Irrational anomalies in one-dimensional Anderson localization

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We revisit the problem of one-dimensional Anderson localization, by providing perturbative expression for Lyapunov exponent of Anderson model with next-nearest-neighbor (nnn) hopping. By comparison with exact numerical results, we discuss the range of validity of the naive perturbation theory. The stability of band center anomaly is examined against the introduction of nnn hopping. New anomalies of Kappus-Wegner type emerge at nonuniversal values of wavelength when hopping to second neighbor is allowed. It is shown that covariances in the first order of perturbation theory, develop singularities at these resonant energies which enable us to locate them.

I. INTRODUCTION

Localization of noninteracting particles in one and quasi-one-dimensional systems can be formulated using transfer matrices. It is also mostly accepted that localization properties in two and three dimensions can be deduced via transfer matrix method combined with finite-size scaling on quasi-one-dimensional geometries. Therefore the problem reduces to calculating growth rates [Lyapunov exponents (LEs)] of products of random matrices. There are a few cases in which analytical expression for LEs can be obtained. Most cases have to be treated numerically. But the limit of arbitrarily weak disorder is not accessible even numerically because the convergence slows down extremely. So it would be of crucial importance to develop a perturbation theory in this limit. Particularly, existence of delocalized states can be judged thereby. Perturbative expansions for LEs are provided[1] for some class of random matrices of the form $\mathbf{T} = \mathbf{A} + \epsilon \mathbf{B}$, where $\mathbf{A}$ is nonrandom matrix and $\epsilon \mathbf{B}$ is small random part. They require the eigenvalues of $\mathbf{A}$ to have different moduli. Many interesting situations which appear in localization do not fulfill this condition.

Using nondegenerate perturbation theory, Thouless[2] obtained a weak disorder expansion of LE for one-dimensional Anderson model. Later numerical results[3] showed 9% increase in localization length at the center of band. This discrepancy was resolved by Kappus and Wegner when they developed a degenerate perturbation theory for the band center.[4] The failure of nondegenerate perturbation theory at the middle of the band is known as Kappus-Wegner (KW) anomaly. The anomaly is a manifestation of spatial periodicity of the system. It is known as commensurability effect between lattice constant and electron wavelength. Description of this effect using phase formalism offers an analogy in classical dynamics.[5,6]

Apart from the mathematical subtlety, there are remarkable physical consequences at this point. Conductance distribution at this anomaly deviates[7] from predicted distribution (log normal) by single-parameter scaling (SPS) theory. The occurrence of anomaly is accompanied with breakdown of reflection phase randomization[5,8] as well, which also is of basic assumptions of SPS theory.[9] Systematic treatment of the band center anomaly as well as anomalies at the energies

$E = 2t \cos(\pi \alpha)$ with α rational, is already established.[10] Quite recently a classification of anomalies is given[11] for 2×2 transfer matrices according to which the anomaly in the band center is of second order. Another study is done via calculation of participation ratio (instead of LE) by means of field theoretic tools which provides full statistics of wave function at the band center anomaly.[12] This leads the authors to conjecture that there is a hidden symmetry responsible for integrability of the problem at this spectral point.

II. MODEL

In more realistic representation of the problem, hopping to the next-nearest neighbors should be taken into account. In this paper we want to address the stability of the anomalies, against the introduction of hopping to next neighbors. We restrict ourselves to hopping to the second neighbor only. Generalization for other neighbors is straightforward. By doing so, the results will be applicable to probing, recently proposed[13] delocalization transition in low-dimensional systems with long-range hopping. We consider the one-dimensional Anderson model

$$t'(\Psi_{n+2} + \Psi_{n-2}) + t(\Psi_{n+1} + \Psi_{n-1}) + \epsilon U_n \Psi_n = E \Psi_n \quad (1)$$

