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A study of one-dimensional correlated disordered systems using the invariant measure method

K Kundu†, D Giri‡ and K Ray§
Institute of Physics, Bhubaneswar 751005, India

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Abstract. The behaviour of electronic states of one-dimensional correlated disordered systems which are modelled by a tight binding Hamiltonian is studied analytically using the invariant measure method. The approach of Bovier is generalized to include the possibility of different site energies and nearest neighbour hopping integrals inside the correlated sites or the cluster. The process is further elaborated by applying to the symmetric random trimer model which contains in it many hitherto known models of this category. An alternative mathematical definition of the exceptional energy (E_S) from the invariant measure density, along with physical arguments substantiating it, is presented. Furthermore, the procedure for obtaining exceptional energies is outlined and applied to the symmetric random trimer model to derive conditions for obtaining doubly degenerate exceptional energies. The Lyapunov exponent ($\gamma(E)$) or the inverse localization length of states around the exceptional energy is found to vary as $\sim(E - E_S)^{2n}$ in the leading order. n denotes the degeneracy of the exceptional energy. The density of states at the exceptional energies are calculated. We further propose that one-dimensional correlated disordered systems can be mapped to a Lloyd model in which the width of the distribution of site energies is determined by the reflection coefficient of the cluster embedded in the lattice of the other constituent. The importance of our results is discussed.

1. Introduction

One of the well established results in condensed matter physics is that all electronic eigenstates of a disordered one-dimensional system are exponentially localized irrespective of the strength of the disorder. The early work of Anderson [1] on uncorrelated site diagonal disorder in the tight binding model (TBM) and of Mott and Twose [2] form the basis of this result. Of course, the results of Anderson and of Mott and Twose, cannot be rigorously valid in one-dimensional systems in which the disorder is correlated. For example, in the context of a TBM it has been shown that correlated off-diagonal disorder [3] cannot localize the state at the band centre. Another example in this category is the model proposed by Dunlap, Kundu and Phillips (DKP) [4]. The best known example in the context of a TBH, however, is the random dimer model (RDM) [5]. This is basically the offspring of the original DKP model. The generalization of the RDM requires the extension of the correlation beyond the nearest neighbour site and the introduction of different nearest neighbour hopping elements among the correlated sites or simply the cluster. Two good but simpler examples in this generalized category are the repulsive binary alloy (RBA) [6] and the symmetric

† E-mail address: kundu@iopb.ernet.in
‡ E-mail address: giri@iopb.ernet.in
§ E-mail address: koushik@iopb.ernet.in

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random trimer model (SRTM) [7]. The SRTM, which is the further generalization of the RBA, yields two exceptional energies. The exceptional energy is the energy at which the reflection coefficient of the cluster embedded in the lattice of the other constituent vanishes. We further note that the number of exceptional energies for a trimer embedded in a one-dimensional lattice of another element cannot exceed two. Another interesting as well as important feature of the SRTM is that the positions of these exceptional energies can be tuned by changing either the hopping element or the site energies of the cluster, and in the limit these two energies can merge. This has actually been shown by Giri, Datta and Kundu (GDK) [7] by conventional analysis of the reflection coefficient and by appropriate numerical simulations. Salient features of the SRTM can be verified by fabricating appropriate layered heterojunctions and also by coupling quantum dots [8]. Another potential area of application of this model is the field of organic conducting polymers [9].

The most commonly used method for studying the electronic properties of one-dimensional correlated systems is to analyse the reflection coefficient of the cluster in the neighbourhood of exceptional energies. Since the system behaves like a weakly disordered system in the neighbourhood of these energies, a very good estimation, albeit not rigorous, of the Lyapunov exponent (inverse localization length) in these neighbourhoods can be obtained from the reflection coefficient. On the other hand an estimation of the density of states (DOS) at an exceptional energy can in principle be obtained from the phase of the transmission coefficient of a single cluster through the Thouless formula [10]. To the best of our knowledge no such effort has been made in this direction. Hence, the DOS and the mean square displacement of the particle are calculated numerically [11] to establish the presence of nonscattered states around these energies.

Another way of looking at this state of affairs is the calculation of the Lyapunov exponent and the integrated density of states (IDOS) of the system from its invariant measure. In an attempt toward understanding the behaviour of the IDOS of the one-dimensional Anderson model in the weak disorder limit, Bovier and Klein [12, 13] developed a scheme for a perturbation expansion of the invariant measure of the model. From the modified perturbative expansion of the invariant measure, Bovier and Klein showed that at all energies $E_0 = 2\cos\alpha\pi$ with α rational, the IDOS of the Anderson model in the weak disordered limit has singularities. This was the extension of the results obtained previously by Kappus and Wegner [14] and Derrida and Gardner [15]. Bovier and Klein [12] further showed that for irrational α, their technique gives unique invariant measure with finite coefficients to all orders of perturbation. This modified expansion has also proved to be a true asymptotic expansion of the invariant measure [16]. This scheme was later applied by Bovier [17] to develop the perturbation series expansion of the invariant measure around the exceptional energies of the RDM. This enabled him to show that the Lyapunov exponent vanishes as ε^2 in energy (ε) in the neighbourhood of the exceptional energies. Furthermore, the IDOS is found to vary as ε within this energy width. This is basically the first rigorous calculation on the RDM confirming the results of [5].

The fundamental characteristic of the cluster correlated disordered systems is the presence of exceptional energies where disorder systems purportedly behave like perfect systems. However, for these systems to play an important role in the transport properties of the materials, there must be a finite DOS at these energies. Hence, to fully characterize these systems, we need rigorous analytical calculations of the Lyapunov exponent around these energies and DOS at these energies. To the best of our knowledge, for these systems, the invariant measure technique is the only technique that can yield the DOS analytically without invoking any approximation. This is primarily the motive to apply this technique to the SRTM which encompasses many hitherto known examples. For this purpose, we generalize

the approach of Bovier [17] to include the possibility of different site energies and nearest neighbour hopping elements in the cluster. We also give here an alternative mathematical definition of the exceptional energy from the invariant measure and derive from it, in the case of the SRTM, an algebraic equation in energy involving relevant parameters of the system. We further show that the equation gives the correct prediction of the possibility of tuning of exceptional energies yielding in the limit a degenerate exceptional energy as noted by GDK [7]. Finally we propose a mapping of these systems to an effective Lloyd model. Such a mapping will be useful in the study of the transport properties of these systems.

The organization of the paper is as follows. In the following section we generalize the approach of Bovier. We then develop equations for the invariant measure density, the Lyapunov exponent and the IDOS. In section 4 we discuss the method for obtaining exceptional energies. Section 5 is devoted to the perturbative calculation of the invariant measure density for the SRTM. In sections 6 and 7 we calculate the leading order behaviour of the Lyapunov exponent and the DOS at exceptional energies respectively. In section 8 we deal with the mapping of the aspect. We conclude the paper by highlighting the major contributions of the paper.

2. Formalism

We study the Hamiltonian

$$H = \sum_n \epsilon_n a_n^\dagger a_n + \sum_n V_{n+1,n}(a_{n+1}^\dagger a_n + a_n^\dagger a_{n+1}) \tag{1}$$

on $l^2(Z)$ where a_n ($a_n^\dagger$) destroys (creates) a particle at the nth site. $V_{n,n+1}$ is the tunnelling matrix connecting the nth site to the $(n+1)$th site. $\{V_{n+1,n}\}$ are taken to be real and positive, although this constraint is not necessary.

The eigenvalue equation [18] associated with H is

$$\epsilon_n C_n + V_{n+1,n}C_{n+1} + V_{n,n-1}C_{n-1} = EC_n. \tag{2}$$

We introduce $z_n = \frac{V_{n,n-1}C_n}{C_{n-1}} \in \dot{\boldsymbol{R}}$ with $\dot{\boldsymbol{R}}$ denoting the compactified real line $\boldsymbol{R} \cup \{\infty\}$. The recursion relation for z_n is then

$$z_{n+1} = E - \epsilon_n - \frac{V_{n,n-1}^2}{z_n} = \xi_{E,\epsilon_n V_{n,n-1}}(z_n). \tag{3}$$

We further note in this connection that the eigenvalue equation for a one-dimensional array of masses $\{m_i\}$ coupled to nearest neighbours by identical harmonic springs is

$$(2 - m_i\Omega^2)u_i = u_{i-1} + u_{i+1} \tag{4}$$

where u_i is the displacement of the ith mass, m_i in the vibration with frequency Ω. All spring constants are taken to be unity without any loss of generality. Now introducing a variable, $z_n = \frac{u_n}{(m_{n-1}u_{n-1})} \in \dot{\boldsymbol{R}}$, we obtain from (4)

$$z_{n+1} = -\Omega^2 + \epsilon_n - \frac{V_{n,n-1}^2}{z_n} \tag{5}$$

where $\epsilon_n = \frac{2}{m_n}$ and $V_{n,n-1} = (m_n m_{n-1})^{-1/2}$. Hence, the behaviour of a one-dimensional array of masses coupled by harmonic springs is mathematically equivalent to the one-dimensional quantum motion of a particle in a TBM [19, 20]. The Lyapunov exponent, $\gamma(E)$ and the IDOS, $N(E)$ are related to the large-n behaviour of z_n. If we define

$$\tilde{\gamma}(E) = \lim_{N\to\infty} \frac{1}{N} \sum_{n=1}^{N} \ln \frac{z_n}{V_{n,n-1}} \tag{6}$$

then

$$\gamma(E) = \operatorname{Re}\tilde{\gamma}(E) \tag{7}$$

and

$$N(E) = \frac{1}{\pi}\operatorname{Im}\tilde{\gamma}(E). \tag{8}$$

To understand the origin of equation (8) we consider a chain of N sites with fixed boundary conditions at both ends. In other words we set $C_{-1} = C_N = 0$. To keep the argument simple, we assume that $\{V_{n,n-1}\}$, $n \in Z$ are real. From equation (3) we get $z_1 = E - \epsilon_1$, a real quantity. So, none of the $\{z_n\}$ can be truly complex. However, $\{\frac{Z_n}{V_{n,n-1}}\}$, $n \in Z$ can be negative real numbers which can be thought of as complex numbers with the minimum phase, π. So the right-hand side of equation (8) picks up a contribution whenever $\frac{z_n}{V_{n,n-1}} = \frac{C_n}{C_{n-1}}$ is negative.

