{s+1} \psi_{s} + \text{h.c.} \]

where \( s \) is the site index, \( \phi \) is the magnetic flux, \( \mu \) and \( \lambda \) represent the nearest and next-nearest-neighbor hopping terms, respectively, of the original 2D square lattice model (figure 1(a)). The second example is that of the 1D Hamiltonian derived from the nearest-neighbour hopping on
In recent years the application of quantum information techniques in the context of quantum phase transitions (QPT) of a many-body system has led to unique insights [16, 17]. In this regard the study of quantum fidelity and fidelity susceptibility have been quite useful in a system where the knowledge of the relevant order parameter and the changes in symmetries are not known [18]. Quantum fidelity (QF) measures the overlap between two ground states with differing parameters, whereas fidelity susceptibility measures the change in QF between two parameters with infinitesimal separation [16–19]. Another important tool is the von Neumann entropy (VNE) which quantifies the entropy of entanglement [20, 21]. These techniques have been implemented to successfully characterise the phase diagram of the extended Harper model obtained by considering a triangular lattice [22].

In this work we have considered a honeycomb lattice with anisotropic hopping in the presence of a uniform magnetic field. While it has been shown that the energy spectrum \( E \) versus \( \phi \) (where \( \phi \) is the magnetic flux) plot for this model exhibits the famous Hofstadter butterfly pattern [23], here we establish the phase diagram of this Hamiltonian as a function of the anisotropic hopping terms. For this purpose, we have focussed on properties of the eigenfunctions, principally the ground state, of this Hamiltonian. The study of edge states by characterizing the gap via the calculation of the bulk Chern number or by counting the number of states between the band gap reveal the topological properties of the model. For a given set of parameters, the topological features undergo drastic modification with change in \( \phi \) [23]. However, the phase diagram we discuss are robust with respect to changes in \( \phi \). We study the effective 1D Hamiltonian as given in equation (6) and show that similar to the case of the triangular lattice, the phase diagram is divided into an insulating region and two metallic regions (see figure 2). However, the phase diagram that emerges here is of a fundamentally different nature in contrast to those obtained from the above two generalized AAH type models. The reason is that while the AAH-type models have quasi-periodic potential terms, our system instead has a modulating hopping term and no potential term at all. A consequence of this is that for the two AAH-type models, cranking up either of the parameters while keeping the other zero is sufficient to induce a phase transition, in sharp contrast to our model where both parameters need to be non-zero for a phase transition to exist.

The techniques used for obtaining the phase diagram include fidelity-susceptibility, fidelity and VNE. These three

\[
H = -t \left[ \sum_s \left( \{1 + \lambda \exp[2\pi i (s + \frac{1}{2})\phi] \}c_s^\dagger c_{s+1} + \text{h.c.} \right) + \mu \sum_s \cos[2\pi \phi s]c_s^\dagger c_s \right].
\]

where \( \mu \) and \( \lambda \) represent the nearest neighbor hopping terms of the original 2D triangular lattice model (figure 1(b)). In both the effective 1D models (equations (2) and (3)), \( \lambda \) represents the 1D hopping while \( \mu \) represents the strength of the on-site potential. Turning off the \( \lambda \) term reduces the two models to the AAH model, since the geometry of the 2D lattice reduces to the nearest neighbor square lattice (figure 1). The phase diagram (see figure 1(c)) for the square lattice problem consists of a localized phase, a metallic and a critical phase separated by critical lines and one bicritical point where the three phases meet. The phase diagram for the triangular lattice has a similar structure as the above—however, the critical region is replaced by a metallic region.

Over the years a number of techniques have been used to characterize these phases. Analytical techniques include calculation of the Lyapunov exponent [10, 11] and measure of the spectrum [12]. Numerical techniques include the study of level statistics, in particular the distribution of normalised energy gaps and bandwidths at the critical lines [8, 9, 13]; in addition multifractal analysis of the spectrum and the wavefunction have proved useful in characterising the critical regions [14, 15].

In this paper we have considered a honeycomb lattice in the presence of uniform magnetic field given by [9]

\[
\left[ \sum_s \left( \{1 + \lambda \exp[2\pi i (s + \frac{1}{2})\phi] \}c_s^\dagger c_{s+1} + \text{h.c.} \right) + \mu \sum_s \cos[2\pi \phi s]c_s^\dagger c_s \right].
\]
techniques complement each other; while fidelity-susceptibility determines the phase boundaries, fidelity and VNE help to characterize the phases. Further, multi-fractal analysis and level statistics approaches allow us to show that the lines separating the three regions are critical. In the last part of the work we show that turning on the NNN hopping destroys the universal features of the phase diagram, while in the absence of NNN coupling all wave-functions at a given non-critical point in the parameter space exhibit either insulating or metallic behavior. We discuss the appearance of mobility edges in this scenario.