with nnn hopping and weak disordered potential ϵU_n, where $\langle U_n \rangle = 0$ and $\langle U_n U_m \rangle = \sigma^2 \delta_{nm}$. This model also can be viewed as a system of two coupled chains in the way that is illustrated in Fig. 1. It is studied extensively[14] as an extension of one-dimensional Hubbard model, called t-t' Hubbard chain, and exhibits a rich phase diagram. Pure chain has a dispersion relation which is quadratic in $\cos k$

$$E(k) = 2t \cos k + 2t' \cos 2k, \quad -\pi < k < \pi, \quad (2)$$

where unit lattice spacing is assumed. We will only consider positive t' on account of symmetry. Dispersion curves for two different ratios of $|\frac{t}{t'}| > 4$ and $|\frac{t}{t'}| < 4$ are plotted in Fig. 1. In the latter case, there are two pairs of wave vectors, carrying the same energy at the bottom of the band. In other word, there are two propagating channels for that part of spectrum. For each case the density of states (DOS) is shown in the right panel. Additional singularity of DOS inside the band for $|\frac{t}{t'}| < 4$ is an internal band edge corresponding to
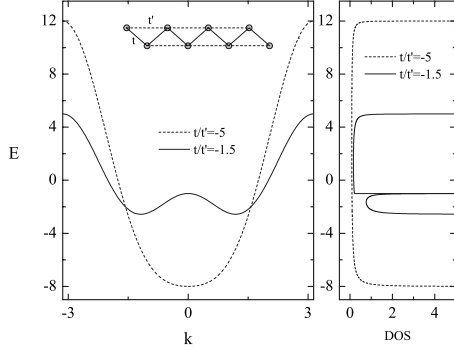
FIG. 1. Dispersion carves (left) and density of states (right) of pure chain for $t=-5$, $t'=1$ (dashed) and $t=-1.5$, $t'=1$ (solid).

new channel. As $|\frac{t}{t'}|$ increases, this singularity moves toward the bottom of the band and disappears at $|\frac{t}{t'}|=4$, after which there will be single channel at entire band.

III. TRANSFER MATRIX

Propagation along the chain according to Eq. (1) can be described by using 4×4 transfer matrices

$$\begin{pmatrix} \Psi_{n+2} \\ \Psi_{n+1} \\ \Psi_n \\ \Psi_{n-1} \end{pmatrix} = \begin{pmatrix} -\dfrac{t}{t'} & \dfrac{E-\epsilon U_n}{t'} & -\dfrac{t}{t'} & -1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} \Psi_{n+1} \\ \Psi_n \\ \Psi_{n-1} \\ \Psi_{n-2} \end{pmatrix}.$$

(3)

The transmission channels of pure system can be distinguished in terms of eigenvalues and corresponding eigenvectors of transfer matrix for $\epsilon=0$. We have four eigenvalues which appear in pairs $\lambda_i, \lambda_i^{-1}$. Each pair corresponds to a right-going and a left-going plane waves. It should be noted that each mode is propagating as long as corresponding eigenvalue has unit norm and is evanescent otherwise. We will return to this point and will give the range of energy for each channel.

In a similar manner, by addition of random potential one obtains pairs of LEs $\pm \gamma_i, i=1,2$ for product of transfer matrices. Each LE has a contribution to conductance but regarding the eigenstates, for which k is not a good quantum number in presence of disorder, the smaller LE gives the localization length. The transfer matrix in Eq. (3) will be used for numerical calculation of LEs.