Consider now the case when $C_n = 0$ for $n \leqslant N$. From equation (3) we obtain

$$z_{n-1} = \frac{V_{n-1,n-2}^2}{E - \epsilon_{n-1}} = E - \epsilon_{n-2} - \frac{V_{n-2,n-3}^2}{z_{n-2}}. \tag{9}$$

Values of E for which this equation (9) is satisfied are the eigenvalues of the system. When $n = N$, we obtain eigenvalues of the system under study. Let us assume that E_l is the lth eigenvalue of the system in ascending order. So, the eigenvector belonging to E_l has $(l-1)$ nodes. This in turn implies that $\frac{z_n}{V_{n,n-1}}$ will also pick up $(l-1)$ negative numbers giving $\operatorname{Im}\frac{1}{N}\sum_{n=1}^{N}\frac{z_n(E_l)}{V_{n,n-1}} = \frac{l-1}{N}$. On the other hand, the number of states up to $E = E_l$, i.e. IDOS (E_l) is l. So, in the limit $N \to \infty$, equation (8) yields the IDOS (E_l). To understand further the behaviour of equation (8) for $E_l < E < E_{l+1}$, we note that $E_l(m) > E_l(N)$ if $m < N$. For E in this limit equation (9) will be satisfied for some m such that $l \leqslant m < N$ and the lth eigenvalue of the reduced system will be obtained. Hence, the number of modes and consequently the number of negative values of $(\frac{Z_n}{V_{n,n-1}})$ will be preserved. We further note that when $E = E_l + \epsilon$ and $\epsilon \to 0$, m will be close to N. When $E = E_{l+1} - \epsilon$, m will be close to l and it will swing back to N for $E = E_{l+1}$. For further discussion on this see [21].

The disorder in the Anderson model can arise from the disorder in diagonal elements (ϵ_n) of H, from the disorder in off-diagonal elements, $V_{n,n+1}$, $n \in Z$ of H or from both. In all these cases equation (3) defines a Markov chain in which states are characterized by the random variable z_n, $n \in Z$. When $V_{n,n+1} = V$, $n \in Z$ and $\{\epsilon_n\}$ are 2D random variables, this Markov chain consists of persistent non-null states [22]. In other words, the chain is ergodic. Frustenberg's theorem [23] then asserts that $\epsilon_n \neq \tilde{\epsilon}$, $\tilde{\epsilon}$ = a constant, $n \in Z$, and there is a unique invariant measure $\mathrm{d}\nu_E(z)$ on $\dot{\boldsymbol{R}}$. This measure satisfies

$$\int_{\dot{\boldsymbol{R}}} \mathrm{d}\nu_E(z)\, f(z) = \boldsymbol{E}\int_{\dot{\boldsymbol{R}}} \mathrm{d}\nu_E(z)\, f\left(E - \epsilon - \frac{1}{z}\right) \tag{10}$$

for all bounded measurable functions, f. Here, $\boldsymbol{E}$ denotes the expectation with respect to the probability distribution of ϵ. Furthermore, this measure is actually continuous and hence is supported by $\boldsymbol{R}$. So, the measure $\mathrm{d}\nu_E(z)$ has a density, i.e. $\mathrm{d}\nu_E(z) = \phi_E(z)\,\mathrm{d}z$, where $\phi_E(z)$ defines the density at $z \in \boldsymbol{R}$. Similarly, if $\epsilon_n = \tilde{\epsilon}$, $n \in Z$ and $\{V_{n,n+1}\}$ are 2D random variables, the resulting Markov chain is also ergodic except at $E = \tilde{\epsilon}$. Hence, in this case also a unique invariant measure exists on $\dot{\boldsymbol{R}}$ [13]. From these established results we conclude that when both $\{\epsilon_n\}$ and $\{V_{n,n+1}\}$ are 2D random variables, the resulting Markov chain also consists of persistent non-null states. So, again a unique invariant measure will exist on $\dot{\boldsymbol{R}}$.

To apply these results to correlated disordered systems some modifications are needed. In order to introduce the required modifications, we first describe the model. The model considered here is a random binary mixture of two types of cluster. Each cluster contains $q \geqslant 2$ elements. In the host cluster all elements are assumed to be the same while in the guest cluster at least one element, if not all, should be distinct from the host element. All site energies and nearest neighbour hopping integrals in the host cluster are set to zero and unity, respectively, without any loss of generality. In the guest cluster site energies and nearest neighbour hopping integrals are allowed to be different. We further assume that the hopping integrals between the end sites of any two clusters are unity. So, diagonal and off-diagonal elements in our model are not totally random. Instead each category is required to satisfy q constraint relations:

$$\tilde{\epsilon}_{qm+l-1} = [\epsilon_{l-1} p_{qm} + \epsilon_{q-l}(1 - p_{qm})]e_{qm} \tag{11}$$

and

$$\tilde{V}_{qm+l,qm+l-1} = 1 - [1 - (V_{l,l-1} p_{qm} + V_{q-1-l,q-l}(1 - p_{qm}))](1 - \delta_{q,l})e_{qm} \tag{12}$$

where $1 \leqslant l \leqslant q$ and $qm \in Z$. The randomness in the model is, therefore, introduced through two Rademacher variables, e_{qm}, $p_{qm} \in \{0, 1\}$. These variables by construction are indeed 2D random variables. Rademacher variables, $\{p_{qm}\}$, are introduced to take into account the asymmetry of the guest cluster. Since a cluster can take only two possible orientations in the lattice, two possible values of $\{p_{qm}\}$, namely zero and unity, occur with probability $\frac{1}{2}$.

Since diagonal elements of H here determine the strength of hopping to and from the sites, the off-diagonal elements are not truly random. In essence this model is similar to the Anderson model of uncorrelated site disorder. However, due to constraints on diagonal and off-diagonal elements of H, $\{Z_n\}$ as such do not form a Markov chain. To form the required Markov chain we need to consider the clusters as unit cells. In other words, we need to define a new random variable $\{X_n\}$ such that

$$\begin{aligned} x_{n+1} &= z_{q(m+1)} \\ &= \prod_{l=1}^{q} \xi_{E,\epsilon_{q(m+1)-l},\tilde{V}_{q(m+1)-l,q(m+1)-(l+1)}}(x_n) \\ &= \boldsymbol{P}_{E,q}(x_n) \end{aligned} \tag{13}$$

We note that in the product of the operators in equation (13), the operator with the lower value of l comes to the left. The Markov chain defined by the random variable, $\{X_n\}$, is ergodic and according to Frustenberg's theorem, a unique invariant measure $\mathrm{d}\nu_E(x)$ for this process will exist on $\dot{\boldsymbol{R}}$. Furthermore, this measure will have density, i.e. $\mathrm{d}\nu_E(x) = \phi_E(x)\,\mathrm{d}x$, when $\phi_E(x) \in L^1_+(\dot{\boldsymbol{R}}, \mathrm{d}x)$. In other words $\phi_E(x)$ belongs to the class of non-negative Lebesgue integrable functions on the compactified real line.

3. Equations for the invariant measure $\phi_E(x)$, the Lyapunov exponent and the integrated density of states

Before defining the equation for determining $\phi_E(x)$, we define an operator ${}^{V_0}T_E$ such that

$$({}^{V_0}T_E f)(x) = \frac{V_0^2}{(E - x)^2} f\left(\frac{V_0^2}{E - x}\right). \tag{14}$$

This is the logical extension of the definition given by Bovier and Klein [12]. This generalization is useful for the more general problem as can be seen in the forthcoming discussion. Some important properties of ${}^{V_0}T_E$ which will be used here are

(i) ${}^{V_0}T_{E-v}\,{}^{V_0}T_{E-u} = T_{E-v}T_{\frac{E-u}{V_0^2}}$

(ii) ${}^{V_0}T_E^{-1}\frac{\mathrm{d}}{\mathrm{d}x}\,{}^{V_0}T_E = \frac{1}{V_0^2}\frac{\mathrm{d}}{\mathrm{d}x}x^2$, including $E = 0$.

