

Spectral degeneracy in the one-dimensional Anderson problem: A Uniform expansion in the energy band

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A uniform quantitative description of the properties of the one-dimensional Anderson model is obtained by mapping that problem onto an infinitely quasidegenerate master equation. This quasidegeneracy is identified as the source of the small-denominator problem encountered before in investigations of this problem. An appropriate quasidegenerate perturbation theory is developed to obtain a uniform asymptotic expansion, in powers of the strength of the noise, for the probability distribution function of the ratio of the value of the wave function at neighboring sites. Well known results, such as those obtained by Thouless, Kappus and Wegner, and Derrida and co-workers are reproduced and systematic corrections to these results as well as some more results are found. In particular, we find internal layers in the above-mentioned distribution function for values of the energy given by $E = 2 \cos \pi \alpha$ with α rational. We also find crossovers in the behavior of the distribution function (and consequently in quantities derived from it) near the band-edge and band-center regions. The properties of the model in the band-edge region were studied by us in detail in a previous publication [Phys. Rev. B **47**, 1918 (1992)].

I. INTRODUCTION

The realization that even the most minute amount of randomness in a physical system can change its properties in a drastic fashion,¹⁻⁴ has had a most significant impact on the understanding of phenomena in disordered materials. It is well understood that unlike ordered materials, disordered environments give rise to localized states and have many unusual transport properties.¹⁻⁹

Perhaps the simplest model describing dynamics in a disordered system is that due to Anderson.⁵ This model, which is based on the tight-binding description of electronic states in solids, has been thoroughly investigated.¹⁰⁻²² One of the important quantities which characterize the Anderson model is the localization length (see, e.g., Refs. 1, 2) or the inverse Lyapunov exponent.^{23,24} Pioneering work, due to Thouless,²⁵ based on a regular perturbation theory, has produced a formula for the leading-order approximation of the Lyapunov exponent for small disorder in one dimension. Higher-order terms in the perturbation theory employed by Thouless are divergent on a dense set of energies in the band. Subsequent work¹³⁻²² has shown that the Thouless formula is correct as a leading-order approximation in the magnitude of the disorder, except in the vicinities of the band center and the band edge. In the former regime, it was found by Kappus and Wegner¹³ that the correct Lyapunov exponent differs by about 10% from Thouless' prediction. Derrida and Gardner¹⁵ proposed a nonlocal linear integrodifferential equation for the probability density function of the ratio of the values of the wave function at neighboring sites. Using an expansion in

terms of a small parameter ϵ , which measures the disorder, they were able to find the Lyapunov exponent in the troublesome band-edge and band-center regions. When attempting to compute the Lyapunov exponent outside these two regions, they encountered difficulties related to the problem of reducing the nonlocal equation to a quasilocal one. A tedious method was then used¹⁵ to obtain the value of the Lyapunov exponent in neighborhoods of certain interior points in the band. The Derrida and Gardner method was generalized in Ref. 19 for the entire interior of the band and the asymptotic convergence of the series obtained by them was established in Ref. 20. The latter work did not produce a direct expansion of the probability distribution function in powers of the strength of the noise for a fixed value of the energy E ; it consists of expansions of the energy around rational values of θ/π in parallel with the expansion of the probability distribution function in powers of the strength of the disorder. In our view, this method, in addition to being very tedious, is not of uniform nature in the energy band, it fails to deal with crossover to the band edge, and it does not reveal the source of the small-denominator problem. The present paper shows how a uniform expansion for the statistical properties of the one-dimensional (1D) Anderson model can be obtained. The result is an asymptotic series in powers of the disorder parameter ϵ whose coefficients are bounded, ϵ -dependent, functions. This series is uniformly valid in the entire band, including the band-edge region. The basic observation leading to the expansion developed here is that the integral equation satisfied by the invariant measure possesses an infinitely degenerate spectrum for rational values of θ/π and an

infinite quasidegenerate spectrum for irrational values in the limit of vanishing disorder. This degeneracy is lifted by the disorder. It is also responsible for internal layers in the invariant measure in the neighborhood of rational values of θ/π and for the crossovers to the band center and band edge. The results of our formalism are used to compute the density of states and the Lyapunov exponent for the Anderson model. The Thouless formula is confirmed as a leading approximation for the Lyapunov exponent everywhere except in the vicinities of the band center and the band edge. This work is, in a way, a generalization of our previous (detailed) study²² of the properties of the 1D Anderson problem for near-band-edge energies. This article is organized as follows. In Sec. II the problem is formulated, the basic equation is presented, and a linear operator is defined, whose eigenfunction corresponding to the eigenvalue 1 is the probability distribution function of the ratio of the values of the wave function at consecutive sites. In Sec. III the problem is recast as a more convenient eigenvalue problem for a linear operator. In Sec. IV a decomposition of the operator is given and a procedure for finding the eigenfunction is described. In Sec. V the formal results of Sec. IV are applied to the general in-band case ($\theta \neq 0, \pi/2$) and a general formula for the invariant measure is presented there. Section VI provides a perturbative solution for the band-center region ($\theta \sim \pi/2$). The transition to the band edge ($\theta \sim 0$) is discussed in Sec. VII. Finally, Sec. VIII provides a summary and discussion.

II. FORMULATION OF THE PROBLEM AND BASIC DEFINITIONS

The discretized Schrödinger equation in one dimension with a random potential $\epsilon\xi_n$ at site n is given by¹⁵

$$\psi_{n+1} + \psi_n = (E + \epsilon\xi_n)\psi_n, \quad (2.1)$$

where $-2 \leq E \leq 2$ is the average "energy" (the physical average energy is $2 - E$ in dimensionless units) and $\{\xi_n\}$ is a sequence of independent identically distributed random variables with a probability distribution function $\rho(\xi) = \text{Prob}(\xi_n = \xi)$. The noise ξ_n is assumed to have zero mean and unit variance, that is, $\langle \xi_n \rangle = 0$ and $\langle \xi_n^2 \rangle = 1$. The parameter ϵ , which measures the strength of the noise, is assumed to be small. It is convenient to define an angle θ by

$$E = 2 \cos \theta. \quad (2.2)$$

When $\epsilon = 0$ Eq. (2.1) with E given by Eq. (2.2) has the bounded (plane wave) solutions $e^{\pm in\theta}$. When $\epsilon \neq 0$, the solutions are localized. We define the variable R_n by

$$R_n \equiv \frac{\psi_n}{\psi_{n-1}}. \quad (2.3)$$

The complex Lyapunov exponent is defined as

$$\gamma(E) \equiv \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{n=1}^N \ln R_n. \quad (2.4)$$

Mathematically, only $\text{Re } \gamma(E)$ is defined to be the Lyapunov

exponent.^{23,24} Following Eqs. (2.1) and (2.3), R_n obeys the recursion relation

$$R_{n+1} = 2 \cos \theta + \epsilon\xi_n - \frac{1}{R_n}. \quad (2.5)$$

In the following, only real values of R_n are considered. This is consistent with (2.5). Since (2.1) is real, the consideration of real R_n 's does not limit generality. Thus only this case is considered henceforward. The sequence $\{R_n\}$ is a Markov process which becomes stationary as $n \rightarrow \infty$.²⁰ Its stationary probability distribution function is defined by

$$p(x) dx \equiv \lim_{n \rightarrow \infty} \text{Prob}(x \leq R_n \leq x + dx). \quad (2.6)$$

It follows from (2.4) that

$$\gamma(E) = \int_{-\infty}^{\infty} p(x) \ln x dx. \quad (2.7)$$

Therefore

$$\text{Re } \gamma(E) = \int_{-\infty}^{\infty} p(x) \ln |x| dx, \quad (2.8)$$

and, since $\arg(\ln x) = i\pi$ for $x < 0$, it is evident that

$$\text{Im } \gamma(E) = \pi \int_{-\infty}^0 p(x) dx. \quad (2.9)$$

The density of states $\tilde{\rho}(E)$ is related to the Lyapunov exponent by^{12,15}

$$\tilde{\rho}(E) = -\frac{d}{dE} \int_{-\infty}^0 p(x) dx = -\frac{1}{\pi} \frac{d \text{Im} \gamma(E)}{dE}. \quad (2.10)$$

Since $\{R_n\}$ is a Markov process its probability distribution function satisfies, following (2.5), the master equation

$$\begin{aligned} p_{n+1}(x) &\equiv \langle \delta(R_{n+1} - x) \rangle \\ &= \left\langle \delta \left(2 \cos \theta + \epsilon\xi_n - \frac{1}{R_n} \right) \right\rangle, \end{aligned} \quad (2.11)$$

where $\langle \dots \rangle$ is the average over the ensemble of realization $\{\xi_j\}$ for $-\infty < j \leq n$. In terms of the probability distribution function $\rho(\xi)$ of the noise, Eq. (2.11) can be rewritten as

$$\begin{aligned} p_{n+1}(x) &= \int_{-\infty}^{\infty} p \left(\frac{1}{2 \cos \theta - x + \epsilon\xi} \right) \frac{\rho(\xi) d\xi}{(2 \cos \theta - x + \epsilon\xi)^2} \\ &\equiv \hat{\mathbf{L}} p_n(x), \end{aligned} \quad (2.12)$$

where the definition of the linear operator $\hat{\mathbf{L}}$ is evident. The stationary probability distribution function $p(x) \equiv \lim_{n \rightarrow \infty} p_n(x)$ satisfies the equation

$$p(x) = \hat{\mathbf{L}} p(x), \quad (2.13)$$

that is, $p(x)$ is an eigenfunction of the operator $\hat{\mathbf{L}}$ corresponding to the eigenvalue 1. Equation (2.13), which is identical to that obtained by Derrida and Gardner,¹⁵ contains two parameters, ϵ and θ . It is our aim to construct an asymptotic solution of (2.13) for small values of ϵ and all values of θ .

III. THE ANGLE REPRESENTATION

The analysis of (2.13) can be significantly simplified by introducing the angular variable ϕ , defined by (see Ref. 13)

$$x = \frac{\sin(\phi + \theta)}{\sin \phi}, \quad 0 < \phi < \pi, \quad (3.1)$$

where θ is the angle defined in (2.2). For each R_n one defines similarly

$$R_n = \frac{\sin(\phi_n + \theta)}{\sin \phi_n}, \quad (3.2)$$

or

$$R_n = \cos \theta + \sin \theta \cot \phi_n. \quad (3.3)$$

The recursion relation (2.5) in the angle representation assumes the form

$$\phi_{n+1} = \arccot[\cot(\phi_n + \theta) + \eta \xi_n], \quad (3.4)$$

where

$$\eta \equiv \frac{\epsilon}{\sin \theta}. \quad (3.5)$$

The parameter η can be considered small as long as $\theta \gg \epsilon$. The stationary probability distribution function of $\{\phi_n\}$ which, without confusion, is denoted by $p(\phi)$, is related to $p(x)$ by

$$p(\phi) = p(x) \frac{dx}{d\phi}, \quad (3.6)$$

where x is related to ϕ by (3.1). In Appendix A it is shown that (2.13) is transformed into

$$p(\phi) = \int_0^\pi \frac{p\{\arccot[\cot(\phi - \eta\xi) - \theta]\}}{1 - \eta\xi \sin 2\phi + \eta^2 \xi^2 \sin^2 \phi} \rho(\xi) d\xi \equiv \hat{\mathbf{L}}p(\phi). \quad (3.7)$$

The operator $\hat{\mathbf{L}}$ acts in the space of π -periodic continuous functions which are absolutely integrable. It is convenient to use the basis $\{e^{2i\phi n}; n = 0, \pm 1, \pm 2\}$ in this space. The Fourier expansion of $p(\phi)$ is denoted by

$$p(\phi) = \sum_{n=-\infty}^{\infty} e^{2i\phi n} p_n. \quad (3.8)$$

The action of the operator $\hat{\mathbf{L}}$, defined in (3.7), on the basis elements $\{e^{2i\phi n}\}$ (see Appendix B) is given by

$$\hat{\mathbf{L}}e^{2i\phi n} = e^{2i\phi n} e^{-2i\theta n} \int_0^\pi \frac{(1 + \eta\xi e^{-i\phi} \sin \phi)^{2n}}{(1 + \eta\xi e^{-i\phi} \sin \phi)^{n+1} (1 + \eta\xi e^{i\phi} \sin \phi)^{n+1}} \rho(\xi) d\xi. \quad (3.9)$$

Equations (2.8) and (2.9) for the Lyapunov exponent are given in terms of the variable ϕ as

$$\text{Re } \gamma(E) = \int_0^\pi [\ln |\sin(\phi + \theta)| - \ln |\sin \phi|] d\phi \quad (3.10)$$

and

$$\text{Im } \gamma(E) = \pi \int_{\pi-\theta}^\pi p(\phi) d\phi. \quad (3.11)$$

The density of states,¹³ $\tilde{\rho}(E)$ can be expressed in terms of $p(\phi)$ as

$$\tilde{\rho}(E) = \frac{1}{\sin \theta} \int_0^\pi p(\phi) \sin^2 \phi p(-\phi - \theta) d\phi. \quad (3.12)$$

Note that with our definition $p(\phi)$ is a π -periodic function, whereas in Ref. 13 it is a 2π -periodic function, accounting for a difference by a factor of 2 in (3.12) between the corresponding formulas.