IV. PERTURBATION THEORY

As usual we define the variables $R_n = \frac{\Psi_{n+1}}{\Psi_n}$ and rewrite Eq. (1) in terms of them. Also it is appropriate to scale energies with t' such that $\frac{t}{t'}=h$, $\frac{U_n}{t'} \to U_n$, and $\frac{E}{t'} \to E$. We have

$$R_{n+1}R_n + \frac{1}{R_{n-1}R_{n-2}} + h\left(R_n + \frac{1}{R_{n-1}}\right) = E - \epsilon U_n.$$

(4)

Following the Ref. 15 we use the ansatz

$$R_n = a e^{B_n \epsilon + C_n \epsilon^2 + \cdots}$$

(5)

and by inserting in Eq. (4) and collecting terms of same order in ϵ we obtain recursive equations for $a, B_n, C_n, \ldots$. Up to second order in ϵ we have

$$a^2 + \frac{1}{a^2} + h\left(a + \frac{1}{a}\right) = E,$$

(6a)

$$a^2(B_{n+1} + B_n) - \frac{1}{a^2}(B_{n-1} + B_{n-2}) + h\left(aB_n - \frac{1}{a}B_{n-1}\right) = -U_n,$$

(6b)

$$a^2\left[C_{n+1} + C_n + \frac{1}{2}(B_{n+1} + B_n)^2\right]$$
$$+ \frac{1}{a^2}\left[-C_{n-1} - C_{n-2} + \frac{1}{2}(B_{n-1} + B_{n-2})^2\right]$$
$$+ h\left[a\left(C_n + \frac{1}{2}B_n^2\right) + \frac{1}{a}\left(-C_{n-1} + \frac{1}{2}B_{n-1}^2\right)\right] = 0.$$

(6c)

The LE is given by

$$\gamma(E) = \lim_{N \to \infty} \frac{1}{N} \sum_{n=1}^{N} \log R_n.$$

(7)

Using Eqs. (5) and (7) an expansion for LE can be obtained as follows:

$$\gamma(E) = \log a + \epsilon \langle B \rangle + \epsilon^2 \langle C \rangle + \cdots.$$

(8)

Angular brackets denote the ensemble average. In order to calculate the averages we take average of both sides of Eqs. (6b) and (6c). Then we get

$$\langle B \rangle = 0,$$

(9)

$$\langle C \rangle = -\frac{\left(a^2 + \dfrac{1}{a^2}\right)[\rho(1) + \rho(0)] + \dfrac{h}{2}\left(a + \dfrac{1}{a}\right)\rho(0)}{2\left(a^2 - \dfrac{1}{a^2}\right) + h\left(a - \dfrac{1}{a}\right)}, \quad (10)$$

where $\rho(\tau)$ is the autocovariance function $\langle B_{n+\tau}B_n \rangle$. Recursive Eq. (6b) is an autoregressive process of third order. Covariances $\rho(\tau)$ can be determined by the following set of Yule-Walker equations for B process:

$$\rho(0) = \phi_1\rho(1) + \phi_2\rho(2) + \phi_3\rho(3) + \frac{\sigma^2}{a^4},$$

(11a)

$$\rho(1) = \phi_1\rho(0) + \phi_2\rho(1) + \phi_3\rho(2),$$

(11b)

$$\rho(2) = \phi_1\rho(1) + \phi_2\rho(0) + \phi_3\rho(1),$$

(11c)

$$\rho(3) = \phi_1\rho(2) + \phi_2\rho(1) + \phi_3\rho(0),$$

(11d)

where $\phi_1 = -(1 + \frac{h}{a})$, $\phi_2 = \frac{1}{a^4} + \frac{h}{a^3}$, and $\phi_3 = \frac{1}{a^4}$.
By solving this set of equations we find

$$\rho(0) = \frac{\sigma^2}{a^4 M}(-1 + \phi_2 + \phi_1 \phi_3 + \phi_3^2), \tag{12a}$$

$$\rho(1) = -\frac{\sigma^2}{a^4 M}(\phi_1 + \phi_2 \phi_3), \tag{12b}$$

$$\rho(2) = -\frac{\sigma^2}{a^4 M}(-\phi_2 + \phi_1^2 - \phi_2^2 + \phi_1 \phi_3), \tag{12c}$$