(iii) ${}^{V_0}T_0\,{}^{V_0}T_0 = \mathrm{I}$

(iv) ${}^{V_0}T_E = \mathrm{e}^{-E\frac{\mathrm{d}}{\mathrm{d}x}}\,{}^{V_0}T_0$

(v) $({}^{V_0}T_E^{-1}f)(x) = \frac{V_0^2}{x^2}f(E - \frac{V_0^2}{x})$.

If $\mathrm{d}\nu_E(x)$ defines the invariant measure with respect to the process described by $\{X_n\}$, introducing equation (13) in equation (10) we obtain

$$\int_{\dot{\boldsymbol{R}}} \mathrm{d}\nu_E(x)\, f(x) = \boldsymbol{E}\int_{\dot{\boldsymbol{R}}} \mathrm{d}\nu_E(x)\, f(\boldsymbol{P}_{E,q}(x)) \tag{15}$$

for all bounded measurable functions. As usual $\boldsymbol{E}$ denotes the expectation with respect to the probability distribution of $\{e_{qm}\}$ and $\{p_{qm}\}$. In our model calculations we take

$$P(e) = \tfrac{1}{2}\delta(e) + \tfrac{1}{2}\delta(e-1). \tag{16}$$

Since $\mathrm{d}\nu_E(x) = \phi_E(x)\,\mathrm{d}x$, introducing this relation in equation (15) and making an appropriate change of variables we obtain

$$\int_{\dot{\boldsymbol{R}}} \phi_E(x)\,\mathrm{d}x = \boldsymbol{E}\int_{\dot{\boldsymbol{R}}} \mathrm{d}x \prod_{l=1}^{q} {}^{\tilde{V}(q,l)}T_{E-\epsilon(q,l)}\phi_E(x) \tag{17}$$

where $\epsilon(q,l)$ and $\tilde{V}(q,l)$ are defined, respectively, by equations (11) and (12) by setting $p_{qm} = p$ and $e_{qm} = e$. Again in the product of these operators, the operator with the lower value of l comes to the left. Since equation (17) should hold good for any arbitrary bounded measurable function, f, we obtain after averaging over e and p

$$\phi_E(x) = \left[\tfrac{1}{2}T_E^q + \tfrac{1}{4}\prod_{l=1}^{q} {}^{V_{q-l,q-(l+1)}}T_{E-\epsilon_{q-l}} + \tfrac{1}{4}\prod_{l=1}^{q} {}^{V_{l-1,l}}T_{E-\epsilon_{l-1}}\right]\phi_E(x). \tag{18}$$

As an example we consider the SRTM. For this model $q = 3$, $\epsilon_2 = \epsilon_0 = v$ and $\epsilon_1 = u$. The hopping between nearest neighbours in the guest cluster is V_0. Since the cluster has a inversion symmetry, two products are identical. So, we have

$$\begin{aligned}\phi_E(x) &= \tfrac{1}{2}[T_E^3 + {}^{V_0}T_{E-v}\,{}^{V_0}T_{E-u}T_{E-v}]\phi_E(x)\\ &= \tfrac{1}{2}[T_E^3 + T_{E-v}T_{(E-u)/V_0^2}T_{E-v}]\phi_E(x).\end{aligned} \tag{19}$$

Before computing the complex Lyapunov exponent, $\tilde{\gamma}(E)$, we note that for disordered systems, including the systems under study, due to the subadditive ergodic theorem [13, 24] the limit in equation (6) exists and is independent of the realization of the disorder, for almost all realizations. In other words, $\tilde{\gamma}(E)$ is self-averaging,

$$\boldsymbol{E}\tilde{\gamma}(E) = \tilde{\gamma}(E) \tag{20}$$

where $\boldsymbol{E}$ denotes the ensemble average. For effective calculation of $\tilde{\gamma}(E)$, we first write

$$\tilde{\gamma}(E) = \lim_{N\to\infty}\tilde{\gamma}_N(E) \tag{21}$$

where $N = qM$ is the total number of sites in the chain. Since

$$\begin{aligned}z_{qm+l} &= \prod_{k=1}^{l}\xi_{E,\epsilon(q,l-k),\tilde{V}(q,l-k)}(z_{qm})\\ &= P_{E,l}(x_n)\end{aligned} \tag{22}$$

(see equation (13)), from equation (6) we obtain

$$\tilde{\gamma}_N(E) = \frac{1}{qM}\sum_{n=0}^{M}\ln x_n + \frac{1}{qM}\sum_{n=0}^{M}\sum_{l=1}^{q-1}\ln P_{E,l}(x_n) - \frac{1}{qM}\sum_{n=0}^{M}\ln\prod_{l=0}^{q-1}\tilde{V}_{qn+l,qn+l-1}. \tag{23}$$

The last term in equation (23) when averaged over all possible realizations of the sample (over e and p) yields

$$\left\langle \frac{1}{qM}\sum_{n=0}^{M}\ln\prod_{l=0}^{q-1}\tilde{V}_{qn+l,qn+l-1}\right\rangle_{e,p} = \frac{1}{2q}\ln\prod_{l=1}^{q-1}V_{l-1,l}. \tag{24}$$

In the limit $N\to\infty$ we apply the subadditive ergodic theorem to equation (23). This in turn yields

$$\tilde{\gamma}(E) = \frac{1}{q}\int_{\dot{\boldsymbol{R}}}\mathrm{d}v_E(x)\ \ln x + \frac{1}{q}\sum_{l=1}^{q-1}\boldsymbol{E}\int_{\dot{\boldsymbol{R}}}\mathrm{d}v_E(x)\ \ln P_{E,l}(x) - \frac{1}{2q}\ln\prod_{l=1}^{q-1}V_{l-1,l} \tag{25}$$

where $\boldsymbol{E}$ denotes the expectation over $\{e\}$ and $\{p\}$. Furthermore, introducing $\mathrm{d}v_E(x) = \phi_E(x)\,\mathrm{d}x$ and making an appropriate change of variables in the second integral of equation (25), we obtain

$$\tilde{\gamma}(E) = \frac{1}{q}\int_{\dot{\boldsymbol{R}}}\mathrm{d}x\ \phi_E(x)\ln x + \frac{1}{q}\sum_{l=1}^{q-1}\boldsymbol{E}\int_{\dot{\boldsymbol{R}}}\mathrm{d}x\ \ln x\prod_{m=0}^{l}{}^{\tilde{V}(q,l-m)}T_{E-\epsilon(q,l-m)}\phi_E(x)$$
$$-\frac{1}{2q}\ln\prod_{l=1}^{q-1}V_{l-1,l}. \tag{26}$$

We again point out that in the product of the operators, the operator with the lowest value of m comes to the left. Furthermore, the product terminates at $m=l$. Equation (26) when averaged over e and p yields

$$\tilde{\gamma}(E) = \frac{1}{q}\int_{\dot{\boldsymbol{R}}}\mathrm{d}x\ \phi_E(x)\ln x + \frac{1}{2q}\sum_{l=1}^{q-1}\int_{\dot{\boldsymbol{R}}}\sum_{l=1}^{q-1}\mathrm{d}x\ \ln x T_E^l\phi_E(x)$$
$$+\frac{1}{4q}\sum_{l=1}^{q-1}\int_{\dot{\boldsymbol{R}}}\mathrm{d}x\ \ln x\prod_{m=1}^{l}{}^{V_{l-m,l-m-1}}T_{E-\epsilon_{l-m}}\phi_E(x)$$
$$+\frac{1}{4q}\sum_{l=1}^{q-1}\int_{\dot{\boldsymbol{R}}}\mathrm{d}x\ \ln x\prod_{m=1}^{l}{}^{V_{q-1-l+m,q-l+m}}T_{E-\epsilon_{q-l+m-1}}\phi_E(x)$$
$$-\frac{1}{2q}\ln\prod_{l=1}^{q-1}V_{l-1,l}. \tag{27}$$

Before applying equation (27) to the SRTM we first observe that

$$\int_{\dot{\boldsymbol{R}}}\mathrm{d}x\ \ln x\,{}^{V_0}T_{E-u}T_{E-v}\phi_E(x) - \ln V_0^2 = \int_{\dot{\boldsymbol{R}}}\mathrm{d}x\ \ln x T_{\frac{(E-u)}{V_0^2}}T_{E-v}\phi_E(x). \tag{28}$$

Decomposing the complex Lyapunov exponent $\tilde{\gamma}(E)$ to real and imaginary parts, we obtain for the IDOS, $N(E)$ of the SRTM

$$N(E) = 1 - \frac{1}{\pi}\,\mathrm{Im}\,\tilde{\gamma}(E)$$
$$= 1 - \tfrac{1}{6}\int_{-\infty}^{0-}\mathrm{d}x\,[2 + T_E + T_E^2 + T_{E-v} + T_{\frac{(E-u)}{V_0^2}}T_{E-v}]\phi_E(x). \tag{29}$$

Furthermore, for the Lyapunov exponent $\gamma(E)$ we get

$$\gamma(E) = \mathrm{Re}\,\tilde{\gamma}(E) = \tfrac{1}{6}\int_{-\infty}^{\infty} \mathrm{d}x\ \ln y(x)[T_{E-v}T_{\frac{(E-u)}{V_0^2}}T_{E-v} - T_E]\phi_E(x)$$
$$+\tfrac{1}{6}\int_{-\infty}^{\infty} \mathrm{d}x\ \ln|x|[T_{E-v} + T_{\frac{(E-u)}{V_0^2}}T_{E-v}]\phi_E(x). \tag{30}$$