On the experimental front, tremendous advancement, especially in the ability to use ultra cold atoms and photonic lattices for controlled simulation of many-body states, has created a lot of excitement [24, 25]. Signatures of the localization-delocalization transition in the AAH model were observed almost a decade ago [26, 27]. More complicated models are being simulated with the help of Raman lasers with inhomogeneous intensity [28, 29], lattice modulation techniques [30, 31] and laser assisted tunneling [32, 33]. These techniques provide non-trivial Berry phases which serve as artificial gauge fields. The latter technique has been utilized to generate large tunable artificial magnetic fields and spatially dependent complex tunneling amplitudes which were successfully used to simulate the 2D square lattice Hofstadter model [34, 35]. With work being done on generating artificial honeycomb lattices for atoms via optical trapping techniques [36, 37], it can be expected that the 2D honeycomb Hofstadter model and its derivative 1D Hamiltonian with modulating hopping terms will be realized soon.

The organization of this paper is as follows. The next section describes the model, and reports the phase diagram obtained. The third section provides details of the quantum information techniques used to arrive at the phase diagram. We also consider multi-fractal analysis and level statistics approaches for characterizing the critical lines. This is followed by a section on the NNN hopping model, and a final section of summary and conclusions.

2. Model

The tight binding Hamiltonian of an electron in a honeycomb lattice in the presence of a uniform magnetic field has the form:

$$H = -\sum_{n+m=\text{even}} \left[ t_1 a_{n+1,m}^\dagger a_{n,m} + t_2 e^{-i2\pi(n+m)} \right] a_{n,m}^\dagger a_{n+1,m} + \text{h.c.},$$

where $a_{n,m}^\dagger$ and $a_{n,m}$ are the creation (annihilation) operators at the $(n,m)$th site, $t_1$, $t_2$ and $t_3$ are real hopping parameters, the gauge choice is $[0,\phi(x+y),0]$, and $2\phi$ is the flux enclosed per unit cell (figure 2(a)). For $\phi = p/2$, where $p$ and $q$ are coprimes, the phase term repeats itself after $q$ (2q) sites along the $x$-direction for $q$ even (odd). The phase factor is attached with the $t_3$ hopping term and for fixed $n+m$ remains invariant for hopping from $(n,m)\to (n,m+1)$ site, consequently, the wave-function amplitude at the $(n,m)$th site can be written as $\Psi_{n,m} = \Psi_{n+m} e^{i(\epsilon_{k_x} + k_y)}$. Therefore the Harper matrix obtained from the Schrödinger equation, $H[\epsilon,k_x,k_y] = \epsilon[\epsilon,k_x,k_y]$, where $[\epsilon,k_x,k_y] = \sum \Psi_{n+m} e^{i(\epsilon_{k_x} + k_y)} |n,m\rangle$, acquires the following form [39]

$$\begin{pmatrix}
-E & B_1 & 0 & \cdots & 0 & B_m^* \\
B_1^\ast & -E & B_1 & 0 & \cdots & 0 \\
0 & B_1 & -E & B_2 & 0 & \cdots & 0 \\
\vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \\
0 & \cdots & 0 & B_{m-1} & -E & B_m & 0 \\
0 & \cdots & 0 & B_m & -E & B_m & 0 \\
B_m^* & 0 & \cdots & 0 & B_{m-1}^* & -E & B_m^* \\
\end{pmatrix} = 0,$$

where $B_m = a_{n,m}$ (a_{nm}) are the creation (annihilation) operators at the $(n,m)$th site, $t_1$, $t_2$ and $t_3$ are real hopping parameters, the gauge choice is $[0,\phi(x+y),0]$, and $2\phi$ is the flux enclosed per unit cell (figure 2(a)). For $\phi = p/2$, where $p$ and $q$ are coprimes, the phase term repeats itself after $q$ (2q) sites along the $x$-direction for $q$ even (odd). The phase factor is attached with the $t_3$ hopping term and for fixed $n+m$ remains invariant for hopping from $(n,m)\to (n,m+1)$ site, consequently, the wave-function amplitude at the $(n,m)$th site can be written as $\Psi_{n,m} = \Psi_{n+m} e^{i(\epsilon_{k_x} + k_y)}$. Therefore the Harper matrix obtained from the Schrödinger equation, $H[\epsilon,k_x,k_y] = \epsilon[\epsilon,k_x,k_y]$, where $[\epsilon,k_x,k_y] = \sum \Psi_{n+m} e^{i(\epsilon_{k_x} + k_y)} |n,m\rangle$, acquires the following form [39]
Figure 3. Scaled entropy (equation (9)) plots for $F_{m=1,2}$ as a function of the parameters $(\mu, \lambda)$ (a) minimum and (b) maximum entropy. Both figures exhibit sharp drop for the parameters exceeding the range $\mu, \lambda > 1$.