$$\rho(3) = -\frac{\sigma^2}{a^4 M}(\phi_3 + 2\phi_1 \phi_2 - \phi_2 \phi_3 - \phi_1 \phi_2^2 - \phi_1 \phi_3^2 + \phi_1^2 \phi_3$$
$$+ \phi_2^2 \phi_3 + \phi_1^3 - \phi_3^3) \tag{12d}$$

with $M = (1 + \phi_1 - \phi_2 + \phi_3)(-1 + \phi_1 + \phi_2 + \phi_3)[1 + \phi_2 + \phi_3(\phi_1 - \phi_3)]$. By inserting Eqs. (12a) and (12b) in Eq. (10) and using Eq. (8) we obtain the LE up to second order (in the original energy scale)

$$\frac{1}{\xi} = \Re(\gamma) = \frac{-\sigma^2 \epsilon^2}{2\left[2t'\left(a^2 - \frac{1}{a^2}\right) + t\left(a - \frac{1}{a}\right)\right]^2}. \tag{13}$$

Note that inside the band, a is pure phase. This expression reduces to the well-known result for Anderson model at the limit $t' \to 0$. All that remains is to find roots of Eq. (6a). Equation (6a) is in fact the characteristic equation for eigenvalues of transfer matrix of pure system. Inside the energy band where we have $a = e^{ik}$, it is nothing but the dispersion relation in Eq. (2), from which we have

$$\cos k_\pm = \frac{1}{4}(-h \pm \sqrt{h^2 + 4E + 8}). \tag{14}$$

Depending on the sign of h, one of branches produces the energy band $-2 - \frac{h^2}{4} < E_1 < 2 + 2|h|$ and the other $-2 - \frac{h^2}{4} < E_2 < 2 - 2|h|$, for $|h| < 4$. We will call them first and second channel, respectively. For $|h| > 4$, second channel gets closed and the first one spans the interval $2 - 2|h| < E_1 < 2 + 2|h|$.

V. POLES OF $\rho(\tau)$ AND ANOMALIES

Perturbation expansion in Eq. (8), diverges in different orders for special energies. As we mentioned, this signals an anomaly and the order of divergent term is related to the order of anomaly. As it is shown for Anderson model, first divergence is showed up in the fourth order at the middle of the band which corresponds to the principal anomaly (KW anomaly). The expansion is finite up to the second order for the model studied here as well.

The point that has not been noticed is the appearance of divergences at the level of covariance functions $\rho(\tau)$. Here we show that covariance functions $\rho(\tau)$ possess some poles on real energy axis, yet the final result in Eq. (13) is finite. By exact numerical calculation we show that the localization length enhances at these poles. Depending on h, there are four situations as follows. Without loss of generality let us consider positive h hereafter.

h > 4. By inserting a small hopping term, t', in the Hamiltonian, results will smoothly deviate from that of ordinary
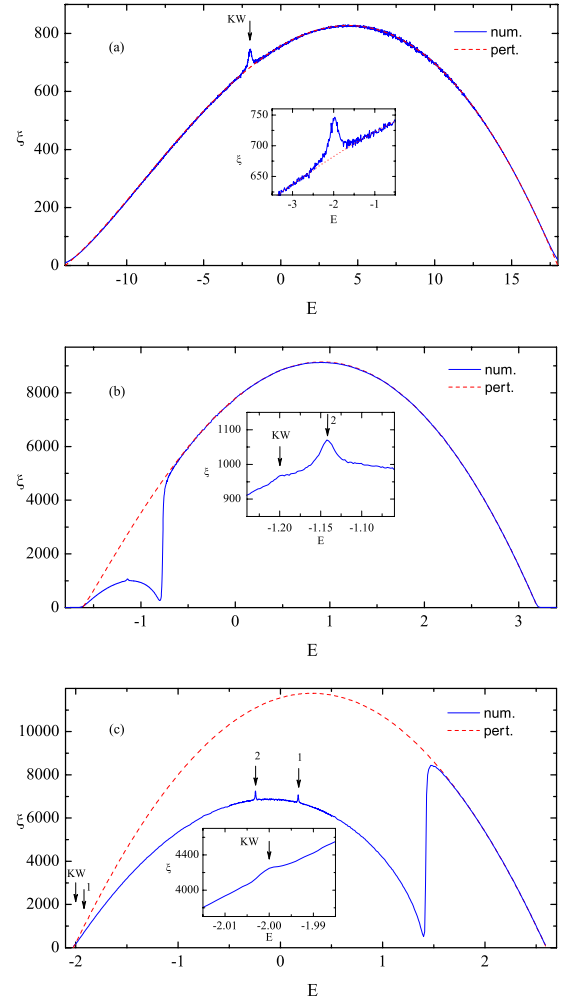