To obtain the first integral of equation (30) we define $y(x) = \sqrt{x^2 - Ex + 1}$ so that $|x| = y(x)/y(E - \frac{1}{x})$. This in turn yields

$$\ln|x| = \ln y(x) - \ln y\left(E - \frac{1}{x}\right) \tag{31}$$

and the integral decomposes into two integrals. In the second integral we replace x by $1/(E - x)$ so that $y(E - \frac{1}{x}) \to y(x)$. Then we combine these integrals and introduce the governing equation of $\phi_E(x)$ (equation (19)) [17] for the final result. We further note that the effect of the guest cluster on $\gamma(E)$ appears in the second integral of equation (30). So the transformation required for this integral will depend on the structure of the guest cluster. For example, consider the example of the RBA. Here, $v = 0$ and $u = (1 - V_0^2)\omega$. For this case we simply introduce equation (31) in equation (30) and after the needful amount of algebra we obtain

$$\gamma(E) = \tfrac{1}{6}\int_{-\infty}^{\infty} \mathrm{d}x\ \ln y(x)(T_{\frac{(E-u)}{V_0^2}} - T_E)T_E\phi_E(x). \tag{32}$$

Equation (32) immediately yields $\gamma(\omega) = 0$, confirming the result of [6]. As a second example, we consider $u = (1+V_0^2)v$ in the SRTM. In this case the system has an exceptional energy at $E = v$. To obtain the behaviour of $\gamma(E)$ in the neighbourhood of v we transform equation (30) to

$$\gamma(E) = \tfrac{1}{6}\int_{-\infty}^{\infty} \mathrm{d}x\ \ln y(x)[T_{E-v}T_{\frac{(E-u)}{V_0^2}}T_{E-v} - T_E]\phi_E(x)$$
$$-\tfrac{1}{6}\int_{-\infty}^{\infty} \mathrm{d}x\ \ln y(x)[1 - T_E]T_0[T_{E-v} + T_{\frac{(E-u)}{V_0^2}}T_{E-v}]\phi_E(x). \tag{33}$$

Since $T_0^2 = \mathrm{I}$ and $T_0T_{-v}T_0 = T_v^{-1}$, from equation (33) we obtain $\gamma(v) = 0$ which is in agreement with the result in [7]. When $V_0 = 1$, this system also has another exceptional energy at $E = 2v$. The calculation of $\gamma(E)$ for this case is facilitated by converting equation (30) to

$$\gamma(E) = \tfrac{1}{6}\int_{-\infty}^{\infty} \mathrm{d}x\ \ln y(x)[T_{E-v}T_{E-2v}T_{E-v} - T_E]\phi_E(x)$$
$$+\tfrac{1}{6}\int_{-\infty}^{\infty} \mathrm{d}x\ \ln|x|[T_{E-v} - T_0T_{E-2v}T_{E-v}]\phi_E(x). \tag{34}$$

We note that when $E = 2v$, $T_{E-v}T_{E-2v}T_{E-v} = T_vT_0T_v = T_{2v}$ and $T_0T_{E-2v}T_{E-v} = T_v$. So, $\gamma(2v) = 0$. This result has also been obtained in [7]. There is another important motivation behind bringing $\ln y(x)$ in the integrals. When $E = 2\cos\alpha\pi$, these integrals can be easily carried out by mapping the compactified real line on the circumference of a circle of circumference $\pi(S_1)$ through the transformation

$$x = \frac{\sin(\theta + \alpha\pi)}{\sin\theta} \tag{35}$$

when $x \in \dot{\boldsymbol{R}}$ and $\theta \in S_1$. As will be shown later, this transformation will also simplify the perturbative calculation of $\phi_E(x)$.

4. Exceptional energy

For the purpose of clarity we discuss this aspect in reference to the SRTM. We have already obtained the governing equation of $\phi_E(x)$ for this model (equation (19)). We note that for the RBA, at $E = \omega$ equation (19) reduces to

$$\phi_\omega(x) = T_\omega^3 \phi_\omega(x). \tag{36}$$

For the SRTM with $u = (1 + V_0^2)v$ we obtain at $E = v$

$$\phi_v(x) = \tfrac{1}{2}[T_v^3 + T_v^{-1}]\phi_v(x) \tag{37}$$

and for $V_0 = 1$ at $E = 2v$, we get

$$\begin{aligned}\phi_{2v}(x) &= \tfrac{1}{2}[T_{2v}^3 + T_v T_0 T_v]\phi_{2v}(x) \\ &= \tfrac{1}{2}[T_{2v}^2 + \mathrm{I}]T_{2v}\phi_{2v}(x).\end{aligned} \tag{38}$$

We note now that $T_E f = f$ always has the normalized solution

$$f_E(x) = \frac{1}{\pi}\frac{\sqrt{1 - E^2/4}}{x^2 - Ex + 1} \tag{39}$$

and $f(x) \in L_+^1(\dot{R}, \mathrm{d}x)$ iff $|\frac{E}{2}| \leqslant 1$. For $E = 2\cos\alpha\pi$, if α is irrational, this solution is unique. On the other hand for $\alpha = p/q$ with p and q prime integers, there exists infinitely many others [7]. But this has no serious implication in our calculation.

It is important to note that the solution $\phi_E(x)$ of equations (36)– (38) is $f_{E_S}(x)$ when $E_S = \omega$, v or $2v$. Keeping this in mind, we define the exceptional energy as the energy at which $\phi_{E_S} = f_{E_S}(x)$. This definition also has a physical origin. Consider two periodic structures, one from the host cluster and the other from the guest cluster. The periodic system from the guest cluster will in principle form q bands. Intersection of the DOS of any one of these bands with the DOS of the periodic system from the host cluster determines the exceptional energy (E_S). Since the invariant measure density of the host system is given by equation (39), the definition ensues. Then, to derive the equation for exceptional energies of the SRTM we need to solve

$$f_E(x) = T_{E-v} T_{\frac{(E-u)}{V_0^2}} T_{E-v} f_E(x). \tag{40}$$

It is relevant at this point to note that if

$$g(x) = \frac{1}{\pi}\frac{a}{(x-b)^2 + a^2} \tag{41}$$

then $T_E g(x)$ is also another Lorentzian distribution centred at b_1 with a half-width a_1, where

$$b_1 + \mathrm{i}a_1 = E - \frac{1}{b + \mathrm{i}a}. \tag{42}$$

Hence, from equation (40) we obtain

$$S = E - v - \frac{1}{\frac{E-u}{V_0^2} - \frac{1}{E-v-\frac{1}{S}}} \tag{43}$$

where $S = \frac{E}{2} + \mathrm{i}\sqrt{1 - E^2/4}$. Equation (43) in turn yields a quadratic equation in S. The required equation is obtained from either $\mathrm{Re}\, S = \frac{E}{2}$ or from $\mathrm{Im}\, S = \sqrt{1 - E^2/4}$. Both will yield identical equations. This procedure for the SRTM yields

$$v(E_S - v)^2 - [v(u - v) + (1 - V_0^2)](E_S - v) + [u - (1 + V_0^2)v] = 0. \tag{44}$$

This equation has already been obtained in [7] by considering the reflection coefficient of a single guest cluster embedded in the host lattice. Full analysis of this equation can also be found there. We note that for $v = 0$ and $u = (1 - V_0^2)\omega$, from equation (44) we obtain $E_S = \omega$. On the other hand if we take $u = (1 + V_0^2)v$, from equation (44) we obtain $E_{s_1} = v$ and $E_{s_2} = (1 + V_0^2)v + (1 - V_0^2)/v$. From these we can immediately see that two exceptional energies in this case will merge at v if $V_0^2 = \frac{1}{1-v^2}$. For $V_0 = 1$, a similar situation can be obtained by setting $u = [v + \frac{2[1-\sqrt{1-v^2}]}{v}]$ and $|v| \leqslant 1$. For this case, two exceptional energies will coincide at $E_S = (u + v)/2$.

We further note that the procedure outlined here can be applied to complicated one-dimensional chains like polyaniline, polythiophene, etc. We first need to apply the real space renormalization procedure to these systems to obtain effective one-dimensional chains [9]. Then we can apply this procedure for finding exceptional energies in these systems.

When the guest cluster is asymmetric $f_E(x)$ has to satisfy two equations for two different orientations of the cluster. This in turn will yield two equations for S, and these need to be identical. This develops further constraints in the parameter space. Because of this extra constraint on the equation for S, the probability of obtaining exceptional energies with an asymmetric guest cluster, particularly if the cluster size is relatively large, is negligible. One example of an asymmetric guest cluster having an exceptional energy has been worked out in [7]. This shows the importance of symmetry in the guest cluster for obtaining exceptional energies. This aspect has also been discussed in [6].