where $m = q/2$ for $q$ even, $m = q$ for $q$ odd, 

$$B_q = -t_1 e^{ik} - t_2 e^{i(2q+1)\phi} \text{ and } B'_q = -t_3 e^{ik}. \quad (6)$$

The corresponding 1D Harper Hamiltonian has the form of a non-interacting chain with anisotropic nearest-neighbor hopping:

$$\hat{H} = \sum_k \Gamma^r_k c_2 k c_2 k + \Gamma^i_k c_{2+1} k c_{2+1} k + \text{ h.c.}, \quad (6)$$

where the left and the right hopping parameters are $\Gamma^r_k = -t_1 e^{ik} - t_2 e^{i(2q+1)\phi}$ and $\Gamma^i_k = -t_3 e^{ik}$, respectively. Invoking the Schrödinger equation, $\hat{H}|\psi_i\rangle = \epsilon_i|\psi_i\rangle$, where $|\psi_i\rangle = \sum \psi_i c_i^\dagger |0\rangle$, the following eigenfunction equations are obtained:

$$\epsilon_i \psi_{2i} = \Gamma^r_i \psi_{2i-1} + \Gamma^i_i \psi_{2i+1} \quad (7)$$

We re-express equation (7) in terms of the parameters $\mu = t_1/t_3$ and $\lambda = t_2/t_3$ and study the phase diagram as a function of $\mu$ versus $\lambda$ for irrational values of $\phi$. We fix $\phi$ to be the inverse of the golden ratio which we approximate as $\phi_n = F_n-1/F_n$, where the Fibonacci number $F_n$ is defined in terms of the recurrence relation $F_0 = 1$, $F_1 = 1$ and in the limit $n \rightarrow \infty$, the ratio $\phi_n$ tends to $(\sqrt{5} - 1)/2$. We find that the phase diagram, as shown in figure 2(b), can be divided into three distinct regions. Each of these phases is separated from the other by a critical line. These lines meet at the bicritical point, which corresponds to all the tunnelling parameters being identical. To characterise these regions we have used multiple techniques. While VNE, fidelity and fidelity susceptibility are able to characterise the regions into insulating or metallic type, we find that multifractal analysis and level statistics approaches are especially helpful for studying the wavefunction and the spectral properties at the critical lines.

3. Phase diagram

3.1. von Neumann entropy

We begin our analysis by studying the von Neumann entropy of the $N$-site wave function averaged over all sites [22]:

$$S_j = -\sum_{i=1}^{N} p_i^j \log_2 p_i^j + (1 - p_i^j) \log_2 (1 - p_i^j), \quad (8)$$

where $p_i^j$ is the occupation probability of the $i$th site of the $j$th wave-function. We note that for delocalised wave functions $p_i^j \sim 1/N$ and hence $S_j \sim \log_2 (N)/N$. On the other hand, $S_j \sim 1/N$ for wave-functions that are localised. Thus the von Neumann entropy serves as an excellent diagnostic tool for distinguishing regions that are localised from those that are delocalised.

It is useful to define the scaled entropies as:

$$\sigma_j = \frac{N}{\log_2 N} S_j. \quad (9)$$

$\sigma_{\text{min}}$ close to unity implies all the states are delocalized, while $\sigma_{\text{max}}$ significantly smaller than unity suggests that all states are localised. In figures 3(a) and (b), we plot the minimum and maximum scaled entropy from the set $\{\sigma_1, ... , \sigma_N\}$ at each parameter value $(\mu, \lambda)$. Interestingly, even for relatively small system sizes (for example $F_{12} = 144$), a clear separation between the extended regions II, III and the localized region I, is seen. Another feature that is illustrated from the near identical phase diagrams of figures 3(a) and (b) is that there are no mobility edges. The wave functions in a given parameter regime are either all localised or all delocalised.

3.2. Fidelity and fidelity susceptibility

Although the VNE approach is able to distinguish regions into metallic and insulating type, the distinction between the two metallic regions remain inconclusive. We find that fidelity and FS techniques are able to further characterise the metallic regions.