FIG. 2. (Color online) Localization length obtained from numerical calculation via transfer matrix method (solid) and analytical perturbation theory (dashed). White noise disorder with uniform distribution and zero mean is used. Arrows indicate the anomalies and their positions are determined from poles of covariance function $\rho(\tau)$. Numbers denote the channel in which the poles show up. (a) $t = 8$, $t' = 1$, $\sigma^2 = \frac{3}{4}$, inset is a closer view of anomaly, (b) $t = 1$, $t' = 0.6$, $\sigma^2 = \frac{1}{300}$, inset is a closer view of anomalies, and (c) $t = 0.3$, $t' = 1$, $\sigma^2 = \frac{1}{300}$, inset: $t = 0.8$, $t' = 1$, $\sigma^2 = \frac{1}{1200}$.

Anderson model. It will cause an asymmetry in the localization length vs. energy about the zero energy. Other surprising fact is that the anomaly at the band center survives and shifts from the center [Fig. 2(a)]. If we suppose that it would occur at the same fraction of wavelength to the lattice spacing, which was seen for Anderson model, we can estimate the energy by using dispersion relation in Eq. (2) for $k = \frac{\pi}{2}$, which gives $E = -2t'$. Now by looking at $\rho(\tau)$ we can see that there is one pole at $E = -2$ (root of the term $1 + \phi_1 - \phi_2 + \phi_3$ in M for first channel) which is the same energy, $E = -2t'$, in the original energy scale. This pole indeed corresponds to the KW anomaly which now appears away from the center. The anomalous behavior of localization length and deviation from perturbative result at this point can be seen clearly in Fig. 2(a). It is also present in other cases but appears weaker. The second channel is evanescent in this case.

$\frac{4\sqrt{6}}{9} < \mathbf{h} < \mathbf{4}$. Third factor in denominator, $1 + \phi_2 + \phi_3(\phi_1 - \phi_3)$, has other roots which satisfy the cubic equation $x^3 = 3px - 2q$, where $p = \frac{2}{3}$, $q = \frac{h}{2}$, and $x = (a + \frac{1}{a}) = 2\cos k_\pm$. Positive and negative signs correspond to first and second channels, respectively. In this case which we have $q^2 - p^3 > 0$, the equation has one real root $x = -(q + \sqrt{q^2 - p^3})^{1/3} - (q - \sqrt{q^2 - p^3})^{1/3}$ which gives a valid energy in second channel only. In the first channel we have one pole so far [Fig. 2(b)].

$\mathbf{h} = \frac{4\sqrt{6}}{9}$. In this case $(q^2 - p^3 = 0)$, the cubic equation has three real roots, one of which has multiplicity 2, $x_1 = -2q^{1/3}, x_2 = x_3 = q^{1/3}$. x_1 is actually the root in previous case and corresponds to the second channel. The other root gives rise to a pole of second order in the first channel.

$\mathbf{h} < \frac{4\sqrt{6}}{9}$. We have three distinct real roots in this case ($q^2 - p^3 \leq 0$), which can be expressed in the standard form, $x_1 = 2\sqrt{p}\cos(u/3)$, $x_2 = 2\sqrt{p}\cos(u/3 + 2\pi/3)$, $x_3 = 2\sqrt{p}\cos(u/3 + 4\pi/3)$, where $\cos u = -q/(p\sqrt{p})$, $0 < u < \pi$. Again one of them is in second channel and other two are in the first channel [Fig. 2(c)]. One of the later poles seems to be absent in numerical results and needs to be discussed beyond the second-order perturbation. These cases are summarized in the Fig. 3.