5. The perturbative calculation of the invariant measure density, $\phi_E(x)$, around the exceptional energy, E_S, for the SRTM

The procedure for the calculation is well documented in the literature. For $E = 2\cos\alpha\pi$, the calculation is facilitated by the transformation given by equation (35). Hence, for the invariant measure density we should have

$$\phi_E(x)\,\mathrm{d}x = h_E(\theta)\,\mathrm{d}\theta. \tag{45}$$

We define an operator J_α such that

$$(J_\alpha\phi_E)(\theta) = \phi_E(x)\frac{\mathrm{d}x}{\mathrm{d}\theta} = h_E(\theta). \tag{46}$$

We also define another operator, $\tau_\alpha = J_\alpha T_E J_\alpha^{-1}$, such that

$$(\tau_\alpha g)(\theta) = g(\theta - \alpha\pi). \tag{47}$$

Furthermore, if $g(x) = \frac{\mathrm{d}f(x)}{\mathrm{d}x}$, we then have

$$(J_\alpha G)(\theta) = g(x)\frac{\mathrm{d}x}{\mathrm{d}\theta} = \frac{\mathrm{d}}{\mathrm{d}\theta}\frac{\mathrm{d}\theta}{\mathrm{d}x}(J_\alpha\hat{f})(\theta) \tag{48}$$

where $(J_\alpha\hat{f})(\theta) = f(x)\frac{\mathrm{d}x}{\mathrm{d}\theta}$. It then follows that

$$J_\alpha\frac{\mathrm{d}}{\mathrm{d}x}J_\alpha^{-1} = \frac{\mathrm{d}}{\mathrm{d}\theta}\frac{\mathrm{d}\theta}{\mathrm{d}x} = -\frac{\mathrm{d}}{\mathrm{d}\theta}\frac{\sin^2\theta}{\sin\alpha\pi}. \tag{49}$$

We now consider the RBA and put $E = \omega + \lambda$. It is transparent from equation (19) that the perturbative calculation will be less cumbersome if we replace ω by $(E - \lambda)$. This yields

$$\phi_{E,\epsilon}(x) = \tfrac{1}{2}[T_E^3 + T_E T_{E-\epsilon} T_E]\phi_{E,\epsilon}(x) \tag{50}$$

when $\epsilon = -\lambda(1 - V_0^2)/V_0^2$. So the problem effectively reduces to the calculation of the invariant measure density of a random binary mixture of two trimeric clusters. The central energy of the guest cluster is ϵ and all nearest neighbour hoppings are unity. We again emphasize that we are seeking $\phi_{E,\epsilon}(x) \in L_+^1(\dot{\boldsymbol{R}}, \mathrm{d}x)$ for $|E| < 2$. To obtain the perturbative solution of $\phi_{E,\epsilon}(x)$ around $\epsilon = 0$, we write

$$\phi_{E,\epsilon}(x) = \sum_{n=0}^{\infty} \frac{\epsilon^n}{n!} \phi_E^{(n)}(x) \tag{51}$$

and $\phi_E^{(n)}(x)$ satisfies $\int_{\dot{\boldsymbol{R}}} \phi_E^{(n)}(x)dx = \delta_{n,0}$. We further note that $\phi_E^0(x) = \frac{1}{2\pi} \frac{\sqrt{4-E^2}}{x^2-Ex+1}$. So,

$$h_E^0(\theta) = \phi_E^0(x) \frac{\mathrm{d}x}{\mathrm{d}\theta} = -\frac{\mathrm{sgn}(\alpha\pi)}{\pi} \tag{52}$$

when $\mathrm{sgn}(\alpha\pi)$ is positive or negative depending on whether α is positive or negative. We know that according to Anderson's theorem, all eigenstates of the system will be exponentially localized for $|\epsilon| > 0$. Furthermore, the Lyapunov exponent, $\gamma(E)$, is the inverse localization length of the eigenstate at E. So, physically $\gamma_\epsilon(E) \geqslant 0$ for $E \in (-2, 2)$. We also know that $\gamma_\epsilon(E)$ is a continuous function of ϵ particularly if $|\epsilon| \ll 1$. So, we can expand $\gamma_{\epsilon_s}(E)$ in a Taylor series around $\epsilon = 0$ to obtain

$$\gamma_\epsilon(E) = \sum_{n=0}^{\infty} \frac{\epsilon^n}{n!} \gamma_n(E). \tag{53}$$

Since $\gamma_0(E) = 0$, $\gamma(E)$ reaches the minimum value at $\epsilon = 0$. So for $|E| < 2$, we must have $\gamma_1(E) = 0$ and the leading order term in the Taylor expansion will be $\mathrm{O}(\epsilon^2)$ with $\gamma_2(E) > 0$. We also note in this context that when $|E| = 2$, although $\gamma_0(E) = 0$, the analytical continuation of $\gamma(E)$ for $|E| > 2$ will, however, yield negative $\gamma(E)$. This naturally follows from the constraint on $\phi_E(x)$. So, in this case $\gamma_1(E)$ will be non-zero. We also see from equation (32) that $\gamma_m(E)$ has no contribution from $\phi_E^{(m)}(x)$. So to calculate the leading order term of $\gamma_\epsilon(E)$, the knowledge of $\phi_E^{(1)}(x)$ will suffice. Similarly for the density of states at E_S, we do not need more than $\phi_E^{(1)}(x)$ (see equation (29)). From equations (50) and (51) for $(J_\alpha \phi_E^{(1)})(\theta) = h_E^{(1)}(\theta)$ we obtain

$$(\mathrm{I} - \tau_\alpha^3) h_E^{(1)}(\theta) = -\frac{1}{2} \frac{\mathrm{d}}{\mathrm{d}\theta} \frac{\sin^2(\theta - \alpha\pi)}{\sin\alpha\pi} \tau_\alpha^3 h_E^0(\theta) \tag{54}$$

The procedure for solving this type of equation is to expand $h_E^n(\theta)$ in the Fourier series in $(\frac{-\pi}{2}, \frac{\pi}{2})$ and then calculate the coefficients from the governing equation. This procedure when applied to equation (54) yields

$$h_E^{(1)}(\theta) = \frac{(-1)}{4\pi} \frac{\cos(2\theta + \alpha\pi)}{|\sin\alpha\pi| \sin 3\alpha\pi}. \tag{55}$$

The second case that we consider is $V_0 = 1$ and $u = 2v$. Here, v and $2v$ are exceptional energies and we have already shown that $\gamma(E_S) = 0$ for $E_S = v$ and $2v$ (see equations (33) and (34)). Since $E_S = E - \lambda$, from equation (19) we get for $|v| \leqslant 1$

$$\phi_{E(E_S),\lambda}(x) = \tfrac{1}{2}[T_E^3 + T_{E-\Sigma_1} T_{E-\Sigma_2} T_{E-\Sigma_1}] \phi_{E(E_S),\lambda}(x) \tag{56}$$

where $\Sigma_1 = E - \lambda$ and $\Sigma_2 = 2(E - \lambda)$ if $E_S = v$. On the other hand, for $E_S = 2v$, we have $\Sigma_1 = \frac{E-\lambda}{2}$ and $\Sigma_2 = E - \lambda$. So here the effective site energies of the guest cluster depend on the energy under consideration. When viewed from a broader perspective, such a situation does arise in the analysis of complex one-dimensional chains like polyaniline, polythiophene etc. But the situation there is a bit more complex. In relation to the localization of

eigenstates, arguments presented for the previous example also hold good here. States which are delocalized for $\lambda = 0$ will be exponentially localized for $\lambda \neq 0$. Again, the Lyapunov exponent, $\gamma_\lambda(E)$, is expected to be $O(\lambda^2)$. So, to obtain the first order term in the perturbative calculation of $\phi_{E(E_S),\lambda}(x)$, we write

$$(J_\alpha \phi_{E(E_S),\lambda})(\theta) = h_{E(E_S),\lambda} = \sum_{n=0}^{\infty} \frac{\lambda^n}{n!} h^{(n)}_{E(E_S)}(\theta). \tag{57}$$

Then from equations (56) and (57) for $E_S = v$ and $2v$ we get

$$(\mathrm{I} - 2\tau_\alpha + \tau_\alpha^4) h^{(1)}_{E(v)}(\theta) = \frac{E^2}{\pi |\sin \alpha\pi|} \sin 2\theta \tag{58}$$

and

$$(2 - \tau_\alpha^3 - \tau_\alpha) h^{(1)}_{E(2v)}(\theta) = -\frac{E^2 \sin 2\theta}{4\pi |\sin \alpha\pi|} \tag{59}$$

respectively. Since we plan to calculate only the IDOS for these cases, we solve for a new function, $f_{E(E_S)}(\theta)$. For $E_S = v$ and $2v$

$$f_{E(v)}(x) = [\mathrm{I} - T_E - {T_E}^2 - {T_E}^3] \phi^{(1)}_{E(v)}(x) \tag{60}$$

and

$$f_{E(2v)}(x) = [2 + T_E + {T_E}^2] \phi^{(1)}_{E(2v)}(x). \tag{61}$$

Now from the governing equation of $h_{E(E_S)}(\theta)$ (i.e. equations (58) and (59)) we find that

$$(\mathrm{I} - \tau_\alpha) \hat{f}_{E(E_S)}(\theta) = \frac{E^2 \sin 2\theta}{C(E_S)\pi |\sin \alpha\pi|} \tag{62}$$

when $C(S) = 1$ and -4 for $E_S = v$ and $2v$, respectively. This equation (62) can be solved by the standard procedure and we obtain

$$f_{E(E_S)}(x) = (J_\alpha \hat{f}_{E(E_S)})(0) = \frac{E^3}{4C(E_S) \sin^2 \alpha\pi} \phi^0_E(x) - \frac{E^3 \pi}{2C(E_S) |\sin \alpha\pi|} {\phi^0_E}^2(x) + \frac{E^2}{2C(E_S)} \frac{\mathrm{d}}{\mathrm{d}x} \phi^0_E(x). \tag{63}$$