Fidelity is defined as the overlap of the ground-state wavefunctions for differing parameters and is given by

$$F(\vec{T}_1, \vec{T}_2) = |\langle \psi_0(\vec{T}_1) | \psi_0(\vec{T}_2) \rangle|, \quad (10)$$

where $|\psi_0(\vec{T}_1)\rangle$ are the ground state wave-functions with parameters $\vec{T}_i = (\mu_i, \lambda_i), i \in \{1, 2\}$. Keeping one of the parameters as the reference point, say $\vec{T}_1$, the other parameter
\( \tilde{T}_2 \), is varied. If the two parameters lie in the same phase the fidelity value is near unity. On the other hand, the ground-state wave-function differs significantly for parameters separated by a quantum critical point/line thus resulting in near vanishing fidelity values. In figures 4(a)–(c), we choose \((0.5, 1)\), \((1, 0.5)\) and \((2, 2)\) respectively, as the reference parameters. These highlight, respectively, insulating and the two metallic regions. Although the data presented is for the lowest energy state, we have checked that the same phase diagram is generated if arbitrary eigenstates are considered.

Fidelity measurements can also highlight the critical lines. When the reference point is taken to be on a critical line, fidelity exhibits its maximum value along that line and a sharp decline away from it. This is best illustrated for the reference point \((1, 1)\) (which is a bicritical point) for which fidelity exhibits peak behaviour (figure 4(d)) along all the critical lines. The above approach to isolate the critical lines, is dependent on the correct positioning of the reference point. It turns out that an efficient alternate way to obtain the critical lines is to calculate fidelity susceptibility, which exhibits a sharp peak at the region separating the different phases. Fidelity susceptibility, \( \chi_F \), is defined in terms of the sub-leading term in the expansion of fidelity between states which are infinitesimally separated in the phase space, i.e. \( F(\tilde{T}, \tilde{T} + \delta \tilde{T}) = 1 - \delta \tilde{T}^2 \chi_F / 2 + \cdots \). From the Taylor-series expansion of

\[
\begin{align*}
[F(\tilde{T}, \tilde{T} + \delta \tilde{T})]^2 &= \left[ 1 + \delta \tilde{T} \sum_a \frac{\partial T_a}{\partial \tilde{T}} \langle \psi_0 | \frac{\partial}{\partial T_a} \psi_0 \rangle \right. \\
&\quad + \frac{\delta \tilde{T}^2}{2} \sum_{ab} \frac{\partial T_a}{\partial \tilde{T}} \frac{\partial T_b}{\partial \tilde{T}} \langle \psi_0 | \frac{\partial}{\partial T_a} \frac{\partial}{\partial T_b} \psi_0 \rangle \bigg] ^2,
\end{align*}
\]

and utilizing the constraint \( \partial \langle \psi_0 | \psi_0 \rangle / \partial T_a = 0 \) (arising from the normalization of the wave-function) one obtains the expression for susceptibility given by \[16–19, 22\]

\[
\chi_F = \sum_{(a,b)=\lambda,\mu} \frac{\partial T_a}{\partial \tilde{T}} \frac{\partial T_b}{\partial \tilde{T}} \left[ \frac{1}{2} \left( \langle \psi_0 | \frac{\partial}{\partial T_a} | \psi_0 \rangle + \langle \psi_0 | \frac{\partial}{\partial T_b} | \psi_0 \rangle \right) \right. \\
&\quad - \left. \langle \psi_0 | \frac{\partial}{\partial T_a} | \psi_0 \rangle \langle \psi_0 | \frac{\partial}{\partial T_b} | \psi_0 \rangle \right].
\]

Further, by inserting the identity operator \( \hat{1} = \sum_n | n \rangle \langle n | \) in the above equation and making use of the identity \( \langle \psi_n | \partial_a \psi_n \rangle = \langle \psi_n | (\partial_a H) | \psi_n \rangle / (\epsilon_n - \epsilon_a) \) one obtains,
as

$$\chi_F = \sum_{(a,b)=\lambda,\mu} \sum_{n\neq 0} \frac{\partial Y_a}{\partial Y} \frac{\partial Y_b}{\partial Y} |\langle \psi_n | \frac{\partial H}{\partial Y_a} | \psi_n \rangle|^2 \frac{1}{(\epsilon_0 - \epsilon_n)^2}. \quad (13)$$

This modified form for the susceptibility is explicitly gauge invariant and particularly suitable for numerical evaluation [18]. The unit vector \( \frac{\partial Y_a}{\partial Y}, \frac{\partial Y_b}{\partial Y} \) represents the direction connecting the two infinitesimally close points. The choice of the unit vector is arbitrary. If the unit vector is chosen to be parallel to one of the critical lines, then all critical lines except for the one parallel to the unit vector will be exposed. In our case, fidelity susceptibility plots obtained by considering at least two choices of non-collinear unit vectors will reveal all the critical lines. In figure 5 we consider \( (1/\sqrt{3}, \sqrt{2}/3) \) as the unit vector; since this vector is not along any of the critical lines, only one plot is sufficient to highlight the position and direction of all the critical lines.