The wave vector of last three poles is given by

$$k = \arccos \frac{x}{2}. \tag{15}$$

Due to the dependence of x on h, wave vector changes continuously by varying the ratio of hopping integrals [Fig. 3(b)]. Thus the value of wavelength at these anomalies will not be necessarily rational.

We shall mention two other essential features in Fig. 2. (i) Apart from in the anomalies, perturbative result deviates significantly from numerical result for those energies at which two channels are open [Figs. 2(b) and 2(c)]. Analytical result based on Eq. (5) presents the perturbation around the solutions with single wave vector while the numerical method produces a mixture of two solutions. The fact that the anomalies are obtained correctly by perturbation theory, supports the above statement.

It is worth mentioning the limit of zero h where the whole spectrum is degenerate. Covariances in Eq. (12) are divergent, however LE in Eq. (13) has a well-defined limit. We have nnn hopping (t') only at this limit and the system transforms to two decoupled chains with nearest-neighbor hopping. So one expects the result of ordinary Anderson model (ξ_A) with doubled lattice constant, i.e., $\xi \rightarrow 2\xi_A$. But the factor is 4 rather than 2. This suggests to use decoupled chains as a starting point to develop the perturbation theory. (ii) The
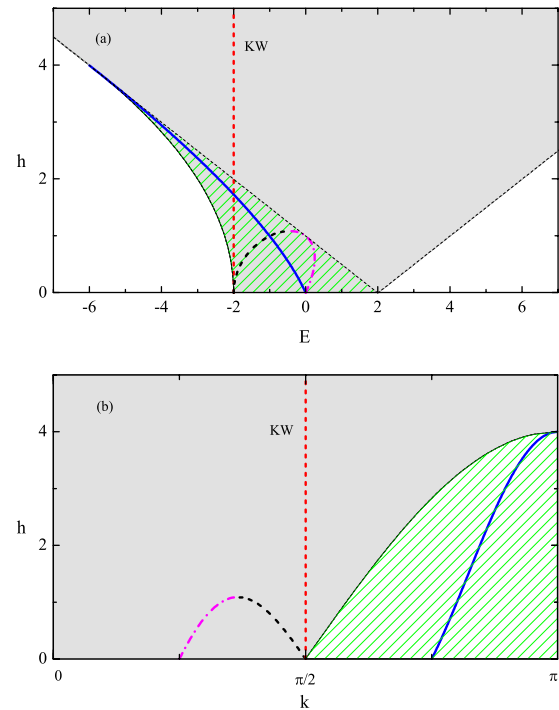

FIG. 3. (Color online) Transmission channels of pure system and trajectory of poles of $\rho(\tau)$. Two channels are specified with gray color (first channel) and green shade (second channel). As it is clear from (b), red dashed (KW), black dashed and dashed-dotted lines correspond to first channel and solid blue line corresponds to the second channel. Thin dashed lines at the band edges in (a) are also nonanalytic poles of $\rho(\tau)$.

sudden change in localization length happens at the internal band edge and is in coincidence with van-Hove singularity in DOS of pure system.

VI. CONCLUSION

In conclusion, we show that KW anomaly exists in presence of nnn hopping, where we have lower symmetry of Hamiltonian for vanishing disorder (broken particle-hole symmetry) and occurs at the same wavelength as in the Anderson model. We also demonstrate that the anomaly could be identified by certain divergences at first order of perturbation theory. Three other singularities turn out to exist which are not attributed to single wavelength and may even correspond to incommensurate ratio of wavelength to the lattice spacing which is in striking contrast to the known anomalies in Anderson model.

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