IV. THE METHOD

A. General formulation

The operator $\hat{\mathbf{L}}$ is represented in the basis $\{e^{2i\phi n}\}$ by an infinite-dimensional matrix. Below, we denote the operator and its representation interchangeably by \mathbf{L} . Its first approximation, corresponding to the noiseless case $\eta = 0$, is obtained from (3.9) as

$$\mathbf{L}^0 e^{2i\phi n} = e^{-2i\theta n} e^{2i\phi n}, \quad (4.1)$$

so that \mathbf{L}^0 can be represented by the diagonal matrix

$$L_{n,m}^0 = e^{-2i\theta n} \delta_{n,m}. \quad (4.2)$$

The k th component of the eigenvector \mathbf{v}_0^n corresponding to the eigenvalue $e^{-2i\theta n}$ is given by $v_{0,k}^n = \delta_{n,k}$. When θ is a rational multiple of π , that is, $\theta = p\pi/q$, where p and q are integers, the eigenvalue 1 of \mathbf{L}^0 is infinitely degenerate, since $e^{-2i\theta n} = 1$ when n is an integral multiple of q . When θ is an irrational multiple of π , there are infinitely many eigenvalues of \mathbf{L}^0 of the form $e^{-2i\theta n}$ in every neighborhood of 1. Thus in this case 1 is an infinitely *quasidegenerate* eigenvalue. The perturbation theory developed below to treat this problem is based on the following projection operator technique.

The eigenvalues are partitioned into two sets, according to their distances from 1. Choosing an arbitrary number δ such that

$$\eta^2 \ll \delta < 1, \quad (4.3)$$

the set \mathbf{s}_δ of indices is defined, for a given value of θ , by

$$\mathbf{s}_\delta \equiv \{n : |e^{-2i\theta n} - 1| < \delta\}. \quad (4.4)$$

The subspace \mathcal{S} spanned by the eigenvectors \mathbf{v}_0^n with $n \in \mathbf{s}_\delta$ corresponds to eigenvalues of \mathbf{L}^0 in a δ neighborhood of 1. The projection operator \mathbf{K} onto \mathcal{S} has the matrix representation

$$K_{n,m} \equiv \begin{cases} \delta_{n,m} & \text{if } n \in \mathfrak{s}_\delta, \\ 0 & \text{otherwise.} \end{cases} \quad (4.5)$$

Next, the matrix \mathbf{M} is defined by $\mathbf{M} = \mathbf{L} - \mathbf{K}$, so that

$$\mathbf{L} = \mathbf{K} + \mathbf{M}. \quad (4.6)$$

The problem of finding $p(\phi)$ is equivalent to that of finding an eigenvector \mathbf{v} of \mathbf{L} with eigenvalue 1, that is,

$$\mathbf{L}\mathbf{v} = \mathbf{v}. \quad (4.7)$$

The projection of \mathbf{v} on the subspace \mathcal{S} is given by

$$\tilde{\mathbf{w}} \equiv \mathbf{K}\mathbf{v} \quad (4.8)$$

and its projection on the complementary subspace is given by

$$\tilde{\mathbf{z}} \equiv \mathbf{v} - \mathbf{K}\mathbf{v} = (\mathbf{I} - \mathbf{K})\mathbf{v}, \quad (4.9)$$

where \mathbf{I} is the identity matrix. Obviously

$$\mathbf{K}\tilde{\mathbf{z}} = \mathbf{0} \quad (4.10)$$

and

$$\mathbf{v} = \tilde{\mathbf{z}} + \tilde{\mathbf{w}}. \quad (4.11)$$

Using (4.6), (4.7), and (4.10) one finds that

$$\mathbf{L}\mathbf{v} = (\mathbf{K} + \mathbf{M})(\tilde{\mathbf{z}} + \tilde{\mathbf{w}}) = \mathbf{M}\tilde{\mathbf{z}} + \tilde{\mathbf{w}} + \mathbf{M}\tilde{\mathbf{w}}, \quad (4.12)$$

and since $\mathbf{L}\mathbf{v} = \mathbf{v} = \tilde{\mathbf{z}} + \tilde{\mathbf{w}}$, it follows from (4.12) that

$$\tilde{\mathbf{z}} = (\mathbf{I} - \mathbf{M})^{-1}\mathbf{M}\tilde{\mathbf{w}}. \quad (4.13)$$

Applying \mathbf{K} to both sides of (4.13) and using (4.10) we obtain

$$\mathbf{K}(\mathbf{I} - \mathbf{M})^{-1}\mathbf{M}\tilde{\mathbf{w}} = \mathbf{0}. \quad (4.14)$$

Moreover, since $\mathbf{K}\tilde{\mathbf{w}} = \tilde{\mathbf{w}}$, (4.14) can be written as

$$\mathbf{K}(\mathbf{I} - \mathbf{M})^{-1}\mathbf{M}\mathbf{K}\tilde{\mathbf{w}} = \mathbf{0}. \quad (4.15)$$

Clearly, the subspace \mathcal{S} is an invariant subspace of the matrix $\tilde{\mathbf{T}}$, given by

$$\tilde{\mathbf{T}} \equiv \mathbf{K}(\mathbf{I} - \mathbf{M})^{-1}\mathbf{M}\mathbf{K}. \quad (4.16)$$

Let $\{n_j\}$ be the set of indices in \mathfrak{s}_δ , ordered in increasing order, that is, $n_k > n_j$ if $k > j$. A reduced matrix \mathbf{T} is defined by

$$T_{j,k} \equiv \tilde{T}_{n_j, n_k}. \quad (4.17)$$

Since $\mathbf{K}\tilde{\mathbf{w}} = \tilde{\mathbf{w}}$ we also define a reduced vector \mathbf{w} as

$$w_j \equiv \tilde{w}_{n_j}, \quad (4.18)$$

with $w_0 = \tilde{w}_0$. Equation (4.15) is thus equivalent to the reduced equation

$$\mathbf{T}\mathbf{w} = \mathbf{0}. \quad (4.19)$$

Clearly, (4.19) is equivalent to the original problem (4.7), since once $\tilde{\mathbf{w}}$ is known $\tilde{\mathbf{z}}$ is obtained from (4.13) which in turn yields \mathbf{v} by (4.11). Below, \mathbf{T} and $\tilde{\mathbf{T}}$ are fre-

quently used, the difference being only in the renaming of indices in the appropriate spaces. The same holds for other quantities, such as \mathbf{w} and $\tilde{\mathbf{w}}$.

Equation (4.19) is a linear homogeneous system for \mathbf{w} in the subspace \mathcal{S} . Upon separating the zeroth component from the others, Eq. (4.19) assumes the form

$$T_{0,0}w_0 + \sum_{j \neq 0} T_{0,j}w_j = 0 \quad (4.20)$$

and

$$\sum_{j \neq 0} T_{k,j}w_j = -T_{k,0}w_0 \quad \text{for } k \neq 0. \quad (4.21)$$

The vector \mathbf{e}_0 , whose components are $e_{0,j} = \delta_{0,j}$, is in the subspace \mathcal{S} . We denote the orthogonal complement of \mathbf{e}_0 in \mathcal{S} by \mathcal{S}' . The reduction of the matrix \mathbf{T} to \mathcal{S}' , by removing its zeroth row and column, is denoted by \mathbf{R} , that is,

$$R_{k,j} \equiv T_{k,j} \quad \text{for } k \neq 0 \text{ and } j \neq 0. \quad (4.22)$$

Next, the vector \mathbf{w} is decomposed into its projection on \mathbf{e}_0 and its complement \mathbf{u} in \mathcal{S}' ,

$$\mathbf{w} = \mathbf{u} + w_0\mathbf{e}_0. \quad (4.23)$$

Finally, the component of the right-hand side of (4.21) in \mathcal{S}' is denoted by \mathbf{g} , that is,

$$g_k \equiv -T_{k,0}w_0. \quad (4.24)$$

In this notation (4.21) can be written as

$$\mathbf{R}\mathbf{u} = \mathbf{g}, \quad (4.25)$$

or

$$\mathbf{u} = \mathbf{R}^{-1}\mathbf{g}, \quad (4.26)$$

assuming \mathbf{R} is nonsingular in \mathcal{S}' (this is shown below). Equation (4.26) can be written as

$$u_k = -\sum_{j \neq 0} \{R^{-1}\}_{k,j} T_{j,0}w_0 \quad \text{for } k \neq 0. \quad (4.27)$$

For the purpose of calculation of \mathbf{v} , we may assume that $w_0 = 1$ or any other nonzero normalization constant. The true value of w_0 is found from the requirement that the integral of $p(x)$ is 1 [see (2.6)].

Equations (4.11)–(4.27) constitute a formal solution of the eigenvalue problem (4.7). Equation (4.27) expresses u_k through w_0 and matrices which are derivable from \mathbf{L} . The vector $\tilde{\mathbf{w}}$ is obtained from (4.23), then $\tilde{\mathbf{z}}$ is obtained from (4.13). Thus the eigenvector \mathbf{v} , given by $\mathbf{v} = \tilde{\mathbf{z}} + \tilde{\mathbf{w}}$, is directly expressible through known matrices. Next we show how this formalism can be employed in a perturbative calculation.

B. Perturbation analysis for small ϵ

The matrix \mathbf{T} plays a fundamental role in our analysis and its properties are studied below. First we con-

sider the matrix \mathbf{M} [see (4.6)]. Let \mathbf{M}^0 represent \mathbf{M} for $\eta = 0$, set $\eta^2\delta\mathbf{M} \equiv \mathbf{M} - \mathbf{M}^0$, and $\eta^2\delta\mathbf{L} \equiv \mathbf{L} - \mathbf{L}^0$. Since $\mathbf{L} = \mathbf{K} + \mathbf{M}$ and \mathbf{K} is independent of η [see (4.5)], we have $\eta^2\delta\mathbf{L} = \eta^2\delta\mathbf{M}$. Note that terms of order η do not appear in the expansion of \mathbf{L} due to the assumption $(\xi_n) = 0$. It follows that

$$\begin{aligned} (\mathbf{I} - \mathbf{M})^{-1} &= (\mathbf{I} - \mathbf{M}^0 - \eta^2\delta\mathbf{L})^{-1} \\ &= [\mathbf{I} - \eta^2(\mathbf{I} - \mathbf{M}^0)^{-1}\delta\mathbf{L}]^{-1} (\mathbf{I} - \mathbf{M}^0)^{-1}. \end{aligned} \quad (4.28)$$

Since both \mathbf{L} and \mathbf{K} are diagonal so is $\mathbf{M}^0 \equiv \mathbf{L}^0 - \mathbf{K}$. From the definitions (4.6) of \mathbf{M} and (4.5) of \mathbf{K} , and the value (4.2) of $L_{n,m}^0$, we have

$$M_{j,j}^0 \equiv \begin{cases} e^{-2i\theta j} - 1 & \text{if } j \in \mathbf{s}_\delta, \\ e^{-2i\theta j} & \text{otherwise.} \end{cases} \quad (4.29)$$

and

$$I - M_{j,j}^0 \equiv \begin{cases} 2 - e^{-2i\theta j} & \text{if } j \in \mathbf{s}_\delta, \\ 1 - e^{-2i\theta j} & \text{otherwise.} \end{cases} \quad (4.30)$$

Expanding (4.28) formally in powers of $\eta^2\delta\mathbf{L}$, where $\delta\mathbf{L}$ depends on η , we see that at order η^{2n} , the expansion contains a product of $n+1$ terms $(\mathbf{I} - \mathbf{M}^0)^{-1}$. From the definitions (4.4) of \mathbf{s}_δ and (4.29) of \mathbf{M}^0 we have $|(\mathbf{I} - \mathbf{M}^0)_{j,j}| \geq \delta$, so that terms of order η^{2n} are bounded by $\eta^{2n}\delta^{-n-1}$, multiplied by products of matrix elements of $\delta\mathbf{L}$ which are $O(\eta^0)$. It follows that for any $\eta^2 \ll \delta$ the perturbative expansion of $(\mathbf{I} - \mathbf{M})^{-1}$ in powers of $\eta^2\delta\mathbf{L}$ is well defined. Moreover, as is shown below, the result is independent of the choice of δ in the range $\eta \ll \delta < 1$. Next, the operator \mathbf{L} in (3.9) can be expanded in a power series in the small parameter η as

$$\mathbf{L} = \mathbf{L}^0 + \eta^2\mathbf{L}^2 + \dots \quad (4.31)$$

Note that $\mathbf{L}^1 \equiv \mathbf{0}$, as can be seen directly from (3.9) and from the assumption $(\xi_n) = 0$. The matrix elements $L_{m,n}^i$ ($i = 2, 3, 4$) are given in Appendix C. Also, it is easy to see that the matrix element $L_{k,0}$ is of order η^k . Using (4.28) and (4.31), the matrix $\tilde{\mathbf{T}}$ can be expanded in powers of η as $\tilde{\mathbf{T}} = \sum_{i=0}^{\infty} \eta^i \tilde{\mathbf{T}}^i$, the leading order being a diagonal matrix with diagonal entries

$$T_{j,j}^0 = \frac{-1 + e^{-2i\theta n_j}}{2 - e^{-2i\theta n_j}}, \quad (4.32)$$

where the indices correspond to the subspace \mathcal{S} . Also, $\tilde{\mathbf{T}}^1 = \mathbf{0}$ since $\mathbf{L}^1 = \mathbf{0}$. It follows from (4.32) that $|\tilde{T}_{j,j}^0| = O(\delta)$. It can vanish, of course, for θ a rational multiple of π and appropriate values of n_j . Following (4.16) and (4.28) one obtains

$$\tilde{\mathbf{T}}^2 = \mathbf{K}(\mathbf{I} - \mathbf{M}^0)^{-1}\mathbf{L}^2(\mathbf{I} - \mathbf{M}^0)^{-1}\mathbf{K}, \quad (4.33)$$

and using $\mathbf{L}^1 = \mathbf{0}$

$$\tilde{\mathbf{T}}^3 = \mathbf{K}(\mathbf{I} - \mathbf{M}^0)^{-1}\mathbf{L}^3(\mathbf{I} - \mathbf{M}^0)^{-1}\mathbf{K}. \quad (4.34)$$