Further insight into the various phases is obtained by studying the limiting scenarios in equation (6). For \( \lambda = t_2/t_1 = 0 \) and \( \mu \neq 0 \), which is part of metallic region I (see figure 2), the 1D Hamiltonian reduces to

$$\tilde{H} = - \sum_{s} (t_1 c_{2s-1}^{\dagger} c_{2s} + t_3 c_{2s+1}^{\dagger} c_{2s}) + \text{h.c.}, \quad (14)$$

where we have set the constant phase part \( k_i = k_j = 0 \). We note that this 1D Hamiltonian is exactly the Su–Schrieffer–Heeger (SSH) model [38] (i.e. hopping Hamiltonian with alternating bond strengths) whose bulk states are all metallic. As borne out by the fidelity plots, all the ground states of region I or \( (\mu > \lambda) \cap (\lambda < 1) \) belong in the same universality class, i.e. the overlap of the wavefunctions is close to one and therefore all of them are metallic. On the other hand the limit \( \mu = t_1/t_2 = 0 \) and \( \lambda \neq 0 \) (belonging to the metallic region II) yields a 1D Hamiltonian

$$\tilde{H} = - \sum_{s} (t_2 e^{i4\pi \phi_0} c_{2s-1}^{\dagger} c_{2s} + t_3 c_{2s+1}^{\dagger} c_{2s}) + \text{h.c.}, \quad (15)$$

where the hopping terms repeat itself after sites \( \propto F_n \) (note \( \phi_n = F_{n-1}/F_n \)). All states of this Hamiltonian are also extended. At the same time all the ground states of region II \( (\mu < \lambda) \cap (\mu < 1) \) have a near-unity overlap with the ground state of this Hamiltonian, and form a separate universality class. Due to the distinct natures of the two Hamiltonians (equations (14) and (15)) above, one would expect the corresponding ground states to be orthogonal to each other.

Extending the argument a step further, we expect the ground states of the entire region II to be orthogonal w.r.t. the ground states of region I. Indeed these expectations are realised as seen from the fidelity plots shown in figure 4. In figures 6(a) and (b), we plot the real part of the wavefunctions of region I with parameters \( (5.5, 0) \) and \( (5.5, 0.4) \) and compare them with the figures 6(c) and (d), where the real part of the wavefunctions of region II with parameters \( (0, 5.5) \) and \( (0.4, 5.5) \) are plotted. As compared to wave-functions of region II, those of region I exhibit periodic behavior with small periodicity.

Finally consider the \( \mu, \lambda \gg 1 \) or the regime-III as shown in figure 2 where the Hamiltonian can be approximated as

$$\tilde{H} = - \sum_{s} (t_1 e^{i4\pi \phi_0} c_{2s-1}^{\dagger} c_{2s} + \text{h.c.}, \quad (16)$$

i.e. the Hamiltonian is equivalent to cutting off of right-hopping from an even-site to an odd-site, thus generating localized islands. All states of the Hamiltonian (16) and also all the states in the entire parameter regime of region III are localized.

3.3. Multifractal analysis

In this section we will briefly mention some key ideas of the multifractal technique useful for analysing the scaling properties of wave functions in different regions of parameter space. Detailed reviews of this topic can be found in papers by Kohmoto and co-workers [9, 14, 15]. The basic point is to express the probability measure of a wave-function at the \( n \)th site, \( \rho_n \), terms of the function \( \phi_n = F_{n-1}/F_n \), where \( N \propto F_n \) is the number of lattice sites at the \( n \)th step. The distribution of \( \alpha_i \)'s thus obtained can be organised in terms of the function \( \Omega_n(\alpha) \) defined as the density of sites with scaling index \( \alpha \), satisfying \( \int \Omega_n(\alpha) d\alpha = N \). Further, \( \Omega_n(\alpha) \) is expressed in terms of the scaling function \( f_n(\alpha) \) such that \( \Omega_n(\alpha) = N f_n(\alpha) \). The above information suffices to make certain qualitative observations regarding the nature of wave-functions.