Finally we note that when $u = (1 + V_0^2)v$ and $V_0^2(1 - v^2) = 1$, two exceptional energies merge at $E = v$ ($\gamma(v) = 0$ (equation (33)). For this case the equation for $\tilde{h}_{E(v),\lambda}(\theta)$ ($\tilde{}$ denotes the merging of two E_S's) is

$$(\mathrm{I} - 2\tau_\alpha + \tau_\alpha^4) \tilde{h}^{(1)}_{E(v)}(\theta) = 0. \tag{64}$$

The solution for this equation is $\tilde{h}^{(1)}_{E(v)}(\theta) = \text{constant}$. Since

$$\int_{-\pi/2}^{\pi/2} \tilde{h}_{E(v),\lambda}(\theta)\, \mathrm{d}\theta = \int_{-\pi/2}^{\pi/2} \tilde{h}^{(0)}_{E(v)}(\theta)\, \mathrm{d}\theta = 1 \tag{65}$$

by construction, we need

$$\tilde{h}^{(1)}_{E(v)}(\theta) = 0 \tag{66}$$

to satisfy the constraint imposed by equation (65).

6. Calculation of the Lyapunov exponent

We consider here the RBA and the SRTM with a degenerate exceptional energy. We choose the first problem because the guest cluster has different hopping elements inside it. On the other hand, the second problem allows us to investigate analytically the effect of a degenerate exceptional energy on $\gamma(E)$ and the IDOS.

6.1. The RBA

Since $T_{E-\epsilon} = \mathrm{e}^{\epsilon \frac{\mathrm{d}}{\mathrm{d}x}} T_E$, from equations (32) and (55) we obtain

$$\gamma_1(E) = \frac{1}{6}\int_{-\infty}^{\infty} \mathrm{d}x\ \ln y(x) \frac{\mathrm{d}}{\mathrm{d}x}\phi_E^0(x) = 0 \tag{67}$$

and

$$\begin{aligned}\gamma_2(E) &= \frac{1}{6}\int_{-\infty}^{\infty} \mathrm{d}x\ \ln y(x) \left(\frac{\mathrm{d}}{\mathrm{d}x}\right)^2 \phi_E^0(x) + \frac{1}{3}\int_{-\infty}^{\infty} \mathrm{d}x\ \ln y(x) \frac{\mathrm{d}}{\mathrm{d}x} T_E^2 \phi_E^1(x) \\ &= \frac{1}{6\pi \sin^2 \alpha\pi} \int_{-\pi/2}^{\pi/2} \mathrm{d}\theta\, [\ln|\sin\alpha\pi| - \ln|\sin\theta|](\cos 2\theta - \cos 4\theta) \\ &\quad - \frac{1}{3\pi|\sin\alpha\pi|}\int_{-\pi/2}^{\pi/2} \mathrm{d}\theta\, [\ln|\sin\alpha\pi| - \ln|\sin\theta|] \frac{\mathrm{d}}{\mathrm{d}\theta} \sin^2\theta\, \tau_\alpha^2 h_E^{(1)}(\theta) \\ &= \frac{1}{12(4-E^2)}.\end{aligned} \tag{68}$$

So for this case we have

$$\gamma(\omega + \lambda) \sim \frac{\lambda^2(1-V_0^2)^2}{24V_0^4(4-\omega^2)} + \mathrm{O}(\lambda^3) \tag{69}$$

when $|\omega| < 2$.

6.2. The SRTM with degenerate exceptional energy

We define an operator, $\tilde{\boldsymbol{O}}(E,\lambda)$, which is the total operator operating on $\phi_E(v)(x)$ in equation (33):

$$\tilde{\boldsymbol{O}}(E,\lambda) = T_\lambda T_{-E+\lambda f(E,\lambda)} T_\lambda - T_E - (1-T_E)T_0[T_\lambda - T_{-E+\lambda f(E,\lambda)}T_\lambda] \tag{70}$$

where $f(E,\lambda) = 2 - E^2 + 2E\lambda + \lambda^2$. To expand $\tilde{\boldsymbol{O}}(E,\lambda)$ around $\lambda = 0$, we write

$$\tilde{\boldsymbol{O}}(E,\lambda) = \sum_{n=0}^{\infty} \lambda^n \boldsymbol{O}_n(E). \tag{71}$$

Now using the standard procedure, we obtain

$$\boldsymbol{O}_0(E) = 0 \tag{72}$$

$$\boldsymbol{O}_1(E) = -\left[\frac{\mathrm{d}}{\mathrm{d}x}(T_E + T_E^{-1} + (2-E^2)\mathrm{I}\right] \tag{73}$$

$$\begin{aligned}\boldsymbol{O}_2(E) &= \frac{1}{2}\left(\frac{\mathrm{d}}{\mathrm{d}x}\right)^2 [T_E - T_E^{-1} + (2-E^2)^2\mathrm{I}] - 2E\frac{\mathrm{d}}{\mathrm{d}x} + (2-E^2)\frac{\mathrm{d}}{\mathrm{d}x}\frac{\mathrm{d}}{\mathrm{d}x}x^2 \\ &\quad + \frac{2\sqrt{1-E^2/4}}{\pi}\frac{\mathrm{d}}{\mathrm{d}x}\frac{\mathrm{d}}{\mathrm{d}x}\frac{1}{\phi_E^0(x)}T_E^{-1}.\end{aligned} \tag{74}$$

From equations (33) and (66) we find that

$$\gamma_1(E) = -\frac{4-E^2}{6}\int_{-\infty}^{\infty} \mathrm{d}x\ \ln y(x)\frac{\mathrm{d}}{\mathrm{d}x}\phi_E^0(x) = 0 \tag{75}$$

and

$$\begin{aligned}\gamma_2(E) = {} & \frac{1}{6}(2-E^2)^2\int_{-\infty}^{\infty}\mathrm{d}x\ \ln y(x)\left(\frac{\mathrm{d}}{\mathrm{d}x}\right)^2\phi_E^0(x) - \frac{2}{3}\int_{-\infty}^{\infty}\mathrm{d}x\ \ln y(x)\frac{\mathrm{d}}{\mathrm{d}x}\phi_E^0(x) \\ & + \frac{(2-E^2)}{3}\int_{-\infty}^{\infty}\mathrm{d}x\ \ln y(x)\frac{\mathrm{d}}{\mathrm{d}x}\frac{\mathrm{d}}{\mathrm{d}x}x^2\phi_E^0(x) \\ = {} & \frac{(2-E^2)^2}{6\pi\sin^2\alpha\pi}\int_{-\pi/2}^{\pi/2}\mathrm{d}\theta\,[\ln|\sin\alpha\pi| - \ln|\sin\theta|](\cos 2\theta - \cos 4\theta) \\ & + \frac{(2-E^2)}{3\pi|\sin\alpha\pi|}\int_{-\pi/2}^{\pi/2}\mathrm{d}\theta\,[\ln|\sin\alpha\pi| - \ln|\sin\theta|] \\ & \times[\cos 2(\theta+\alpha\pi) - \cos(4\theta+2\alpha\pi)] \\ = {} & 0. \end{aligned} \tag{76}$$

Since $\gamma_2(v) = 0$ for this case, in principle further calculation is needed to find the leading non-zero term in the expansion of $\gamma(E)$. However, the leading term can be obtained through a simple argument. For any arbitrary V_0, the original system will yield two exceptional energies, E_{S_1} and E_{S_2} provided $|E_{S_i}| \leqslant 2$ for $i = 1, 2$. If $|v| \leqslant 1$, so that V_0^2 is positive, for E_{S_2} to be the second exceptional energy we need

$$\frac{1-|v|}{1+|v|} \leqslant V_0^2 \leqslant \frac{1+|v|}{1-|v|}. \tag{77}$$

Now from equation (30) we find that

$$\begin{aligned}\gamma(E_{S_2}) = {} & \tfrac{1}{6}\int_{-\infty}^{\infty}\mathrm{d}x\ \ln|x|[T_{E_{S_2}-v} + T^{-1}_{E_{S_2}-v}]\phi^0_{E_{S_2}}(x) \\ = {} & 0. \end{aligned} \tag{78}$$

Furthermore, $\gamma(v) = 0$. Since $\gamma(E)$ reaches the minimum value at v and E_{S_2}, it must possess a maximum in between these points. As we bring E_{S_2} towards v by tuning V_0, this maximum also moves towards v and the value of $\gamma(E)$ at the maximum simultaneously reduces. In the limit when $V_0^2(1-v^2) = 1$, two minima and a maximum merge at v. So it is an inflection point of $\gamma(E)$ and $\frac{\mathrm{d}^2\gamma}{\mathrm{d}E^2}|_{E=v}$ should be zero. This is precisely obtained. Since for $|v| < 2$, $\gamma(v)$ must be a positive semidefinite quantity with the leading order term determining the sign, $\frac{\mathrm{d}^3\gamma}{\mathrm{d}E^3}|_{E=v}$ must be zero and we should have $\gamma(E) \sim (E-v)^4$. This prediction can be tested by rigorous calculation. We shall, however, present an alternative justification. Since, around the exceptional energies, the system behaves like a weak disordered system, around these energies $\gamma(E) \sim |r(E)|^2$, when $|r(E)|^2$ is the reflection coefficient of a simple guest cluster in the host lattice [7]. For this system $|r(E)|^2$ can be found in [7]. The Taylor series expansion of $|r(E)|^2$ around v for $|v| < 2$ yields

$$|r(E)|^2 \sim \frac{v^2(1-v^2)^2}{(4-v^2)}(E-v)^4 + \mathrm{O}[(E-v)^5] \tag{79}$$

This is consistent with our arguments.