According to the discussion following (4.30) $\tilde{\mathbf{T}}^0 = O(\delta)$, $\eta^2\tilde{\mathbf{T}}^2 = O(\eta^2)$, and $\eta^3\tilde{\mathbf{T}}^3 = O(\eta^3)$. The coefficient

of η^4 in the expansion of $\tilde{\mathbf{T}}$ is

$$\begin{aligned} \tilde{\mathbf{T}}^4 &= \mathbf{K}(\mathbf{I} - \mathbf{M}^0)^{-1}\mathbf{L}^2(\mathbf{I} - \mathbf{M}^0)^{-1}\mathbf{L}^2(\mathbf{I} - \mathbf{M}^0)^{-1}\mathbf{K} \\ &\quad + \mathbf{K}(\mathbf{I} - \mathbf{M}^0)^{-1}\mathbf{L}^4(\mathbf{I} - \mathbf{M}^0)^{-1}\mathbf{K} \end{aligned} \quad (4.35)$$

and $\eta^4\tilde{\mathbf{T}}^4 = O(\eta^4\delta^{-1})$. In general, at order η^{2n} , $n \geq 2$, we have $\eta^{2n}\tilde{\mathbf{T}}^{2n} = O(\eta^{2n}\delta^{-n+1})$ and $\eta^{2n+1}\tilde{\mathbf{T}}^{2n+1} = O(\eta^{2n+1}\delta^{-n+1})$. A similar statement is true for the matrix \mathbf{T} and the matrices \mathbf{T}^i , which contain only indices corresponding to the subspace \mathcal{S} . Since by assumption $\delta \gg \eta^2$, we can separate \mathbf{T} into

$$\mathbf{T} = \mathbf{A} + \mathbf{B}, \quad (4.36)$$

where

$$\mathbf{A} = \mathbf{T}^0 + \eta^2\mathbf{T}^2 \quad (4.37)$$

and

$$\mathbf{B} = \eta^3\mathbf{T}^3 + \eta^4\mathbf{T}^4 + \dots \quad (4.38)$$

The term \mathbf{A} is a sum of an $O(\eta^2)$ contribution and one that is $O(\delta)$, i.e., \mathbf{T}^0 , and it can be dominated by either one of them. The terms in \mathbf{B} are $O(\eta^3)$ or $O(\eta^4\delta^{-1})$, depending on η and δ , and they are easily seen to be of subdominant order with respect to \mathbf{A} . Thus

$$R_{k,j} = A_{k,j} + B_{k,j}, \quad k \neq 0, j \neq 0, \quad (4.39)$$

where \mathbf{R} is defined in (4.22) and \mathbf{R}^{-1} can be written as

$$\mathbf{R}^{-1} = \sum_{n=0}^{\infty} (-\mathbf{A}^{-1}\mathbf{B})^n \mathbf{A}^{-1}, \quad (4.40)$$

provided \mathbf{A}^{-1} exists, which is shown below. Using (4.31)–(4.33) and the expression (C4) (see Appendix C) we obtain

$$\begin{aligned} A_{k,j} &= \delta_{k,j} \frac{-1 + e^{-2i\theta n_j}}{2 - e^{-2i\theta n_j}} \\ &\quad + \eta^2 \frac{L_{n_k, n_j}^2}{(2 - e^{-2i\theta n_k})(2 - e^{-2i\theta n_j})}. \end{aligned} \quad (4.41)$$

Recall that j and k are indices in \mathcal{S}' , and therefore do not vanish, whereas n_j and n_k are the corresponding indices in the original space. Since $L_{n, n \pm i}^2 = 0$ for $i > 2$ (see Appendix C), the matrix \mathbf{L}^2 is diagonal, unless

$$|e^{-2i\theta n} - 1| < \delta$$

$$\text{and either } |e^{-2i\theta(n+2)} - 1| < \delta$$

$$\text{or } |e^{-2i\theta(n+1)} - 1| < \delta \quad (4.42)$$

for some n . The latter can be avoided if

$$\delta < \min\{|\sin 2\theta|, |\sin \theta|\}. \quad (4.43)$$

When $\theta - k\pi/2 = o(\epsilon^2)$ ($k = 0, 1, 2$), no choice of $\delta > \epsilon^2$ can satisfy condition (4.42). Consequently, the matrix \mathbf{L}^2 is not diagonal. The cases $k = 0, 2$ correspond to the band edge and are considered in Sec. VII. The case $k = 1$ corresponds to the band center and is considered

in Sec. VI. If θ is neither in the band center nor in the band edge, \mathbf{L}^2 is diagonal (in \mathcal{S}'), hence so are \mathbf{T}^2 and \mathbf{A} . Also, in the subspace \mathcal{S}' the diagonal elements of the matrix \mathbf{T} are nonvanishing since $L_{n,n}^2$ is proportional to n^2 and $n \neq 0$ (see Appendix C). For θ in the vicinity of the band center, that is, $\theta \approx \pi/2$, the matrix \mathbf{T}^2 is tridiagonal.

Note that the construction of the perturbation expansion is based on Eq. (4.40). Thus, as long as one can (technically) invert the matrix \mathbf{A} , the perturbative scheme is well defined and can be implemented. This scheme is then uniformly valid *throughout the band*. The above specification of the value of δ satisfying inequality (4.43) is made for the sake of simplifying the procedure, since obviously it is easy to invert a diagonal matrix. Since this simplification cannot be achieved in the band-edge and band-center regions for any choice of δ , one must invert, in the latter regions, a tridiagonal matrix. The physical results, in any case, should be (and indeed are) independent of the choice of δ .

Next, at order η^3 the matrix \mathbf{L}^3 connects the index n to indices $n+j$, for $-3 \leq j \leq 3$. Thus \mathbf{T}^3 is diagonal, unless there is an n such that

$$|e^{-2i\theta n} - 1| < \delta \quad \text{and} \quad |e^{-2i\theta(n+3)} - 1| < \delta. \quad (4.44)$$

Hence \mathbf{T}^3 is diagonal if

$$\delta < |\sin 3\theta|. \quad (4.45)$$

By assumption (4.42) the subspace \mathcal{S}' does not contain indices differing by less than 3. When θ is in an $O(1)$ neighborhood of $\pi/3$ or $2\pi/3$ such that

$$|\sin 3\theta| < \delta < |\sin 2\theta|, \quad (4.46)$$

\mathbf{T}^3 is not diagonal. In general, for any angle θ and any given value of δ , the smallest n for which \mathbf{T}^n is not diagonal is obtained as follows. First the smallest integer q is determined such that there is an index n for which the inequalities

$$|e^{-2i\theta n} - 1| < \delta \quad \text{and} \quad |e^{-2i\theta(n+q)} - 1| < \delta \quad (4.47)$$

hold simultaneously, e.g., $\theta = p\pi/q + \delta\sigma/q$ with $0 \leq \sigma \leq 1$. The matrix \mathbf{T}^i for this particular angle θ is diagonal in \mathcal{S}' for $i < q$ and ceases to be diagonal for $i \geq q$. Moreover, it is easy to see that the off-diagonal part of \mathbf{T} is $O(\eta^q)$. This implies that $\mathbf{g} = O(\eta^q)$ [see (4.24)]. All in all, the required vector \mathbf{u} , that is, the projection of $\tilde{\mathbf{w}}$ on \mathcal{S}' , is given by

$$u_k = -w_0 \sum_{j \neq 0} \eta^q A_{k,j}^{-1} (T^q)_{j,0} + \text{higher-order terms in } \eta \quad (4.48)$$

and $u_k = O(\eta^{q-2})$ or $u_k = O(\eta^q \delta^{-1})$, depending on θ and j . As mentioned above, it is found below that the final result is independent of the choice of δ . Different choices of δ correspond to different decompositions of \mathbf{v} into $\tilde{\mathbf{w}} + \tilde{\mathbf{z}}$. As already mentioned, inside the band, that is, for $|\theta - \pi/2| > \delta$, the problem simplifies, because \mathbf{A} is then diagonal and can be trivially inverted.

Finally, the Fourier series corresponding to the vectors

$\tilde{\mathbf{w}}, \tilde{\mathbf{z}}, \mathbf{v}$ define the functions $\tilde{w}(\phi), \tilde{z}(\phi)$, and the probability distribution function $p(\phi)$ in the form

$$p(\phi) = \sum_{j=-\infty}^{\infty} v_j e^{2ij\phi}, \quad (4.49)$$

$$\tilde{w}(\phi) = \sum_{j=-\infty}^{\infty} \tilde{w}_j e^{2ij\phi}, \quad \text{with } \tilde{w}_j = 0 \text{ for } j \notin \mathbf{s}_\delta, \quad (4.50)$$

and

$$\tilde{z}(\phi) = \sum_{j=-\infty}^{\infty} z_j e^{2ij\phi}, \quad \text{with } z_j = 0 \text{ for } j \in \mathbf{s}_\delta. \quad (4.51)$$

Obviously

$$p(\phi) = \tilde{w}(\phi) + \tilde{z}(\phi) \quad (4.52)$$

[see (2.13)].

V. THE IN-BAND CASE: RESULTS

It has been shown in Sec. IV that, as long as θ is not close to the band center or to the band edge, the matrix \mathbf{A} in (4.41) is diagonal. Its j th diagonal element is given by

$$A_{j,j} = \frac{-1 + e^{-2i\theta n_j}}{2 - e^{-2i\theta n_j}} - \frac{3}{4} \eta^2 n_j^2 \frac{e^{-2i\theta n_j}}{(2 - e^{-2i\theta n_j})^2}. \quad (5.1)$$

Note that $A_{j,j}$ is proportional to η^2 when $e^{2i\theta j} = 1$, otherwise $A_{j,j} = O(\delta + \eta^2)$. The expansion given in (4.40) is in powers of $\mathbf{A}^{-1}\mathbf{B}$. Since, by Eq. (4.38), $\mathbf{B} = O(\eta^3)$ when \mathbf{T}^3 contains a nonvanishing $O(1)$ contribution (otherwise \mathbf{B} is of higher order than η^3), the mentioned expansion (4.40) is not a power series expansion in η . Rather, it is an expansion in a family of functions of the form

$$\frac{O(\eta^3)}{O(\delta) + O(\eta^2)} = \eta \frac{O(\eta^2)}{O(\delta) + O(\eta^2)}. \quad (5.2)$$

Therefore (4.40) is not a naive series expansion in powers of η , but rather a singular perturbation expansion which is asymptotic in the sense of Poincaré. The coefficients contain layer terms which peak at values of θ , for which $\theta = \pi\alpha$ and α is a rational number. These terms are analytic functions of θ in the band as long as $\eta \neq 0$, i.e., $\epsilon \neq 0$. Obviously, an expansion in powers of ϵ yields coefficients which are discontinuous functions of θ .¹⁹ As θ approaches $\pi\alpha$ with α a rational number, a term $A_{j,j}$, for some j , is dominated by the η^2 term in (5.2). Accordingly, a term in the expansion which may seem to be of order η^q is actually of order η^{q-2} at this θ . This is the manifestation of the internal layer structure of the probability distribution function $p(\phi)$.

In this section the probability distribution function $p(\phi)$ is calculated perturbatively in η for in-band angles θ . As explained in Sec. IV, the pertinent perturbation theory encounters no singularities at any order. Explicit expressions for the perturbation terms are derived below up to second order in η .

The first step consists in finding the smallest values of p and q such that

$$\theta = \frac{p}{q}\pi + \sigma\delta, \quad q \geq 3 \text{ and } 0 \leq \sigma < 1. \quad (5.3)$$

From (4.27) the components of \mathbf{u} are found to be

$$u_k = -\eta^q w_0 \sum_{j=-\infty}^{\infty} [\mathbf{A}^{-1} - \mathbf{A}^{-1}\mathbf{B}\mathbf{A}^{-1} + \dots]_{k,j} \times \left(T_{j,0}^q + \eta T_{j,0}^{q+1} + \dots \right), \quad (5.4)$$

where $q \geq 3$. The right-hand side of (5.4) can be expanded in a power series in η and η^2/δ and is of the form

$$\mathbf{u} = \frac{O(\eta^q)}{O(\delta) + O(\eta^2)}, \quad (5.5)$$

and the nonzero components of the vector \mathbf{w} are w_0 and $w_{n_j} = u_j$. Next the leading terms in (5.4) are considered. For $q = 3$ (5.4) is written as

$$\begin{aligned} \mathbf{u} &= -\eta^3 w_0 [(\mathbf{I} - \mathbf{A}^{-1}\mathbf{B})\mathbf{A}^{-1}\mathbf{T}_0^3 + \eta\mathbf{A}^{-1}\mathbf{T}_0^4 \\ &\quad - \eta\mathbf{A}^{-1}\mathbf{B}\mathbf{A}^{-1}\mathbf{T}_0^4 + \dots] \\ &\equiv \tilde{\mathbf{w}}^{\pi/3} + \eta\tilde{\mathbf{w}}^{\pi/4} + \text{higher-order terms}, \end{aligned} \quad (5.6)$$

where \mathbf{T}_0^i is the zeroth column of the corresponding matrix. The first term in (5.6), $\tilde{\mathbf{w}}^{\pi/3} \equiv -\eta^3 w_0 (\mathbf{I} - \mathbf{A}^{-1}\mathbf{B})\mathbf{A}^{-1}\mathbf{T}_0^3$, can be $O(\eta)$, if θ is close to $\pi/3$, or $O(\eta^3)$ otherwise. Similarly, the term $\tilde{\mathbf{w}}^{\pi/4} \equiv \eta^4 w_0 \mathbf{A}^{-1}\mathbf{T}_0^4$ is $O(\eta^2)$ if θ is close to $\pi/4$, or $O(\eta^4)$ otherwise. The higher-order terms constitute a remainder which is uniformly $O(\eta^3)$ for all θ in the band. Converting back to the Fourier space, the asymptotic form of $w(\phi)$ up to $O(\eta^3)$ is given by

$$w(\phi) = w_0 + w^{\pi/3}(\phi) + w^{\pi/4}(\phi) + O(\eta^3), \quad (5.7)$$

where, as mentioned above, $w^{\pi/3}(\phi)$ peaks at $\theta = \pi/3$ and $w^{\pi/4}(\phi)$ peaks at $\theta = \pi/4$. Note that (5.7) holds with uniform error in the band, away from the band-center and the band-edge regions.