With the increase in step-size \( n \), the minimum of the scaling index \( \alpha_{\text{min}} \) approaches distinct limits for wave-functions that are extended, localised and critical (for illustration see figure 7). Let us first consider the case for which the states are extended. For this scenario, we expect that the probability measure at a typical point to scale as \( p_i \sim 1/N \) and consequently \( \alpha_{\text{min}} \to 1 \) (since \( \alpha_i = -\ln p_i/\ln N \)). Since for almost all points \( \alpha_i \to \alpha_{\text{min}} \) it is expected that the density of states at \( \alpha_{\text{min}} \) scales as \( \Omega(\alpha_{\text{min}}) \sim N \), therefore \( f(\alpha_{\text{min}}) = \ln \Omega(\alpha_{\text{min}})/\ln N \to 1 \). Now contrast these expectations from those for the localised states. By definition, the probability measure for localised states are concentrated at...
only few points. At these points the probability measure is finite (or in other words $\pi_i \sim \pi_1$) therefore $\alpha_i \sim 1/\ln N$ and in the limit $N \to \infty$, $\alpha_i \to 0$. Therefore for localised states we expect $\alpha_{\min} \to 0$, whereas the points that are unoccupied ($p_i \to 0$) result in $\alpha_{\max} \to \infty$. In the limit of $N \to \infty$, the density of points where the measure is finite (or where $\alpha_i \approx \alpha_{\min} \sim 1/\ln N$) vanishes, therefore $f(\alpha_{\min}) \to 0$. At the same time the density of states where the measure vanishes goes as $\Omega(\alpha_{\max}) \sim N$, therefore $f(\alpha_{\max}) \to 1$. A critical state is characterised by $0 < \alpha_{\min} < 1$ and $f(\alpha)$ defined between the intervals $[\alpha_{\min}, \alpha_{\max}]$.

We consider the wave-functions at the lowest end of the spectra and numerically evaluate $\alpha_{\min}$ for Fibonacci indices $n$ and extrapolate them as $n \to \infty$. The plots of $\alpha_{\min}$ versus $1/n$ are obtained for parameter points on the critical lines and away from it (see figure 8). The plots of $\alpha_{\min}$ versus $1/n$ for the parameter points $(\mu, \lambda) = (0.5, 0.4), (1, 0.9)$ from metallic region I and $(\mu, \lambda) = (0.7, 2), (0.9, 1.1)$ from metallic region II, exhibit $\alpha_{\min} \to 1$ as $n \to \infty$ a behaviour consistent with extended states. For $(\mu, \lambda) = (1.1, 1.1), (2, 3)$ which are in region III, $\alpha_{\min}$ approaches 0 as $n \to \infty$, which is what we expect for an insulating phase. Finally, we consider the behavior at the critical points $(\mu, \lambda) = (1, 1)$ and $(2, 1)$; we see from figure 8 that in the $n \to \infty$ limit, the exponent $\alpha_{\min}$ approaches a limit different from the metallic and insulating ones and lies between $0 < \alpha_{\min} < 1$. At the same time as seen in figure 9, $f(\alpha)$ acquires a dome like feature for the allowed values of $\alpha$ thus confirming the multifractal nature at the critical points [9].

3.4. Level statistics

As an alternative quantitative test for the universal features, we investigate the level statistics along the critical lines by studying the behavior of the spectral distribution function $P(\omega)$ as $\omega \to 0$. The normalizations used to define the distribution function are $\int_0^\infty P(\omega) d\omega = 1$ and $\int_0^\infty \omega P(\omega) d\omega = \langle \omega \rangle = 1$. We find that along the critical lines $P(\omega)$ diverges as $\omega^{-\delta}$ ($\delta > 0$), a behaviour analogous to

Figure 6. Ground state wave functions (real part) plotted as a function of site index for the parameter regimes $(\mu, \lambda)$: (a) $(5.5, 0)$ and (b) $(5.5, 0.4)$ both of which are in the metallic regime-I. The fidelity between the two states is $F = 0.95$. The figures (c) $(0, 5.5)$, and (d) $(0.4, 5.5)$ are in the metallic regime-II, and the fidelity between those two states is also $F = 0.95$. However, the fidelity between states of regime-I and -II is close to zero. In all these plots, $\phi = 377/610$.
earlier studies on the gap distribution functions along critical lines for 1D quasi-periodic systems [9, 40].

Figure 10 shows the distribution of levels for \( n = 24 \) and critical points \((\mu, \lambda) = (0.5, 0.5)\) and \((\mu, \lambda) = (1, 2)\). These can be fitted to the generic form:

\[
\log[P(w)] = -\delta \log(w) - \beta.
\]  

(17)

For \((\mu, \lambda) = (0.5, 0.5)\) and \((\mu, \lambda) = (1, 2)\), \(\delta = 1.52, 1.51\) respectively. We obtain a similar plot for \((\mu, \lambda) = (1, 1)\), with slope \(\delta = 1.52\). Thus along the critical lines the estimated value of \(\delta\) is \(\sim 1.5\), lending further support to universality along the critical lines.