Before concluding this section we show that for the SRTM with $V_0^2 = 1$, $u = 2v$ and $|v| < 1$, $\gamma_1(v)$ and $\gamma_2(2v)$ are indeed zero. Consider first the case of v. From equation (33)

we obtain

$$\gamma_1(E) = -\frac{1}{6}\int_{-\infty}^{\infty} \mathrm{d}x\ \ln y(x)\frac{\mathrm{d}}{\mathrm{d}x}[T_E^{-1} + T_E + 2]\phi_E^0(x)$$
$$= -\frac{2}{3}\int_{-\infty}^{\infty} \mathrm{d}x\ \ln y(x)\frac{\mathrm{d}}{\mathrm{d}x}\phi_E^0(x)$$
$$= 0. \tag{80}$$

On the other hand for $2v$, from equation (34) we obtain

$$\gamma_1(E) = -\frac{1}{12}\int_{-\infty}^{\infty} \mathrm{d}x\ \ln y(x)\frac{\mathrm{d}}{\mathrm{d}x}\left[T_E^{-1} + T_E + 2\left(\frac{E}{2} - x\right)^2 T_E\right]\phi_E^0(x)$$
$$+\frac{\lambda}{6}\int_{-\infty}^{\infty} \mathrm{d}x\ \ln|x|\frac{\mathrm{d}}{\mathrm{d}x}x^2 T_{E/2}\phi_E^0(x)$$
$$= -\frac{E^2}{24}\int_{-\infty}^{\infty} \mathrm{d}x\ \ln y(x)\frac{\mathrm{d}}{\mathrm{d}x}\phi_E^0(x) - \frac{1}{6}\left(1 - \frac{E^2}{4}\right)\int_{-\infty}^{\infty} \mathrm{d}x\ \ln|x|\frac{\mathrm{d}}{\mathrm{d}x}T_{E/2}\phi_E^0(x)$$
$$= 0. \tag{81}$$

This is so because both integrals involve an odd function of x. Hence, around $E_S = v$ and $2v$, $\gamma(E) \sim \frac{\gamma_2}{2}(E - E_S)^2$. The direct calculation of γ_2 for these cases, albeit possible, is however quite complicated. But as mentioned earlier, a good estimate of γ_2 can be obtained from the reflection coefficient of the single guest cluster.

7. Density of states at the exceptional energy

7.1. The RBA

From equation (29) we get

$$N(E = \omega + \lambda) = 1 - \int_{-\infty}^{0-} \mathrm{d}x\,\phi_E^0(x)$$
$$-\frac{\varepsilon}{3}\int_{-\infty}^{0-} \mathrm{d}x\ (\mathrm{I} + T_E + T_E^2)\phi_E^{(1)}(x) - \frac{\varepsilon}{6}\phi_E^0(0) + \mathrm{O}(\varepsilon^2). \tag{82}$$

Again from the governing equation of $h_E^{(1)}(\theta)$, i.e. equation (54), we obtain

$$\hat{f}_E(\theta) = (I + \tau_\alpha + \tau_\alpha^2)h_E^{(1)}(\theta)$$
$$= -\frac{\cos(2\theta - \alpha\pi)}{4\pi\,\sin\alpha\pi\,|\sin\alpha\pi|}. \tag{83}$$

This equation, in turn, yields

$$f(x) = \hat{f}_E(\theta)\frac{\mathrm{d}\theta}{\mathrm{d}x} = \frac{E}{8\sin^2\alpha\pi(E^2 - 1)}\phi_E^0(x) + \frac{1}{4(E^2 - 1)}\frac{\mathrm{d}}{\mathrm{d}x}\phi_E^0(x)$$
$$-\frac{E\pi}{4|\sin\alpha\pi|(E^2 - 1)}{\Phi_E^0}^2(x). \tag{84}$$

Required integrals for the calculation of $N(E)$ can be easily performed. The DOS at ω, $\rho(\omega)$ is

$$\rho(\omega) = \frac{\mathrm{d}N(E)}{\mathrm{d}E}|_{E=\omega}$$
$$= \frac{1}{\pi\sqrt{4 - \omega^2}} + \frac{(1 - V_0^2)}{6V_0^2\pi\sqrt{4 - \omega^2}}. \tag{85}$$

7.2. The SRTM with a degenerate exceptional energy

We have already shown in this case $\tilde{\phi}_E^{(1)}(x) = 0$. Furthermore, to obtain the DOS at $E = v$, we need the coefficient of $(E - v) = \lambda$ in the Taylor series expansion of $N(E)$. So, we write from equation (29)

$$N_0(E = v + \lambda) = 1 - \tfrac{2}{3}\int_{-\infty}^{0-} \phi_E^0(x)\,\mathrm{d}x - \tfrac{1}{6}\int_{-\infty}^{0-} \mathrm{d}x\,[T_{E-v} + T_{\frac{E-u}{V_0^2}}\,T_{E-v}]\phi_E^0(x)$$
$$= \frac{1}{2} + \frac{2}{3\pi}\tan^{-1}\frac{E}{\sqrt{4-E^2}} + \frac{1}{6\pi}\tan^{-1}\frac{E-2v}{\sqrt{4-E^2}} + \frac{1}{6\pi}\tan^{-1}\frac{b(E)}{a(E)} \tag{86}$$

where

$$b(E) = \frac{E-u}{V_0^2} - \frac{E-2v}{2(v^2 - Ev + 1)}$$

and

$$a(E) = \frac{\sqrt{4-E^2}}{2(v^2 - Ev + 1)}.$$

Now expanding $N_0(E)$ in the Taylor series around $E = v$, we get for the DOS, $\rho(v)$

$$\rho(v) = \frac{1}{\pi\sqrt{4-v^2}} - \frac{v^2}{6\pi\sqrt{4-v^2}}. \tag{87}$$

We consider now the case of the SRTM where $V_0^2 = 1$ and $u = 2v$, and $|v| < 1$. For this case the DOS at $E = v$ and $2v$ has been calculated numerically. We present here the analytical results. We write for these cases

$$N(E = E_S + \lambda) \approx N_0(E = E_S + \lambda) + \frac{\lambda}{6}N_1(E = E_S + \lambda) + \mathrm{O}(\lambda^2) \tag{88}$$

when $N_0(E = E_S + \lambda)$ is obtained from equation (86).

Furthermore,

$$N_1(E) = \int_{b(E)}^{\infty} \mathrm{d}x\, f_{E(E_S)}(x) \tag{89}$$

and $b(E) = E$ and 0 for $E_S = v$ and $2v$, respectively. $f_{E(E_S)}$ is given by equation (63). After performing the required integral and combining the coefficient of λ in the expansion of $N(E)$ we get

$$\rho(v) = \frac{1}{\pi\sqrt{4-v^2}} + \frac{v^2}{4\pi\sqrt{4-v^2}} + \frac{v^2(1-2v^2)}{24\pi\sqrt{4-v^2}} \tag{90}$$

and

$$\rho(2v) = \frac{1}{2\pi\sqrt{1-v^2}} - \frac{v^2}{12\pi\sqrt{1-v^2}}. \tag{91}$$

Finally combining the results of the two sections we find that the number of states having localization length superior to the sample size is $\sim\rho(E_S)[\frac{2}{M\gamma_{2n}(E_S)}]^{1/2n}$, where M is the size of the sample. n denotes the degeneracy of the exceptional energy. Consequently, the mean square displacement of an electron should go as $t^{2\gamma}$ with $\gamma = (1 - \frac{1}{4n})$. This prediction matches very nicely with exponents obtained from numerical simulations [5, 11, 25].

8. One-dimensional correlated disordered system as an effective Lloyd model

We have already proved that the invariant measure $\phi_E^0(x)$ of the system at the exceptional energies is a Lorentzian distribution centred at $E_S/2$ with a half-width $\sqrt{1-E_S^2/4}$. We have also seen through examples that the DOS at E_S in the near-perfect limit to a good approximation is the DOS of the perfect system. It is also a well established result that the Lyapunov exponent, $\gamma(E)$ around E_S can be approximated to a fair degree by $|r(E)|^2$ where $|r(E)|^2$ is the reflection coefficient of a single guest cluster in the host lattice and $|r(E_S)|^2 = 0$.