First we consider $w^{\pi/3}(\phi)$. In this case $T_{j,0}^3 \neq 0$ only if $j = \pm 1$, which corresponds to $n_{\pm 1} = \pm 3$ and to

$$|e^{\pm 6i\theta} - 1| < \delta. \quad (5.8)$$

This in turn corresponds to values of θ in an $O(\delta)$ neigh-

borhood of $\pi/3$ or of $2\pi/3$ [cf. (4.45)]. Note that, due to the construction of the subspace \mathcal{S} , $\tilde{\mathbf{w}}^{\pi/3}$ vanishes if (5.8) is not satisfied. Thus $\tilde{\mathbf{w}}$ is not an analytic function of θ . However, together with its complement $\tilde{\mathbf{z}}$ it adds up to the analytic function \mathbf{v} (see Ref. 21). Thus, when (5.8) holds, $n_0 = 0$, $n_{\pm 1} = \pm 3$, $n_{\pm 2} = \pm 4$, $n_{\pm 3} = \pm 6$. Now from (4.34) and (C5) it follows that

$$\begin{aligned} \tilde{w}_3^{\pi/3} &= -w_0 \left\{ 1 - \frac{1}{1 - M_{3,3}^0} \eta^3 L_{3,3}^3 \frac{1}{1 - M_{3,3}^0} \frac{1}{A_{3,3}} \right\} \\ &\quad \times \left\{ \frac{1}{1 - M_{3,3}^0} \eta^3 L_{3,0}^3 \frac{1}{1 - M_{0,0}^0} \frac{1}{A_{3,3}} \right\} + O(\eta^3), \end{aligned} \quad (5.9)$$

and $\tilde{w}_{-3}^{\pi/3} = \tilde{w}_3^{\pi/3*}$, where $*$ denotes complex conjugation. Similarly,

$$\begin{aligned} \tilde{w}_6^{\pi/3} &= -w_0 \left\{ \frac{1}{1 - M_{6,6}^0} \eta^3 L_{6,3}^3 \frac{1}{1 - M_{3,3}^0} \frac{1}{A_{6,6}} \right\} \\ &\quad \times \left\{ \frac{1}{1 - M_{3,3}^0} \eta^3 L_{3,0}^3 \frac{1}{1 - M_{0,0}^0} \frac{1}{A_{3,3}} \right\} + O(\eta^3). \end{aligned} \quad (5.10)$$

Using (5.1), one obtains

$$\begin{aligned} \mathcal{X} &\equiv \left\{ \frac{1}{1 - M_{3,3}^0} \frac{1}{1 - M_{0,0}^0} \frac{1}{A_{3,3}} \right\} \\ &= \frac{2e^{6i\theta} - 1}{6 \sin^2 3\theta - (27\langle \xi^2 \rangle / 4)\eta^2 - i \sin 6\theta}, \end{aligned} \quad (5.11)$$

and $\tilde{w}_{-6}^{\pi/3} = \tilde{w}_6^{\pi/3*}$. Again, from (C5) one finds that

$$\begin{aligned} L_{3,0}^3 &= -i \frac{\langle \xi^3 \rangle}{8}, \quad L_{3,3}^3 = 23ie^{-6i\theta} \langle \xi^3 \rangle, \\ L_{6,3}^3 &= -\frac{5i}{2} e^{-6i\theta} \langle \xi^3 \rangle, \quad L_{6,6}^2 = -27e^{-12i\theta} \langle \xi^2 \rangle. \end{aligned} \quad (5.12)$$

Hence

$$\tilde{w}_3^{\pi/3} = \frac{i\eta^3 w_0 \langle \xi^3 \rangle}{8} \left(1 - \frac{23\eta^3 i e^{-6i\theta} \langle \xi^3 \rangle}{2e^{6i\theta} - 1} \mathcal{X} \right) \mathcal{X}, \quad (5.13)$$

and

$$\tilde{w}_6^{\pi/3} = \frac{5\eta^6 w_0 \langle \xi^3 \rangle^2}{16} \frac{\cos 6\theta + 3i \sin 6\theta}{(2 - e^{-6i\theta})(6 \sin^2 6\theta - i \sin 12\theta - 27\eta^2 \langle \xi^2 \rangle)} \mathcal{X}. \quad (5.14)$$

Note that when $\theta - \pi/3 = O(\eta^2)$ or $\theta - 2\pi/3 = O(\eta^2)$, the denominator in (5.11) is proportional to η^2 so that $\mathcal{X} = O(\eta^{-2})$. It follows that $\tilde{w}_3^{\pi/3} = O(\eta)$. Similarly, $\tilde{w}_6^{\pi/3} = O(\eta^2)$. In the Fourier space one obtains

$$w^{\pi/3}(\phi) = 2\text{Ree}(\tilde{w}_3^{\pi/3} e^{6i\phi} + \tilde{w}_6^{\pi/3} e^{12i\phi}). \quad (5.15)$$

Note that (5.15) is not uniformly $O(\eta^3)$, since due to internal layers it may be $O(\eta)$ for certain values of θ . It is the leading-order term in the asymptotic expansion of $w(\phi)$ only for θ near $\pi/3$ and becomes subdominant to $w^{\pi/4}(\phi)$ for θ near $\pi/4$, as shown below. The layer behavior of $w(\phi)$ as a function of θ for $\theta - \pi/3 = O(\eta^2)$ is best exhibited in terms of the layer variable

$$y \equiv \frac{\pi/3 - \theta}{\eta^2} \quad (5.16)$$

as

$$w(\phi) = w_0 + \frac{w_0 \eta \langle \xi^3 \rangle}{3(64y^2 + 81)} (8y \cos 6\phi + 9 \sin 6\phi) + O(\eta^2). \quad (5.17)$$

This behavior is due to the contribution of $w_3^{\pi/3}(\phi)$, since $w_6^{\pi/3}(\phi) = O(\eta^2)$ in this neighborhood. As y becomes $O(\eta^{-1})$ the leading-order correction to w_0 in Eq. (5.17) is $O(\eta^2)$.

Next we consider $w^{\pi/4}(\phi)$. When δ is chosen sufficiently small [though $O(1)$ for small η] to ensure that \mathbf{A} is diagonal for a large range of values of θ , it is obvious that for θ near $\pi/4$ or $3\pi/4$ it is impossible to satisfy inequality (5.8). Instead, the requirement is

$$|e^{\pm 8i\theta} - 1| < \delta. \quad (5.18)$$

Similarly to the previous case, if (5.18) is not satisfied, $\tilde{\mathbf{w}}^{\pi/4} = 0$. The lowest-order term in (5.4) has the coefficient η^4 for θ in a δ neighborhood of $\pi/4$. Since \mathbf{A} is diagonal the leading-order term in the expansion of \mathbf{B} yields

$$\tilde{w}_4^{\pi/4} = -\eta^4 w_0 \mathbf{A}_{4,4}^{-1} \tilde{T}_{4,0}^4, \quad (5.19)$$

and $\tilde{w}_{-4}^{\pi/4} = \tilde{w}_4^{\pi/4*}$. From (4.35)

$$T_{4,0}^4 = \frac{1}{1 - M_{4,4}^0} L_{4,2}^2 \frac{1}{1 - M_{2,2}^0} L_{2,0}^2 \frac{1}{1 - M_{0,0}^0} + \frac{1}{1 - M_{4,4}^0} L_{4,0}^4 \frac{1}{1 - M_{0,0}^0}. \quad (5.20)$$

Using (C4) and (C6) in (5.20) one obtains

$$\tilde{w}_4^{\pi/4} = -\frac{\eta^4 w_0}{16} \left(\frac{\langle \xi^4 \rangle}{2} + \frac{3\langle \xi^2 \rangle^2 e^{-2i\theta}}{2i \sin 2\theta} \right) \times \frac{1}{6 \sin^2 4\theta - i \sin 8\theta - 12\eta^2 \langle \xi^2 \rangle} + O(\eta^3). \quad (5.21)$$

The remainder term is uniformly $O(\eta^3)$. As in the case considered above, if $\theta - \pi/4 = O(\eta^2)$ or $\theta - 3\pi/4 = O(\eta^2)$, then $\tilde{w}_4^{\pi/4} = O(\eta^2)$. The contribution of $\tilde{w}_3^{\pi/3}$ and $\tilde{w}_6^{\pi/3}$ in these neighborhoods is $O(\eta^3)$ so that it is contained in the remainder term. Similarly, the term of order η^4 in (5.21) is contained in the remainder term in (5.13) for θ near $\pi/3$ or $2\pi/3$. Thus $w^{\pi/4}(\phi)$ is given by

$$w^{\pi/4}(\phi) = -\frac{\eta^4 w_0}{8} \operatorname{Re} \sum_{\lambda=\pm 1} \left(\frac{\langle \xi^4 \rangle}{2} + \frac{3\langle \xi^2 \rangle^2 e^{-2i\theta\lambda}}{2i \sin 2\theta\lambda} \right) \times \frac{e^{8i\phi}}{6 \sin^2 4\theta\lambda - i \sin 8\theta\lambda - 12\eta^2 \langle \xi^2 \rangle}. \quad (5.22)$$

If for a given δ and θ both (5.8) and (5.18) are satisfied, then $w^{\pi/3}(\phi)$ and $w^{\pi/4}(\phi)$ do not vanish. It is obvious that for such θ both terms are $O(\eta^3)$.

It is evident that the expansion (5.4) with $q = 3$ can be continued to obtain a uniform asymptotic representation of $w(\phi)$ for all θ in the band with arbitrarily small

error. However this is not the most efficient method for expanding $w(\phi)$ for a given θ and a given order of accuracy. A more efficient way is first to determine q as the smallest positive integer such that $|\sin q\theta| < \delta$. Then the leading-order contribution to \mathbf{B} is $O(\eta^q)$ or $O(\eta^{q-2})$, depending on whether $|\sin q\theta| = O(1)$ for small η or not. For $q > 4$ this construction yields terms which are uniformly of higher order than η^2 .

In order to construct the full vector \mathbf{v} , it remains to calculate the vector $\tilde{\mathbf{z}}$ in (4.9) (in the subspace \mathcal{S}). Using the obvious identity

$$(\mathbf{I} - \mathbf{M})^{-1}(\mathbf{M} - \mathbf{I} + \mathbf{I}) = -\mathbf{I} + (\mathbf{I} - \mathbf{M})^{-1} \quad (5.23)$$

in (4.28) we obtain from (4.9)

$$\begin{aligned} \tilde{\mathbf{z}} = & -\tilde{\mathbf{w}} + (\mathbf{I} - \mathbf{M}^0)^{-1} \tilde{\mathbf{w}} + \eta^2 [(\mathbf{I} - \mathbf{M}^0)^{-1} \\ & \times \delta \mathbf{L} (\mathbf{I} - \mathbf{M}^0)^{-1}] \tilde{\mathbf{w}} \\ & + \eta^4 [(\mathbf{I} - \mathbf{M}^0)^{-1} \delta \mathbf{L} (\mathbf{I} - \mathbf{M}^0)^{-1} \delta \mathbf{L} (\mathbf{I} - \mathbf{M}^0)^{-1}] \tilde{\mathbf{w}} \\ & + \dots \end{aligned} \quad (5.24)$$

Recall that, by definition, $\tilde{\mathbf{z}}$ is orthogonal to \mathcal{S} . It follows that the leading contribution in (5.24) is $O(\eta^2)$. From (4.23) $\tilde{\mathbf{w}} = \mathbf{u} + w_0 \mathbf{e}_0$, so that the leading-order term is $\tilde{\mathbf{w}} = w_0 \mathbf{e}_0 + O(\eta)$. Therefore (5.24) can be written as

$$\tilde{\mathbf{z}} = \eta^2 w_0 (\mathbf{I} - \mathbf{M}^0)^{-1} \mathbf{e}_0 + \mathbf{r}_2, \quad (5.25)$$

where $\mathbf{r}_2 = o(\eta^2)$. Denoting the first term on the right-hand side of (5.25) by $\tilde{\mathbf{z}}^2$ one obtains for the components \tilde{z}_j of $\tilde{\mathbf{z}}$ the expressions

$$\tilde{z}_1^2 = \frac{\eta^2}{1 - M_{1,1}^0} L_{10}^2 \frac{1}{1 - M_{0,0}^0} = \frac{\eta^2}{2} \frac{1}{1 - e^{-2i\theta}} \quad (5.26)$$

and

$$\tilde{z}_2^2 = \frac{\eta^2}{4} \frac{1}{1 - e^{-4i\theta}}. \quad (5.27)$$

Also $\tilde{z}_{-m}^2 = (\tilde{z}_m^2)^*$, where $*$ denotes the complex conjugate. The remaining components of $\tilde{\mathbf{z}}^2$ vanish. The function corresponding to $\tilde{\mathbf{z}}^2$ is given by

$$z^2(\phi) = \frac{\eta^2 w_0}{2} \operatorname{Re} \left[\frac{e^{2i\phi}}{1 - e^{-2i\theta}} - \frac{e^{4i\phi}}{1 - e^{-4i\theta}} \right]. \quad (5.28)$$