4. Next nearest neighbour hopping

In our study so far, we observe that all the eigenfunctions in each of the phases exhibit features similar to the corresponding
ground state eigenfunction. In other words, the nearest neighbor hopping model we considered is characterised by a lack of mobility edge.

Here we will study the role of next-nearest-neighbor hopping on the localization-delocalization transition. For this purpose we will consider the following Harper equation [41]:

$$ E\Psi_n = D_n \Psi_n + R_n \Psi_{n+1} + R_{n-1}^\dagger \Psi_{n-1}. $$

$$ (18) $$

Here $D_n$ and $R_n$ are $2 \times 2$ matrices,

$$ D_n = \begin{pmatrix} a_n & c_n \\ c_n^\dagger & b_n \end{pmatrix}, \quad R_n = \begin{pmatrix} d_n & 0 \\ f_n & e_n \end{pmatrix}, $$

where at $k_x = k_y = 0$, the matrix entries are given in terms of the NNN hopping parameter $t$ and the NN hopping parameters $t_1, t_2, t_3$ as:
\[ a_n = 2t \sin[2\pi(n + 1/6)\phi], \quad b_n = -2t \sin[2\pi(n + 1/6)\phi], \]
\[ d_n = -ie^{i2\pi(n+1/3)\phi}(1 - e^{i2\pi(n+1/3)\phi}), \]
\[ e_n = i e^{i2\pi(n+2/3)\phi}(1 - e^{i2\pi(n+2/3)\phi}), \]
\[ c_n = t_2 + t_1 e^{i2\pi\phi}, \quad f_n = t_3 e^{-i2\pi\phi(n+1/2)}. \]

We note that our spinless Harper equation is a modified version of the one originally proposed by Beugeling et al \[41\] for spinfull fermions with isotropic NN hopping and the NNN hopping terms being of the intrinsic spin–orbit (ISO) and Rashba types, which correspond to spin conserving and non-conserving processes, respectively. In the intrinsic spin–orbit term, the up and down-spin terms have opposite sign in front of the tunnelling amplitude term. We have considered only the ISO type of hopping process corresponding to spinless fermions.

The effective one dimensional model as before has anisotropic NN hopping; in addition, the NNN hopping in the original hexagonal lattice manifests itself as an on site potential and NNN hopping along the chain. The Hamiltonian has the following form:

\[ H = \sum_x (a_x \alpha_x^\dagger \alpha_x + b_x \alpha_{x+1}^\dagger \alpha_x + c_x \alpha_{x+1}^\dagger \alpha_{x+1} + d_x \alpha_{x+3}^\dagger \alpha_{x+2} + f_x \alpha_{x+2}^\dagger \alpha_{x+1} + \text{h.c.}) + \sum_n (e_n^x \alpha_n^\dagger \alpha_n + f_n^x \alpha_{n-1}^\dagger \alpha_{n+1} + \text{h.c.}) \quad (19) \]

In the absence of the NNN term we recover identically the earlier plots for the phase diagram, von Neumann entropy, fidelity and fidelity-susceptibility. However, turning on the NNN term leads to features that are not universal. In the absence of \( t \), the fidelity plots for reference parameters \( (\mu = 2, \lambda = 0.5) \) will reproduce figure 4(b), however, when \( t = 0.08 \), and 0.12, the ground state fidelity yields plots as given in figures 11(a) and (b), respectively. These plots are significantly different from each other as well as from the \( t = 0 \) case, indicating strong dependence of the nature of the ground state on the NNN hopping parameter.

Figure 12. Scaled entropy (equation (9)) plots for the NNN model for a range of parameters \((t_1, t_2)\) (same as \((\mu, \lambda)\) as we have taken \( t_3 = 1 \)) as a function of the NNN coupling \( t \). Note that for \( t = 0 \) the parameters chosen correspond to the insulating regime, i.e. all the states are localized. (a) Shows the maximum entropy among all the eigenstates. As \( t \) is increased, \( \sigma_{\text{max}} \) increases and therefore the plot suggests that some of the states exhibit a localization-delocalization transition. (b) Shows that the minimum entropy does not change much in the range of \( t \) considered, which suggests that not all states become delocalized.

Figure 13. Scaled entropy (equation (9)) plots for all the energy states of the NNN model for \( t_1 = 4 \) and \( t_2 = 3.8 \) (note that for \( t = 0 \) this parameter choice lies deep in the insulating regime with all states localized) and NNN hopping parameters (a) \( t = 1.2 \) and (b) \( t = 10 \). For the above two choices of the NNN hopping parameter some states are localized (\( \sigma \approx 0.6 \)) and some delocalized (\( \sigma \approx 1 \)). While for \( t = 1.2 \), states with energies \(-3 \lesssim \epsilon \lesssim 3 \) are localized, for \( t = 10 \) there is no clear separation in the energy scales.