The Lloyd model [26], on the other hand, is the uncorrelated site disordered Anderson model where the probability distribution of the site energies $\{\epsilon_n\}$, $P(\epsilon_n)$ is

$$P(\epsilon_n) = \frac{1}{\pi}\frac{\epsilon_1}{(\epsilon_n-\epsilon_0)^2+\epsilon_1^2}. \tag{92}$$

The invariant measure $\phi_E(x)$ for this model is

$$\phi_E(x) = \frac{1}{\pi}\frac{\epsilon_1^*}{(x-\epsilon_0^*)^2+\epsilon_1^{*2}} \tag{93}$$

where

$$\epsilon_0^* = \frac{E}{2} + \frac{1}{2}\,\mathrm{Re}\sqrt{(E+\mathrm{i}\epsilon_1)^2-4} = \frac{E}{2}\left[1+\frac{\tilde\epsilon_1}{\sqrt{A}}\right] \tag{94}$$

$$\epsilon_1^* = \frac{\sqrt{4-E^2}}{2} + [\tilde\epsilon_1+\sqrt{A}] \tag{95}$$

$$A = \frac{1+\tilde\epsilon_1^2+\sqrt{(1+\tilde\epsilon_1^2)^2+4E^2\tilde\epsilon_1^2}}{2} \tag{96}$$

and

$$\tilde\epsilon_1 = \frac{\epsilon_1}{\sqrt{4-E^2}}. \tag{97}$$

We note that all nearest neighbour hopping matrices have been assumed to be unity. The Lyapunov exponent and the DOS for this model can be found in the literature [19]. We simply quote the results.

$$4\cosh\gamma(e) = |2+E|\left[1+\frac{2-E}{2+E}\tilde\epsilon_1^2\right]^{1/2} + |2-E|\left[1+\frac{2+E}{2-E}\tilde\epsilon_1^2\right]^{1/2} \tag{98}$$

and

$$\rho(E) = \frac{1}{\pi}\mathrm{e}^{2\gamma(E)}\left[\epsilon_1^*\frac{\mathrm{d}\epsilon_0^*}{\mathrm{d}E} - \epsilon_0^*\frac{\mathrm{d}\epsilon_1^*}{\mathrm{d}E}\right]. \tag{99}$$

Now in the limit $\tilde\epsilon_1 \to 0$, we find that $\epsilon_0^*(E) = \frac{E}{2}$, $\frac{\mathrm{d}\epsilon_0^*(E)}{\mathrm{d}E} = \frac{1}{2}$, $\epsilon_1^*(E) = \frac{1}{2}\sqrt{4-E^2}$ and $\frac{\mathrm{d}\epsilon_1^*(E)}{\mathrm{d}E} = -\frac{E}{2\sqrt{4-E^2}}$. Consequently, we obtain

$$\phi_E(x) = \frac{1}{\pi}\frac{\sqrt{1-E^2/4}}{x^2-Ex+1} \tag{100}$$

$$\gamma(E) = 0 \tag{101}$$

and

$$\rho(E) = \frac{1}{\pi\sqrt{4-E^2}}. \tag{102}$$

So, all the characteristic features of one-dimensional correlated disordered systems around the exceptional energies are recovered. To develop an effective Lloyd model for one-dimensional correlated disordered systems, we need then $\tilde{\epsilon}_1 = f(E)$ such that $f(E_S) = 0$ for $|E_S| \leqslant 2$ and $f(E)$ should also contain in it the information about the guest cluster. We further note that for $\tilde{\epsilon}_1 \sim 0$, equation (98) yields $\gamma(E) \sim |\tilde{\epsilon}_1|$. But we have shown that for a nondegenerate exceptional energy, $\gamma(E) \sim (E - E_S)^2$. So, $f(E)$ should also satisfy this condition. Inasmuch as $|r(E)|^2$ satisfies all these criteria, we propose that $\tilde{\epsilon}_1 = |r(E)|^2$. This proposal in turn implies that

$$P(\epsilon) = \frac{1}{\pi} \frac{\sqrt{4 - E^2}|r(E)|^2}{\epsilon^2 + (4 - E^2)|r(E)|^4} \tag{103}$$

in the effective Lloyd model. Finally we note that many methods [9] are developed to study the electrical conductivity of uncorrelated site disordered systems. So, these methods can be applied to the systems considered here through the proposed mapping.

9. Summary

The behaviour of electronic states of one-dimensional correlated disordered systems around exceptional energies (E_S) is studied analytically using the invariant measure method. The RDM is the simplest example in this category, and this has been studied by this method by Bovier. The basic approach of Bovier is generalized thoroughly and rigorously to take into consideration more structure in the guest cluster. The formalism is further elaborated by applying to the SRTM. Another useful contribution is the alternative mathematical definition of the exceptional energy from the invariant measure. This definition is further substantiated by physical arguments. Furthermore, from our definition of exceptional energy we obtain an equation constraining the parameters of the guest cluster. The same equation has also been obtained by setting $|r(E)|^2 = 0$. This clearly shows an intimate relationship between the invariant measure and $|r(E)|^2$. This relationship is further highlighted here by mapping these systems to an effective Lloyd model. This equation further shows how the structure of the guest cluster can be modulated to tune positions of exceptional energies. We also obtain through it the condition for a degenerate exceptional energy. Hence, the importance of the method is further illustrated.

In relation to the localization of the eigenstate we find as expected $\gamma(E) \sim (E - E_S)^2$ for cases with a nondegenerate exceptional energy. In the case of a degenerate resonance, $\gamma_2(E_S)$ along with $\gamma_1(E_S)$ are shown to be identically zero. These results are further substantiated by rigorous analytical arguments. Further analytical arguments are presented to show that $\gamma(E) \sim (E - E_S)^4$ for this case. Although a system containing a degenerate exceptional energy has been studied previously by us, this is, however, the most rigorous analysis.

In the RDM $\rho(v)$ is the DOS of the perfect system at $E = v$. Further structure in the guest cluster is found to be manifested in $\rho(E_S)$ through correction terms. However, the universality in the mathematical expression of $N_1(E)$ should not be overlooked. This exemplifies further the universality of one-dimensional correlated disordered systems around exceptional energies. We finally add that the real significance of our work along with that of Bovier on the RDM is that this firmly establishes the anomalous behaviour of one-dimensional correlated disordered systems around exceptional energies.

References

[1] Anderson P W 1958 *Phys. Rev.* **109** 1492
[2] Mott N F and Twose W D 1961 *Adv. Phys.* **10** 107
[3] Ziman T A L 1982 *Phys. Rev. Lett.* **49** 337
Evangelou S N and Katsanos D E 1992 *Phys. Lett.* **164A** 456
[4] Dunlap D H, Kundu K and Phillips P 1989 *Phys. Rev.* B **40** 10 999
[5] Dunlap D H, Wu H-L and Phillips P 1990 *Phys. Rev. Lett.* **65** 88
Datta P K, Giri D and Kundu K 1993 *Phys. Rev.* B **47** 10 727; **48** 16 347
[6] Wu H-L and Phillips P 1990 *J. Chem. Phys.* **93** 7369
[7] Giri D, Datta P K and Kundu K 1993 *Phys. Rev.* B **48** 14 113
[8] Heinrich H, Bauer G and Kuchar F 1988 *Physics and Technology of Submicron Structures* vol 83 (Berlin: Springer)
[9] Wu H-L and Phillips P 1991 *Phys. Rev. Lett.* **66** 1366
Galvao D S, dosSantos D A, Laks B, deMelo C P and Caldas M J 1989 *Phys. Rev. Lett.* **63** 786
Giri D, Kundu K, Majumdar D and Bhattacharyya S P 1996 *Preprint*
[10] Pendry J B 1994 *Adv. Phys.* **43** 461
Thouless D 1972 *J. Phys. C: Solid State Phys.* **25** 77
[11] Giri D, Datta P K and Kundu K 1995 *Physica* B **210** 26
[12] Bovier A and Klein A 1988 *J. Stat. Phys.* **51** 501
[13] Bovier A 1989 *J. Stat. Phys.* **56** 645
[14] Kappus M and Wegner F 1981 *Z. Phys.* B **45** 15
[15] Derrida B and Gardner E 1984 *J. Physique* **45** 1283
[16] Campanino M and Klein A 1990 *Commun. Math. Phys.* **130** 441
[17] Bovier A 1992 *J. Phys. A: Math. Gen.* **25** 1021
[18] Economou E N 1990 *Green's Functions in Quantum Physics* (Heidelberg: Springer)
[19] Matsuda H and Ishii K 1970 *Suppl. Prog. Theor. Phys.* **45** 56
Ishii K 1973 *Suppl. Prog. Theor. Phys.* **53** 77
[20] Datta P K 1995 *PhD Thesis*
[21] Dean P 1959 *Proc. Phys. Soc.* **73** 413; 1960 *Proc. R. Soc.* A **254** 507; 1961 *Proc. R. Soc.* A **260** 263; 1969 *J. Phys. Soc.* **26** 20
[22] Feller W 1991 *An Introduction to Probability Theory and its Applications* vol I (New York: Wiley) ch XV
[23] Fürstenberg H 1963 *Trans. Am. Math. Soc.* **108** 377
[24] Ruelle D 1979 *IHES Publ.* **50** 275
[25] Datta P K and Kundu K 1995 *Phys. Rev.* B **51** 6287
[26] Lloyd P 1969 *J. Phys. C: Solid State Phys.* **2** 1717