By (5.24) the remainder term \mathbf{r}_2 in (5.25) can be written as

$$\mathbf{r}_2 = \eta^3 (\mathbf{I} - \mathbf{M}^0)^{-1} \mathbf{L}^3 (\mathbf{I} - \mathbf{M}^0)^{-1} \mathbf{w}^0 + \eta^2 (\mathbf{I} - \mathbf{M}^0)^{-1} \mathbf{L}^2 (\mathbf{I} - \mathbf{M}^0)^{-1} \mathbf{u} + \mathbf{r}_3. \quad (5.29)$$

We keep in (5.29) only the leading term in the expansion of \mathbf{u} [see (5.9) and (5.19)]. Since $\mathbf{u} = O(\eta)$ for $\theta = \pi/3$ and $\mathbf{u} = O(\eta^2)$ if (5.8) does not hold, the second term in (5.29) is at worst $O(\eta^3)$, so that $\mathbf{r}_3 = o(\eta^3)$ uniformly for all θ in the band. If (5.8) does not hold, $\mathbf{u} = O(\eta^2)$ and the second term in (5.29) is $O(\eta^4)$. Defining

$$\mathbf{z}^3 \equiv \mathbf{r}_2 - \mathbf{r}_3, \quad (5.30)$$

one finds that when $q > 3$, that is, if (5.8) does not hold, then the second term in (5.29) can be included in the remainder and \mathbf{z}_k^3 reduces to

$$z_k^3 = \eta^3 w_0 \frac{L_{k,0}^3}{1 - M_{k,k}^0}, \quad \text{for } k = \pm 1, \pm 2, \pm 3. \quad (5.31)$$

To facilitate the notation the quantities

$$Z_k^3 \equiv \eta^3 w_0 \frac{L_{k,0}^3}{1 - M_{k,k}^0} \quad \text{for } k = \pm 1, \pm 2, \pm 3 \quad (5.32)$$

are introduced. Then (C5) gives

$$\begin{aligned} Z_1^3 &= \frac{\eta^3 - iw_0 \langle \xi^3 \rangle}{8} \frac{1}{1 - e^{-2i\theta}}, \\ Z_2^3 &= \frac{\eta^3 + iw_0 \langle \xi^3 \rangle}{4} \frac{1}{1 - e^{-4i\theta}}, \\ Z_3^3 &= \frac{\eta^3 - iw_0 \langle \xi^3 \rangle}{8} \frac{1}{1 - e^{-6i\theta}}, \end{aligned} \quad (5.33)$$

and $Z_{-k}^3 = (Z_k^3)^*$. When $q = 3$ the nonvanishing components of \mathbf{z} are

$$\begin{aligned} z_1^3 &= Z_1^3 + \frac{\eta^2}{1 - M_{1,1}^0} L_{1,3}^2 \frac{1}{1 - M_{3,3}^0} u_1, \\ z_2^3 &= Z_2^3 + \frac{\eta^2}{1 - M_{2,2}^0} L_{2,3}^2 \frac{1}{1 - M_{3,3}^0} u_1, \end{aligned} \quad (5.34)$$

$$\begin{aligned} z_4^3 &= \frac{\eta^2}{1 - M_{4,4}^0} L_{4,3}^2 \frac{1}{1 - M_{3,3}^0} u_1, \\ z_5^3 &= \frac{\eta^2}{1 - M_{5,5}^0} L_{5,3}^2 \frac{1}{1 - M_{3,3}^0} u_1. \end{aligned} \quad (5.35)$$

The term z_3^3 vanishes, since for $q = 3$ the component ± 3 belongs to \mathcal{S} . Also here $z_{-k}^3 = (z_k^3)^*$. Using (5.13) and (C4) in (5.34) one finds that

$$\begin{aligned} z_1^3 &= Z_1^3 - \eta^5 w_0 \frac{i \langle \xi^3 \rangle}{32} \frac{1}{1 - e^{-2i\theta}} \\ &\quad \times \frac{1}{6 \sin^2 3\theta + (27 \langle \xi^2 \rangle / 4) \eta^2 - i \sin 6\theta} \end{aligned} \quad (5.36)$$

$$\begin{aligned} z_2^3 &= Z_2^3 + \eta^5 w_0 \frac{5i \langle \xi^3 \rangle}{16} \frac{1}{1 - e^{-4i\theta}} \\ &\quad \times \frac{1}{6 \sin^2 3\theta + (27 \langle \xi^2 \rangle / 4) \eta^2 - i \sin 6\theta}, \\ z_4^3 &= \eta^5 w_0 \frac{7i \langle \xi^3 \rangle}{8} \frac{1}{1 - e^{-8i\theta}} \\ &\quad \times \frac{1}{6 \sin^2 3\theta + (27 \langle \xi^2 \rangle / 4) \eta^2 - i \sin 6\theta}, \end{aligned} \quad (5.37)$$

$$\begin{aligned} z_5^3 &= -\eta^5 w_0 \frac{5i \langle \xi^3 \rangle}{16} \frac{1}{1 - e^{-10i\theta}} \\ &\quad \times \frac{1}{6 \sin^2 3\theta + (27 \langle \xi^2 \rangle / 4) \eta^2 - i \sin 6\theta}. \end{aligned}$$

The terms of order η^5 peak to $O(\eta^3)$ when the denominator is $O(\eta^2)$, that is, when $\theta - \pi/3 = O(\eta^2)$ or $\theta - 2\pi/3 = O(\eta^2)$.

In conclusion, a hierarchy of approximations is constructed such that

$$\mathbf{z} = \mathbf{z}^2 + \mathbf{r}_2 \quad \text{and } \mathbf{r}_2 = o(\eta^2), \quad (5.38)$$

$$\mathbf{z} = \mathbf{z}^2 + \mathbf{z}^3 + \mathbf{r}_3 \quad \text{and } \mathbf{r}_3 = o(\eta^3)$$

and so on. This sequence of approximations constitutes an asymptotic expansion of \mathbf{z} . A similar expansion is constructed for \mathbf{w} .

The probability distribution function $p(\phi)$ can be represented asymptotically as

$$p(\phi) = w_n(\phi) + z_n(\phi) + r_n(\phi) + s_n(\phi), \quad (5.39)$$

where $r_n(\phi)$ and $s_n(\phi)$ are the remainders in the expansions of $z(\phi)$ and $w(\phi)$, respectively. The last terms in the expansions $z_n(\phi)$ and $w_n(\phi)$ are at worst $O(\eta^n)$ and the remainders are uniformly $o(\eta^n)$.

Finally, the asymptotic expansion of $p(\phi)$ yields asymptotic expressions for the Lyapunov exponent and for the density of states. The normalization

$$\int_0^\pi p(\phi) d\phi = 1 \quad (5.40)$$

fixes $w_0 = 1/\pi$. In terms of the original variable the leading term in the expansion of $p(x)$ is given by the Lorentzian

$$p_0(x) = p(\phi) \frac{d\phi}{dx} = \frac{1}{\pi} \frac{\sin \theta}{(x - \cos \theta)^2 + \sin^2 \theta}. \quad (5.41)$$

Its contribution to the Lyapunov exponent, as given in (2.7), vanishes, so that the main contribution comes from terms of order η^2 in the expansion of $p(\phi)$. The calculations are simplified by writing $\text{Re } \gamma(E)$ as

$$\text{Re } \gamma(E) = \int_0^\pi \ln(\sin \phi) [p(\phi - \theta) - p(\phi)] d\phi, \quad (5.42)$$

and $\text{Im } \gamma(E)$ as

$$\text{Im } \gamma(E) = \pi \int_{\pi-\theta}^\pi p(\phi) d\phi. \quad (5.43)$$

Using the expansion of $p(\phi)$ and scaling $\langle \xi^2 \rangle$ back into the problem one finds that with $E = 2 \cos \theta$ (see Appendix D)

$$\text{Re } \gamma(E) = \frac{\epsilon^2 \langle \xi^2 \rangle}{8 \sin^2 \theta} + O(\epsilon^4), \quad (5.44)$$

which is the Thouless formula.²⁵ Note that at $O(\epsilon^3)$ there is no contribution to $\text{Re } \gamma(E)$ (this is also valid for $\theta \approx \pi/3$). For $\text{Im } \gamma(E)$ one finds from (5.43)

$$\text{Im } \gamma(E) = \theta - \frac{\epsilon^3 \langle \xi^3 \rangle}{24 \sin^3 \theta} + O(\epsilon^4), \quad (5.45)$$

valid for all θ in the band. For the density of states $\tilde{\rho}(E)$, formulas (2.10) and (5.45) yield

$$\tilde{\rho}(E) = \frac{1}{2\pi \sin \theta} - \epsilon^3 \frac{\langle \xi^3 \rangle \cos \theta}{32\pi \sin^5 \theta} + O(\epsilon^4). \quad (5.46)$$

We conclude this section with a discussion of the role of δ in our asymptotic procedure. Obviously, the result

at any order in η (i.e., in ϵ) must be independent of the choice of δ . We have assumed $\delta \gg \eta$ in order for the scheme to be consistent, otherwise the divisors would be too small and the series would not be asymptotic. We have chosen for convenience δ small enough for the matrix \mathbf{A} [see (4.37)] to be diagonal. The main effect of changing the value of δ (without violating the above-mentioned limitations) is to redefine the subspace \mathcal{S} , thereby changing the vectors \mathbf{w} and \mathbf{z} . The vector \mathbf{v} ($= \tilde{w} + \tilde{z}$) is, of course, left unchanged. Thus one can choose $\delta = \eta^\alpha$ with $0 \leq \alpha < 2$ provided $\delta \ll 1$.

In Ref. 21, where an expansion of the form

$$p(x) \sim \sum_{n=0}^{\infty} \epsilon^n p_n(x, E, \epsilon) \quad (5.47)$$

was used, no use of δ was made in balancing the equations in the asymptotic procedure. The expansion in Ref. 21 contains the same terms as the expansion presented here, but some terms are shifted from the remainder into the expansion.

In the band edge and in the band center, that is, for $\theta \approx \pi/2$, the requirements that $1 > \delta \gg \eta^2$ and that \mathbf{A} be diagonal are contradictory and one faces the nontrivial task of inverting a tridiagonal matrix. Once this is done, the calculations proceed as in the in-band case.

VI. THE BAND-CENTER CASE: RESULTS

In the present section the case $\theta \approx \pi/2$ is considered. We recall that in this case the leading term in the expansion of the matrix \mathbf{A} is no longer diagonal, and thus an additional difficulty is introduced. To overcome it we first define the variable x by

$$\theta = \frac{\pi}{2} - \frac{x}{2}, \quad (6.1)$$

$$S_{\pm 2} \approx \left\{ n_k = 2k + 1 : k \geq 0, \left[\frac{\pi - \delta}{2x} - \frac{1}{2} \right] < k < \left[\frac{\pi - \delta}{2x} + \frac{1}{2} \right] \right\}. \quad (6.6)$$

The matrix \mathbf{A} is block diagonal; its blocks are either diagonal or tridiagonal. The block in the matrix \mathbf{A} belonging to S_1 is tridiagonal; this block defines a submatrix \mathbf{S}_1 . The next block, whose indices range from $\max(k \in S_1) + 1$ to $\min(k \in S_1) - 1$, is diagonal, defining a submatrix \mathbf{D}_1 , followed by a tridiagonal block, \mathbf{S}_2 for $k \in S_2$, and so on. The structure of the matrix is unchanged under the transformation $k \rightarrow -k$. When $x = 0$ the matrix \mathbf{A} consists of two (infinite) blocks \mathbf{S}_{-1} and \mathbf{S}_1 . As x increases the angle θ approaches the in-band region. The nondiagonal blocks shrink down to single elements and the matrix \mathbf{A} tends to a diagonal matrix. The problem of the exact inversion of \mathbf{A} , as given in (4.41), leads to a rather involved algebraic procedure. To overcome this difficulty we use the following device. The matrix \mathbf{A} is expanded in powers of η as

where $|x| < 1$. Due to symmetry it suffices to consider only $x > 0$. When for some n_k both

$$|e^{-2i\theta n_k} - 1| \leq \delta \quad \text{and} \quad |e^{-2i\theta(n_k \pm 2)} - 1| \leq \delta \quad (6.2)$$

are satisfied, then $n_{k+1} = n_k + 2$ and $L_{n_k, n_k \pm 2}^2 \neq 0$. In this case the matrix \mathbf{A} , given by (4.41), is not diagonal. When $x = 0$ the set \mathbf{s}_δ [see (4.4)] consists of all the even integers $-\infty < n_k \equiv 2k < \infty$. When $x \neq 0$ the set \mathbf{s}_δ consists of all the even integers satisfying

$$|(-1)^{n_k} e^{ixn_k} - 1| \leq \delta, \quad (6.3)$$

$$|(-1)^{n_k} e^{ix(n_k \pm 2)} - 1| \leq \delta.$$

For $x \ll \delta$ the set \mathbf{s}_δ is of the form

$$\mathbf{s}_\delta = \{0\} \cup S_1 \cup S_{-1} \cup S_2 \cup S_{-2} \cup \dots \quad (6.4)$$

where the first index in S_1 is $n_1 = 2$ if (6.2) holds. Then $S_1 = \{2, 4, \dots, 2(K-1)\}$, where (6.2) holds for all indices in S_1 , but not for $n_K = 2K$. Similarly, $S_{-1} = \{-2, -4, \dots, -2(L-1)\}$, where (6.3) is satisfied for all elements in S_{-1} , but not for $n_L = -2L$. The first index in S_2 is the smallest odd integer $n_M = 2M+1 > 2K$, such that (6.3) holds. Then $S_2 = \{2M+1, 2M+3, \dots, 2N-1\}$, where (6.3) holds for all elements in S_2 , but not for $n_N = 2N+1$. The set S_{-2} is defined in an analogous manner. The first element in S_3 is the smallest even integer $n_P = 2P > 2N+1$, such that (6.2) holds. Then $S_3 = \{2P, 2P+2, \dots, 2(Q-1)\}$, where (6.2) holds for all elements of S_3 but not for $n_Q = 2Q$, and so on. The above partition of \mathbf{s}_δ into subsets can be simplified using the smallness of δ to

$$S_{\pm 1} \approx \left\{ n_k = 2k : \pm k > 0, |k| \leq \left[\frac{\delta}{2x} \right] \right\}, \quad (6.5)$$

where $[\dots]$ denotes the integer part of a number. Also

$$\mathbf{A} \sim \eta^2 \mathbf{A}^2 + \eta^4 \mathbf{A}^4 + \dots \quad (6.7)$$