It turns out that unlike the NN model, the ground state here is atypical; there are other eigenstates which are dramatically different from the ground state. To show this, we once again study the maximum and minimum values of the...
scaled entropy, just like in figure 3 for the NN problem, where \( \sigma_{\text{min}} \) and \( \sigma_{\text{max}} \) were qualitatively the same. In sharp contrast, figure 12 shows that in the presence of NNN coupling, the dependence as a function of \( t \) of \( \sigma_{\text{min}} \) and \( \sigma_{\text{max}} \) are markedly different. As \( t \) is increased there exists a critical \( t_c \), dependent on the parameters (\( \mu, \lambda \)), beyond which the states corresponding to the maximum entropy exhibit a localisation–delocalisation transition (for large \( n \) the transition is sharper). For large \( t \), \( S_{\text{max}} \sim \log_2 N/N \) implying some of the states become delocalised. There is no such signature seen with \( \sigma_{\text{min}} \). This is an indication of the presence of mobility edges in the spectrum.

A closer look at the plateau region of figure 12(a) is illuminating. Fixing \( t \) to be in the plateau region and \( t_1 = 4, t_2 = 3.8 \), let us study the scaled entropy for all the eigenstates as a function of energy. Two different cases of \( t = 1.2 \) and \( t = 10 \) are shown in figure 13. In each of these cases, it is possible to discern spread-out energy windows where \( \sigma \sim 1 \) corresponding to extended states, and other energy windows where \( \sigma \ll 1 \) corresponding to localized states. For \( t = 1.2 \) a mobility edge separating localized and delocalized states can be identified to be around \( \epsilon \approx 3 \). However, such sequential behaviour is not universal as particularly evidenced for \( t = 10 \), wherein the behaviour exhibited is more complex. There are multiple closely separated energy bands at various energy scales wherein the wavefunctions manifest different behaviour: delocalized, localized and critical.

5. Conclusions

An effective 1D model derived from a 2D honeycomb lattice with anisotropic nearest neighbour hopping in the presence of a uniform magnetic field is studied. Unlike the generalized-AAH type models which have a quasiperiodic on-site potential term, the model we considered can be thought of as a modified version of the SSH model with a modulating hopping term and no potential term. A clue regarding the various phases supported by this model is obtained by studying limiting scenarios. For \( \lambda = 0 \), the 1D Hamiltonian is metallic with unit-cell made of just two sites, whereas for the \( \mu = 0 \) case, the unit cell is \( \infty \) \( \alpha \)-sites and thus corresponds to an altogether different metallic phase. The \( \mu \gg 1 \) and \( \lambda \gg 1 \) regime is insulating since it is equivalent to cutting off of right-hopping from an even-site to an odd-site, thus generating localized islands. These expectations are confirmed employing a variety of techniques. The phase diagram is found to comprise of one insulating region and two metallic regions; von Neumann entropy, averaged over all sites, is useful as a marker of the phase boundaries. The task of distinguishing between the two metallic phases, is accomplished with the help of fidelity, and fidelity susceptibility. An alternative perspective is provided by multifractal analysis, which allows for a finite-size scaling confirmation of the phase diagram. The study of level statistics reveals universal features along the critical lines.

Finally, a variant Hamiltonian which incorporates next nearest neighbour hopping, is found to exhibit mobility edges in contrast to the earlier model. In this model, there are no well-marked parameter-regimes where all states are localized/delocalized. Moreover, even for a fixed set of parameters, the mobility edges are themselves manifest at multiple energy scales in a highly non-trivial manner. These features are worthy of further exploration.

While the present work has focussed on statics, a dynamical perspective is suggested by recent work [42] which has reported on certain driving protocols that can couple between groups of localized states and convert them into extended states. It would be interesting to explore such effects in our model on the honeycomb lattice, which provides a rich phase diagram. The possibility of many-body localization when interaction is turned on [43], and other many-particle effects [44], provides impetus for including interaction in our model.

Acknowledgments

SG would like to thank Diptiman Sen for helpful discussions. We thank the anonymous referees for constructive comments and suggestions. We thank Surajit Sarkar for help with some of the schematic figures. AS and SG are grateful to SERB for the support via grants YSS/2015/001696 and EMR/2016/002646, respectively. We thank the HPC facility of IISER, Bhopal, where part of the computational work was carried out.

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