The construction of the vector \mathbf{u} in (4.26) is now different than that presented in Sec. V. The operator \mathbf{T} is now split as

$$\mathbf{T} = \eta^2 \mathbf{A}^2 + \mathbf{B}, \quad (6.8)$$

where \mathbf{B} is now given by

$$\mathbf{B} \sim \eta^3 \mathbf{T}^3 + \eta^4 (\mathbf{A}^4 + \mathbf{T}^4) + \dots \quad (6.9)$$

As in Sec. IV we obtain

$$u_k = -w_0 \sum_{j \neq 0} R_{k,j}^{-1} T_{j,0} \quad \text{for } k \neq 0, \quad (6.10)$$

where

$$\mathbf{R}^{-1} = \sum_{n=0}^{\infty} \{-\eta^{-2}[\mathbf{A}^2]^{-1}\mathbf{B}\}^n \eta^{-2}[\mathbf{A}^2]^{-1}. \quad (6.11)$$

It follows that to leading order in η [see (4.48)]

$$u_k = -w_0 \sum_{j=\pm 1} [A^2]_{k,j}^{-1} T_{j,0}^2 + O(\eta^2) = O(1). \quad (6.12)$$

Note that to leading order in η the sum in (6.10) reduces to $j = \pm 1$ because $T_{j,0}^2$, being proportional to $L_{n_j,0}^2$, vanishes for $n_j > 2$. Because of the block-diagonal structure of \mathbf{A} (and therefore of \mathbf{A}^2) it is sufficient to invert $\mathbf{S}_{\pm 1}$ in order to calculate $[A^2]_{k,\pm 1}^{-1}$. The matrix \mathbf{S}_1 is considered first and it is assumed that the block size $N \equiv [\delta/2x]$ is a large number. Using the expressions given in Appendix C for the elements of \mathbf{L}^2 , (4.36), (4.37), and (4.33) one finds that the nonvanishing elements of \mathbf{A}^2 are

$$A_{k,j}^2 = \begin{cases} iyn_j - \frac{3}{4}n_j^2 & \text{if } n_k = n_j, \\ -\frac{1}{8}(n_j + 1)(n_j + 2) & \text{if } n_k = n_j + 2, \\ -\frac{1}{8}(n_j - 1)(n_j - 2) & \text{if } n_k = n_j - 2. \end{cases}$$

where $x = y\eta^2$.

To simplify the notation we denote the first column of $[A^2]_{k,1}^{-1}$ as the vector \mathbf{C} , that is,

$$C_k \equiv [A^2]_{k,1}^{-1}. \quad (6.13)$$

Hence, using (6.13) and that $n_j = 2j$ in the first block, the identity

$$\sum_{j=1}^N A_{k,j}^2 [A^2]_{j,l}^{-1} = \delta_{k,l} \quad (6.14)$$

takes the form

$$\sum_{j=1}^N \left[\frac{2k(2k-1)}{8} C_j \delta_{j,k-1} + (-2iyk + 3k^2) C_j \delta_{k,j} + \frac{2k(2k+1)}{8} C_j \delta_{j,k+1} \right] = -\delta_{k,1} \quad (6.15)$$

yielding the homogeneous system of difference equations

$$\frac{2k(2k-1)}{8} C_j \delta_{j,k-1} + (-2iyk + 3k^2) C_j \delta_{k,j} + \frac{2k(2k+1)}{8} C_j \delta_{j,k+1} = 0 \quad (6.16)$$

for $k = 2, \dots, N-1$, with the boundary conditions

$$(-iy + 3)C_1 + \frac{3}{4} = -1 \quad (6.17)$$

and

$$\frac{2N(2N-1)}{8} C_{N-1} + (4iyN + 3N^2)C_N = 0. \quad (6.18)$$

The case $y \ll N$ is considered first. The case $y \gg N$ is treated separately below.

Case I: $y \ll N$. The asymptotic behavior of the solution C_k of (6.16) for $k \gg y$ is determined from the reduced equation

$$C_{k-1} + 6C_k + C_{k+1} \sim 0, \quad (6.19)$$

that is,

$$C_k \sim A\lambda_1^k + B\lambda_2^k, \quad (6.20)$$

where

$$\lambda_{1,2} = -3 \pm \sqrt{8}, \quad \text{with } |\lambda_1| < 1 \text{ and } |\lambda_2| > 1. \quad (6.21)$$

The boundary condition (6.18) at $k = N$ becomes

$$C_{N-1} + 6C_N \sim 0, \quad (6.22)$$

yielding

$$\frac{B}{A} \sim - \left(\frac{\lambda_1}{\lambda_2} \right)^{N-1} \left(\frac{1 - 6\lambda_1^2}{1 - 6\lambda_2^2} \right). \quad (6.23)$$

The general solution of (6.16) is a linear combination of two solutions, G_k and H_k , where G_k is the exponentially increasing solution, that is, $G_k = O(\lambda_2^k)$, and H_k is the exponentially decaying solution, that is, $H_k = O(\lambda_1^k)$, for $k \gg y$. Hence

$$C_k = AG_k + BH_k. \quad (6.24)$$

Substituting (6.24) into the boundary condition (6.17) at $k = 1$, we obtain

$$(-2iy + 3)(AG_1 + BH_1) + \frac{3}{4}(AG_2 + BH_2) = -1. \quad (6.25)$$

From (6.23) it follows that $A \sim 0$ for $k \gg y$, so that (6.25) gives

$$B \sim - \frac{1}{(-2iy + 3)H_1 + \frac{3}{4}H_2}. \quad (6.26)$$

The error introduced at the boundary $k = N$ is then exponentially small in N , provided $B = O(1)$ for large N . The latter is self-consistently satisfied (see below). Thus the problem has been reduced to that of determining the exponentially decaying solution of (6.16), which is considered next.

First (6.16) is solved in the domain $-\infty < k < \infty$. Multiplying (6.16) by $e^{ik\alpha}$ and summing over all k a differential equation for the generating function $H(\alpha)$ of C_k is obtained

$$(3 + \cos \alpha)H''(\alpha) - (-2y + \frac{3}{2} \sin \alpha)H'(\alpha) - \frac{1}{2} \cos \alpha H(\alpha) = 0. \quad (6.27)$$

Noting that (6.27) can be written as

$$[(3 + \cos \alpha)H'(\alpha) - (-2y + \frac{1}{2} \sin \alpha)H(\alpha)]' = 0, \quad (6.28)$$

one finds easily the solution

$$F_1(\alpha) \equiv \frac{1}{\sqrt{3 + \cos \alpha}} \exp \left(\frac{iy}{\sqrt{2}} I(\alpha) \right), \quad (6.29)$$

where

$$I(\alpha) \equiv \ln \left[\frac{e^{i\alpha}(\sqrt{2} + 1) + (\sqrt{2} - 1)}{e^{i\alpha}(\sqrt{2} - 1) + (\sqrt{2} + 1)} \right]. \quad (6.30)$$

The second solution of (6.27) is given by

$$F_2(\alpha) \equiv F_1(\alpha) \int_0^\alpha \exp \left(\frac{iy}{\sqrt{2}} I(t) \right) \frac{dt}{\sqrt{3 + \cos t}}. \quad (6.31)$$

Setting

$$I(z) \equiv \ln \left[\frac{z(\sqrt{2}+1) + (\sqrt{2}-1)}{z(\sqrt{2}-1) + (\sqrt{2}+1)} \right], \quad (6.32)$$

one finds that $I(z)$ is an analytic function in the complex z plane with branch points at the points

$$z_1 = -\frac{\sqrt{2}-1}{\sqrt{2}+1} \quad \text{and} \quad z_2 = -\frac{\sqrt{2}+1}{\sqrt{2}-1}. \quad (6.33)$$

As α increases from 0 to 2π , z moves on a closed contour enclosing z_1 (note that $|z_1| < 1$) and $H(\alpha)$ is multiplied by the factor

$$\exp\left(2\pi \frac{iy}{\sqrt{2}}\right) = e^{-\pi y \sqrt{2}}. \quad (6.34)$$

It follows that the generating functions $F_1(\alpha)$ and $F_2(\alpha)$ are not 2π -periodic in α because of the branch point at $z = z_1$. However it is possible to find a suitable linear combination of F_1 and F_2 ,

$$H(\alpha) = Q[F_1(\alpha) + KF_2(\alpha)], \quad (6.35)$$

so that the branch point at z disappears, rendering $H(\alpha)$ a 2π -periodic function of α . The constant K is then determined from the requirement

$$F_1(0) + KF_2(0) = F_1(2\pi) + KF_2(2\pi), \quad (6.36)$$

or, using (6.29) and (6.31),

$$F_1(0) = e^{-\pi y \sqrt{2}} \left[1 + K \int_0^{2\pi} \exp\left(\frac{iy}{\sqrt{2}} I(t)\right) \times \frac{dt}{\sqrt{3 + \cos t}} \right] F_1(0), \quad (6.37)$$

yielding

$$K = \left(e^{\pi y \sqrt{2}} - 1 \right) / \int_0^{2\pi} \exp\left(\frac{iy}{\sqrt{2}} I(t)\right) \frac{dt}{\sqrt{3 + \cos t}}. \quad (6.38)$$

Thus a 2π -periodic generating function for (6.16) has been constructed. It follows from Parseval's inequality that the coefficients H_k of the Fourier expansion of $H(\alpha)$ decay exponentially and can be calculated from

$$H_k = \frac{1}{2\pi} \int_0^{2\pi} H(\alpha) e^{-ik\alpha} d\alpha, \quad (6.39)$$

with $H(\alpha)$ given by (6.35) and (6.38). The constant Q in (6.35) is fixed by the boundary condition (6.17),

$$(-2iy + 3)H_1 + \frac{3}{4}H_2 = -1. \quad (6.40)$$

The coefficient H_0 is determined next. The difference equation (6.16) for $k = 1$ is

$$\frac{1}{4}H_0 + (-2iy + 3)H_1 + \frac{3}{4}H_2 = 0, \quad (6.41)$$

which combined with (6.40) yields $H_0 = 4$. The constant Q can now be determined from (6.35). The coefficients of the generating function $H(\alpha)$ satisfy both (6.16) and the boundary conditions (6.17) at $k = 1$ and (6.18) at $k = N$.

This determines the coefficients C_k for $k \in S_1$, that is, for $k > 0$. Next we show that the same solution, for $k < 0$, satisfies the boundary conditions (6.17) at $k = -1$ and (6.18) at $k = -N$, therefore determining C_k for $k \in S_{-1}$, that is, for $k < 0$.

First, the boundary condition (6.17) at $k = -1$ for the block S_{-1} is

$$(2iy + 3)C_{-1} + \frac{3}{4}C_{-2} = -1. \quad (6.42)$$

The difference equation (6.16) for H_k holds for $k = -1$ as well, hence

$$\frac{3}{4}H_{-2} + (2iy + 3)H_{-1} + \frac{1}{4}H_0 = 0, \quad (6.43)$$

or, since $H_0 = 4$,

$$\frac{3}{4}H_{-2} + (2iy + 3)H_{-1} = -1, \quad (6.44)$$

which is the boundary condition (6.42). Now the Fourier coefficients H_k are the matrix elements $[A^2]_{k,1}^{-1}$ for indices k in $S_{\pm 1}$. From (4.33) we find

$$T_{\pm 1}^2 = -\frac{1}{4}, \quad (6.45)$$

so that the leading-order term in the expansion (6.10), which is $O(1)$, is given by

$$u_k = \frac{w_0}{4} H_k \quad \text{for } 0 < |k| \leq N. \quad (6.46)$$

Finally, using (4.23), the leading-order term \mathbf{w}^0 in the expansion of \mathbf{w} is given by

$$w_{2k}^0 = \begin{cases} u_k + w_0 & \text{for } 0 < |k| \leq N, \\ 0 & \text{otherwise.} \end{cases} \quad (6.47)$$

In terms of the variable ϕ the leading term $w^0(\phi)$ in the expansion of $w(\phi)$ is given by

$$w^0(\phi) = \frac{w_0}{4} [H(4\phi) - H_0] + w_0. \quad (6.48)$$

Note that the generating function corresponding to u_k is $H(4\phi) - H_0$ and not $H(4\phi)$ because $u_0 = 0$ by definition. Using $H_0 = 4$, Eq. (6.48) reduces to

$$w^0(\phi) = \frac{w_0}{4} H(4\phi), \quad (6.49)$$

and the constant Q need not be calculated since it can be absorbed in w_0 which is fixed by the overall normalization of $p(\phi)$. For small y the constant K in (6.38) is expanded as

$$K = \pi y \sqrt{2} / \int_0^{2\pi} \frac{dt}{\sqrt{3 + \cos t}} + O(y^2) \\ = 2y \sqrt{\pi} \frac{\Gamma(3/4)}{\Gamma(1/4)} + O(y^2). \quad (6.50)$$

Finally, using (6.35) and expanding for small y , one finds that

$$w^0(\phi) = \frac{w_0}{\sqrt{3 + \cos 4\phi}} \times \left[1 + \frac{iy}{\sqrt{2}} \ln \frac{e^{4i\phi}(\sqrt{2} + 1) + (\sqrt{2} - 1)}{e^{4i\phi}(\sqrt{2} - 1) + (\sqrt{2} + 1)} + y \frac{8\sqrt{\pi}\Gamma(3/4)}{\Gamma(1/4)} \int_0^\phi \frac{dt}{\sqrt{3 + \cos t}} \right] + O(y^2). \quad (6.51)$$

The result (6.51) coincides with that obtained in Ref. 15. The case $y \gg N$ is considered next.

Case II: $y \gg N$. It is still assumed that $x \ll \delta$, that is, $y\eta^2 \ll 1$. Note that when $y\eta^2 = O(1)$ the condition (6.3) is violated and \mathbf{A} is fully diagonal, reducing to the in-band case of Sec. V. One observes that, in each row, the diagonal elements of the matrices $\mathbf{S}_{\pm 1}$ are much larger than the off-diagonal ones. The off-diagonal elements can be viewed as perturbations about the diagonal matrix. In such a case Jacobi's iterative method for inversion is appropriate. The iterations are known to converge to the unique fixed point of the scheme, provided the modulus of the diagonal terms is larger than the sum of the moduli of the off-diagonal elements in the same row. Equation (6.16) shows that this is indeed the case. In matrix form (6.16) is

$$\mathbf{A}^2 \mathbf{C} = \mathbf{e}_1, \quad (6.52)$$

where $e_{1,k} = \delta_{k,1}$. The diagonal elements of \mathbf{A}^2 form a matrix \mathbf{D} whose elements are

$$D_{k,j} = (2iy + 3k^2)\delta_{k,j}, \quad (6.53)$$

so that (6.52) can be written as

$$\mathbf{C} = \mathbf{D}^{-1}[\mathbf{D} - \mathbf{A}^2]\mathbf{C} + \mathbf{D}^{-1}\mathbf{e}_1. \quad (6.54)$$

The iterative scheme for the solution of (6.54) is

$$\mathbf{C}^{n+1} = \mathbf{D}^{-1}[\mathbf{D} - \mathbf{A}^2]\mathbf{C}^n + \mathbf{D}^{-1}\mathbf{e}_1 \quad (6.55)$$

with the obvious choice

$$\mathbf{C}^0 = \mathbf{D}^{-1}\mathbf{e}_1. \quad (6.56)$$

The nonvanishing terms in the consecutive iteration are given by

$$C_1^1 = \frac{1}{2iy} + \frac{12}{16y^2} + O\left(\frac{1}{y^3}\right), \quad (6.57)$$

$$C_2^1 = \frac{3}{16y^2} + O\left(\frac{1}{y^3}\right),$$

and $C_{-k}^1 = (C_k^1)^*$, $k = 1, 2$. Further iterations preserve the leading terms in (6.57) and introduce terms of higher order in $1/y$. Once C_k is known u_k can be calculated and then w_k . Thus finally

$$w^0(\phi) = w_0 \left[1 + \frac{1}{4y} \sin 4\phi - \frac{1}{32y^2} (12 \cos 4\phi + 3 \cos 8\phi) + O\left(\frac{1}{y^3}\right) \right]. \quad (6.58)$$

Note that when $y \gg 1$ the in-band solution is recovered, as expected.

The higher-order contributions to \mathbf{w} can be calculated by means of (6.10) and (6.11). It is easy to see that $w(\phi)$ is of the form

$$w(\phi) = w^0(\phi) + \eta w^1(\phi) + \eta^2 w^2(\phi) + O(\eta^3), \quad (6.59)$$

and that $w^1(\phi)$ and $w^2(\phi)$ are $\pi/2$ -periodic functions. Since they contribute neither to the Lyapunov exponent nor to the density of states [see (3.10)–(3.12)], their calculation is not presented here.

The nonvanishing contribution to the Lyapunov exponent comes from $z(\phi)$, which by definition is not a $\pi/2$ -periodic function, being orthogonal to $w(\phi)$. The leading-order nonvanishing contribution to $z(\phi)$ is of order η^2 , that is,

$$z(\phi) = \eta^2 z^2(\phi) + O(\eta^3), \quad (6.60)$$

where $z^2(\phi)$ is the Fourier series corresponding to the vector \mathbf{z}^2 , given by

$$\mathbf{z}^2 = (\mathbf{I} - \mathbf{M}^0)^{-1} \mathbf{L}^2 \mathbf{w}^0, \quad (6.61)$$

where \mathbf{w}^0 is given in Eqs. (6.52) and (6.58). In addition, $z^2(\phi)$ has only “odd” components, that is,

$$z^2(\phi) = \sum_{k=-\infty}^{\infty} z_{2k+1}^2 e^{2i\phi(2k+1)}. \quad (6.62)$$

Therefore we have

$$z_{2k+1}^2 = \frac{1}{2} L_{2k+1,2k}^2 w_{2k}^0 + L_{2k+1,2k+2}^2 w_{2k+2}^0. \quad (6.63)$$

Using (C4), multiplying (6.63) by $\exp\{4i\phi k\}$, and summing over k , one finds that

$$z^2(\phi) = \frac{1}{8} \frac{d}{d\phi} \left(\sin 2\phi w^0(\phi) - \cos 2\phi \frac{dw^0}{d\phi} \right). \quad (6.64)$$

Using (6.28) it can be shown that $w^0(\phi)$ satisfies

$$\frac{d}{d\phi} \left[2y w^0(\phi) + \left(\frac{3 + \cos 4\phi}{4} \right) \frac{dw^0(\phi)}{d\phi} - \frac{1}{2} \sin 2\phi w^0(\phi) \right] = 0. \quad (6.65)$$

It follows that at order η^2 we can write

$$z^2(\phi) = \frac{1}{8} \frac{d}{d\phi} F(\phi), \quad (6.66)$$

where

$$F(\phi) \equiv 2yw^0(\phi) + \left(\frac{3 + \cos 4\phi - 4 \cos 2\phi}{4} \right) \frac{dw^0(\phi)}{d\phi} + (\sin 2\phi - \frac{1}{2} \sin 4\phi)w^0(\phi). \quad (6.67)$$

Note that these results differ from those of Ref. 15 by the term

$$\frac{y}{4} \left(\sin 2\phi - \frac{1}{2} \cos 2\phi \frac{d}{d\phi} \right) w^0(\phi). \quad (6.68)$$

The leading-order approximation is $p(\phi) = w^0(\phi) + o(1)$. In the band center $w^0(\phi)$ is given by (6.51) with $y = 0$, that is,

$$w^0(\phi) = \frac{w_0}{\sqrt{3 + \cos 4\phi}}, \quad (6.69)$$

where the normalization constant is given to leading order by

$$w_0 = \frac{4\sqrt{\pi}}{\Gamma^2(1/4)}. \quad (6.70)$$

In terms of the original variable the leading-order approximation to $p(x)$ is given by

$$p(x) = \frac{2\sqrt{\pi}}{\Gamma^2(1/4)} \frac{1}{\sqrt{1+x^4}} + O(\epsilon). \quad (6.71)$$

We can now calculate the leading-order approximations to the Lyapunov exponent and to the density of states. The calculations follow closely those given in Ref. 15 and are presented here for the sake of completeness. First we note that

$$p\left(\phi + \frac{\pi}{2}\right) - p(\phi) = 2\eta^2 z^2(\phi) + O(\eta^3). \quad (6.72)$$

Then, using $\theta = \pi/2 - y\eta^2/2$ and (6.72) in (3.10) we obtain

$$\begin{aligned} \text{Re } \gamma(E) = \int_0^\pi \ln \sin \phi \left[2\eta^2 z^2(\phi) \right. \\ \left. - \frac{y\eta^2}{2} \frac{dw^0(\phi)}{d\phi} + O(\eta^3) \right] d\phi. \end{aligned} \quad (6.73)$$

The last term in (6.73) vanishes because of the $\pi/2$ -periodicity of $w^0(\phi)$, hence

$$\text{Re } \gamma(E) = 2\eta^2 \int_0^\pi \ln \sin \phi z^2(\phi) d\phi + O(\eta^3). \quad (6.74)$$

Now, using (6.66) and integration by parts, (6.74) becomes

$$\text{Re } \gamma(E) = \frac{\eta^2}{8} \int_0^\pi (1 + \cos 4\phi)w^0(\phi) d\phi + O(\eta^3), \quad (6.75)$$

where $w^0(\phi)$ is given in (6.51) or (6.58) and w_0 is a y -dependent normalization constant for $w^0(\phi)$. It is convenient to define the constant

$$\alpha \equiv \left[\frac{\Gamma(3/4)}{\Gamma(1/4)} \right]^2 \quad (6.76)$$

so that the leading-order approximation to the Lyapunov exponent (6.75) can be expressed as

$$\text{Re } \gamma(E) = \eta^2 [\alpha + O(y)] \approx 0.114 \ 24\eta^2 \quad \text{for } y \ll 1 \quad (6.77)$$

$$\text{Re } \gamma(E) = \eta^2 \left[\frac{1}{8} - \frac{3}{128y^2} \right] + O\left(\frac{1}{y^2}\right) \quad \text{for } y \gg 1. \quad (6.78)$$

The imaginary part of $\gamma(E)$ can be calculated from (3.11) in the form

$$\text{Im } \gamma(E) = \pi \int_{\pi/2}^\pi p(\phi) d\phi - \pi \int_{\pi/2}^{\pi/2+y\eta^2/2} p(\phi) d\phi, \quad (6.79)$$

which, using the identity

$$\int_{\pi/2}^\pi p(\phi) d\phi = \frac{1}{2} + \frac{1}{2} \int_{\pi/2}^\pi \left[p(\phi) - p\left(\phi - \frac{\pi}{2}\right) \right] d\phi, \quad (6.80)$$

can be written in the form

$$\begin{aligned} \text{Im } \gamma(E) = \frac{\pi}{2} + \frac{\pi}{2} \int_{\pi/2}^\pi \left[p(\phi) - p\left(\phi - \frac{\pi}{2}\right) \right] d\phi \\ - \frac{\pi y \eta^2}{2} p\left(\frac{\pi}{2}\right) + O(\eta^4). \end{aligned} \quad (6.81)$$

Thus

$$\text{Im } \gamma(E) = \frac{\pi}{2} + \pi \eta^2 \int_{\pi/2}^\pi z^2(\phi) d\phi - \frac{\pi y \eta^2}{2} w^0(0) + O(\eta^3). \quad (6.82)$$

Finally, using (6.64) in (6.82) one finds that

$$\text{Im } \gamma(E) = \frac{\pi}{2} - \pi \eta^2 \left[w^0(0) + \frac{1}{2} \frac{dw^0(0)}{d\phi} \right] + O(\eta^3), \quad (6.83)$$

which is equivalent to Eq. (76) in Ref. 15. The results are therefore

$$\text{Im } \gamma(E) = \frac{\pi}{2} \left[1 - \eta^2 y \alpha \sqrt{8} \right] + O(y^2) \quad \text{for } y \ll 1, \quad (6.84)$$

$$\text{Im } \gamma(E) = \frac{\pi}{2} \left\{ 1 - \eta^2 \left[\frac{y}{\pi} + \frac{1}{32\pi y} + O\left(\frac{1}{y^2}\right) \right] \right\} \quad \text{for } y \gg 1. \quad (6.85)$$

Using (2.10) one finds the approximation to the density of states as

$$\bar{\rho} \left(\frac{\pi}{2} - \frac{y\eta^2}{2} \right) = \alpha \sqrt{2} + O(y) \quad \text{for } y \ll 1, \quad (6.86)$$

$$\bar{\rho} \left(\frac{\pi}{2} - \frac{y\eta^2}{2} \right) = \frac{1}{2\pi} \left(1 - \frac{1}{32y^2} \right) + O\left(\frac{1}{y^3}\right) \quad \text{for } y \gg 1. \quad (6.87)$$

These results agree with those of Refs. 13 and 15.

VII. TRANSITION TO THE BAND EDGE

As long as the expansion parameter around the noiseless dynamics, η , is small the expansion presented above can be used. However when the perturbation becomes comparable with the spacing between the eigenvalues of the unperturbed system, a crossover to a different expansion can be expected. Specifically, the separation between the consecutive (leading order in ϵ) eigenvalues is

$$|e^{2i(n+1)\theta} - e^{2in\theta}| = O(\theta). \quad (7.1)$$

Since the small parameter of the expansion around the noiseless dynamics is $\eta^2 = \epsilon^2/\sin^2\theta$, the obvious condition for the validity of the expansion developed in the previous sections is that $\theta \gg \eta^2$. This condition is equivalent to $\theta \gg \epsilon^{2/3}$, which thus defines the in-band region. Nevertheless, even when $\theta = O(\epsilon^{2/3})$, that is, inside the band-edge region, the expansion method used above can be extended with minor modifications. Specifically, similarly to the band-center case, the operator \mathbf{A} in Eq. (4.41) is no longer diagonal. It is necessary therefore to invert it as was done for the operator in the band-center case.

Recall that the condition for the operator \mathbf{A} in Eq. (4.41) to be diagonal is that the inequality (4.3) and Eq. (4.43) are satisfied, that is,

$$\eta^2 < \delta < |2\sin\theta|, \quad (7.2)$$

which is equivalent to

$$\epsilon^{2/3} < C\theta, \quad (7.3)$$

where C is a constant. Clearly, in the band-edge region Eq. (7.3) cannot hold. Upon relaxing the condition $\delta < |2\sin\theta| \sim 2|\theta|$ in the inequality (7.2) one finds that the two terms on the right-hand side of Eq. (4.41) may be comparable so that \mathbf{A} is not diagonal to leading order, similarly to the band-center case. The structure of \mathbf{A} is now as follows.

The condition (4.4), i.e., $\{|e^{-2i\theta n} - 1| < \delta\}$, defines a

set of blocks for the linear operator $\hat{\mathbf{L}}$ and the operators derived from it (e.g., \mathbf{A}). The first block is defined by the set of indices for which $|2n\theta| < \delta + O(\theta^2)$, the second block is defined by the set of values of n for which $|2n\theta - 2\pi| < \delta + O(\theta^2)$, and so on.

Consider now the first block. The first block of \mathbf{A} , corresponding to indices k and j satisfying

$$|k|, |j| < \frac{\delta}{2\theta}, \quad (7.4)$$

is not diagonal. To leading order in η we have to solve

$$u_k = -w_0\eta^2 \sum_{j \neq 0} \{A^{-1}\}_{kj} T_{j0}^2, \quad (7.5)$$

for $|k| < \delta/2\theta$, where $\{A^{-1}\}_{kj}$ is a matrix element of the inverse of the matrix defined in Eq. (4.41), that is, of

$$A_{k,j} = \delta_{k,j} \frac{-1 + e^{-2i\theta n_j}}{2 - e^{-2i\theta n_j}} + \eta^2 \frac{L_{n_k, n_j}^2}{(2 - e^{-2i\theta n_k})(2 - e^{-2i\theta n_j})}. \quad (7.6)$$

Note that η is still assumed to be a small parameter, i.e., $\epsilon < \theta$. The range $\epsilon < \theta < \epsilon^{2/3}$ is in the band-edge region though it does not reach the band edge. It is possible to consider the region $0 < \theta < \epsilon$ as well. Since this was done in detail in Ref. 22 we refrain here from considering the latter region. It turns out that the probability distribution function in the latter domain has the same functional dependence on θ and ϵ as for $\theta > \epsilon$.

In the first block defined above the projection operator \mathbf{K} reduces to the identity operator so that to leading order in θ the matrix element T_{j0}^2 is reduced to L_{j0}^2 . We also note that $\mathbf{z} = \mathbf{0}$ so that defining $u_0 = w_0$ we have $\mathbf{u} = \mathbf{w}$.

Next we derive a differential equation for $w(\phi)$. Multiplying Eq. (7.5) by $A_{nk} \exp\{2in\phi\}$ and summing over k and n we obtain, using the the matrix elements of \mathbf{L}^2 from Appendix C,

$$-\theta w'(\phi) + \eta^2 \left\{ \frac{1}{16} [\cos 4\phi - 4\cos 2\phi + 3] w''(\phi) + \frac{3}{8} [2\sin 2\phi - \sin 4\phi] w'(\phi) + \frac{1}{2} [\cos 2\phi - \cos 4\phi] w(\phi) \right\} \sim 0. \quad (7.7)$$

Equation (7.7) was derived by letting $|k| \rightarrow \infty$ in the first block of \mathbf{A} . As in the case of the band center, the error is exponentially small in the block length. Obviously, the solution of Eq. (7.7) matches the in-band solution $w(\phi) = \text{constant}$ when $\eta^2 \ll \theta$. An exact solution of Eq. (7.7) is found as follows.^{15,21} Setting

$$z \equiv \frac{x-1}{\theta}, \quad (7.8)$$

using Eq. (3.1), $w(\phi)d\phi = p(x)dx$, and defining $P(z)dz = p(x)dx$, Eq. (7.7) is transformed into

$$\theta \left[(z^2 + 1)^2 \frac{dP(z)}{dz} + 2z(z^2 + 1)P(z) \right] + \frac{\eta^2}{2} (z^2 + 1) \frac{d^2P(z)}{dz^2} \sim 0. \quad (7.9)$$

The integrable solution of Eq. (7.9) is given by

$$P(z) = C e^{-2t(z^3/3+z)} \int_{-\infty}^z e^{2t(z'^3/3+z')} dz', \quad (7.10)$$

where $t \equiv \theta/\eta^2$, and the normalization factor is

$$C = \left[\int_{-\infty}^{\infty} e^{-2t(z^3/3+z)} \int_{-\infty}^z e^{2t(z'^3/3+z')} dz' dz \right]^{-1}. \quad (7.11)$$

The case $\theta \ll \epsilon$ was considered in Ref. 21. The full study of the statistical properties of the wave function in the band edge is given in Ref. 22.

VIII. CONCLUSION

The analysis of the Anderson problem has invariably led to a problem of small denominators. When the value of the energy considered is of the form $2 \cos \pi n/N$ (in one dimension), one obtains vanishing denominators in perturbation theory beyond the N th order and its multiples. When the energy is of the form $2 \cos \theta$ with θ not a rational multiple of π , one obtains small denominators at finite orders in perturbation theory. In the present work we have investigated in detail the structure of the theory which underlies the perturbative approach in the case at hand. We have traced the source of the above-mentioned difficulties to the fact that, in the Fourier representation, the matrix to be diagonalized has an infinitely quasidegenerate spectrum in the absence of noise, if θ is a rational multiple of π , and an infinitely quasidegenerate spectrum, if θ is not such a multiple. Both cases are similar and are treated by the same method. To overcome the problem of degeneracy we have developed a degenerate perturbation theory, which is suitable for the (infinitely) quasidegenerate case at hand. The essence of this theory is the use of a projection method which projects the matrix into the subspace of quasidegenerate states. Once this is done, the resulting perturbation theory is free of divergent terms and one can use it to calculate physical quantities, such as the Lyapunov exponents and densities of states, to desired orders in perturbation theory. Thus one obtains a systematic method for solving for the relevant quantities associated with the Anderson model in an asymptotic series for small noise variance. The asymptotic expansion shows that the probability distribution function and consequently the quantities derived from it, is an analytic function of θ as long as noise is present. It develops singularities only in the limit of vanishing noise. Our expansion reveals the internal layer structure of the probability distribution function which is the root cause of the anomalies one encounters in a power series expansion.

Using the method developed here, we have reproduced the known results for the Lyapunov exponents and densities of states for $\theta \approx 0, \pi/2, \pi/3$, and confirmed the Thouless formula as the leading-order approximation everywhere in the band, except at $\theta \approx 0, \pi/2$, where this formula indeed fails. Corrections to this result can be found in a straightforward though tedious manner. The resulting theory produces a uniform expression for the probability distribution function (and other desired quantities) in the entire band, including the band edge. It is possible that some of the ideas and techniques bear some relevance to the higher-dimensional Anderson models. In particular, it is conceivable that the exploitation of degeneracies is a key ingredient in the study of these models. This possibility is presently under active study.

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APPENDIX A: DERIVATION OF (3.7)

Using (3.4) it follows that

$$\langle \delta(\phi_{n+1} - \phi) \rangle = \langle \delta\{\text{arccot}[\cot(\phi_n + \theta) + \eta\xi_n - \phi]\} \rangle, \quad (\text{A1})$$

where $\langle \dots \rangle$ is the average over all the ξ_i 's with $0 \leq i \leq n$. Defining

$$p_{n+1}(\phi) \equiv \langle \delta(\phi_n - \phi) \rangle, \quad (\text{A2})$$

one finds, in view of the Markovian property of the process ϕ_n , that

$$p_{n+1}(\phi) = \int_{-\infty}^{\infty} \rho(\xi) d\xi \int_0^{\pi} p_n(\phi_n) \times \delta\{\text{arccot}[\cot(\phi_n + \theta) + \eta\xi] - \phi\} d\phi_n. \quad (\text{A3})$$

In the large- n limit, it is assumed that $p_n(\phi) \rightarrow p(\phi)$. Furthermore,

$$\begin{aligned} & \delta\{\text{arccot}[\cot(\phi_n + \theta) + \eta\xi] - \phi\} \\ &= \{1 + [\cot(\phi_n + \theta) + \eta\xi]^2\} \sin^2(\phi_n + \theta) \delta(\phi_n - \phi'), \end{aligned} \quad (\text{A4})$$

where ϕ' is the unique solution of

$$\text{arccot}[\cot(\phi' + \theta) + \eta\xi] = \phi, \quad (\text{A5})$$

implying

$$\phi' = \text{arccot}[\cot \phi - \eta\xi] - \theta. \quad (\text{A6})$$

Hence

$$\begin{aligned} & \{1 + [\cot(\phi' + \theta) + \eta\xi]^2\} \sin^2(\phi' + \theta) \\ &= \frac{1 + \cot^2 \phi}{1 + (\cot \phi - \eta\xi)^2} \\ &= \frac{1}{1 - \eta\xi \sin 2\phi + \eta^2 \xi^2 \sin^2 \phi}. \end{aligned} \quad (\text{A7})$$

Substituting (A7) into (A3) we obtain (3.7).

APPENDIX B: DERIVATION OF (3.9)

Using the definition of \mathbf{L} we have

$$\begin{aligned} \mathbf{L}e^{2i\phi n} &= e^{-2i\theta n} \int_{-\infty}^{\infty} \frac{\exp\{2in[\text{arccot}(\cot \phi - \eta\xi)]\}}{1 - \eta\xi \sin 2\phi + \eta^2 \xi^2 \sin^2 \phi} \\ &\quad \times \rho(\xi) d\xi. \end{aligned} \quad (\text{B1})$$

Defining

$$\begin{aligned} u &\equiv \cot \phi - \eta\xi, \quad f \equiv \cos \operatorname{arccot} u, \\ g &\equiv \sin \operatorname{arccot} u, \end{aligned} \quad (\text{B2})$$

we obtain the identities

$$g = \frac{1}{\sqrt{1+u^2}} = \frac{\sin \phi}{(1 - \eta\xi \sin 2\phi + \eta^2 \xi^2 \sin^2 \phi)^{1/2}} \quad (\text{B3})$$

$$f = \frac{u}{\sqrt{1+u^2}} = \frac{\cos \phi - \eta\xi \sin \phi}{(1 - \eta\xi \sin 2\phi + \eta^2 \xi^2 \sin^2 \phi)^{1/2}},$$

hence

$$\exp\{2in[\operatorname{arccot}(\cot \phi - \eta\xi)]\} = (f + ig)^{2n} = e^{-2i\phi n} = \frac{(1 - \eta\xi e^{-i\phi})^{2n}}{(1 - \eta\xi \sin 2\phi + \eta^2 \xi^2 \sin^2 \phi)^n}. \quad (\text{B4})$$

Substituting in (B1) we obtain

$$\begin{aligned} \mathbf{L}e^{2i\phi n} &= e^{-2i\theta n} e^{-2i\phi n} \\ &\times \int_{-\infty}^{\infty} \frac{(1 - \eta\xi e^{-i\phi})^{2n}}{(1 - \eta\xi \sin 2\phi + \eta^2 \xi^2 \sin^2 \phi)^{n+1}} \\ &\times \rho(\xi) d\xi. \end{aligned} \quad (\text{B5})$$

The denominator in (B5) factors into

$$\begin{aligned} 1 - \eta\xi \sin 2\phi + \eta^2 \xi^2 \sin^2 \phi \\ = (1 + \eta\xi e^{-i\phi} \sin \phi)(1 + \eta\xi e^{i\phi} \sin \phi), \end{aligned} \quad (\text{B6})$$

yielding (3.9).

APPENDIX C: THE MATRIX ELEMENTS OF \mathbf{L}

The matrix elements $L_{m,n}$ are defined by

$$\mathbf{L}e^{2i\phi n} = \sum_{m=-\infty}^{\infty} L_{m,n} e^{2i\phi m}, \quad (\text{C1})$$

and upon expanding (3.7) in powers of η

$$L_{m,n} = L_{m,n}^0 + \eta L_{m,n}^1 + \eta^2 L_{m,n}^2 + \dots, \quad (\text{C2})$$

the matrices $\{L_{m,n}^i\}$ are defined. Using (B5) we find that

$$L_{m,n}^0 = e^{-2i\theta n} \delta_{m,n}. \quad (\text{C3})$$

At order η the matrix \mathbf{L} vanishes since $\langle \xi_n \rangle = 0$. At order η^2 we have

$$\begin{aligned} L_{m,n}^2 = e^{-2i\theta n} \langle \xi^2 \rangle \left(-\frac{(n+1)(n+2)}{8} \delta_{m,n+2} + \frac{(n+1)(2n+1)}{4} \delta_{m,n+1} - \frac{3n^2}{4} \delta_{m,n} \right. \\ \left. + \frac{(n-1)(2n-1)}{4} \delta_{m,n-1} - \frac{(n-1)(n-2)}{8} \delta_{m,n-2} \right). \end{aligned} \quad (\text{C4})$$

At order η^3

$$\begin{aligned} L_{m,n}^3 = \frac{ie^{-2i\theta n} \langle \xi^3 \rangle}{8} \left(-\frac{(n+1)(n+2)(n+3)}{6} \delta_{m,n+3} + (n+1)^2 (n+2) \delta_{m,n+2} \right. \\ - \frac{(n+1)(5n^2 + 5n + 2)}{2} \delta_{m,n+1} + \frac{2n(5n^2 + 1)}{3} \delta_{m,n} - \frac{(n-1)(5n^2 - 5n + 2)}{2} \delta_{m,n-1} \\ \left. + (n-1)^2 (n-2) \delta_{m,n-2} - \frac{(n-1)(n-2)(n-3)}{6} \delta_{m,n-3} \right), \end{aligned} \quad (\text{C5})$$

and at order η^4 we have

$$\begin{aligned}
L_{m,n}^4 = \frac{e^{-2i\theta n} \langle \xi^4 \rangle}{16} & \left\{ \frac{(n+1)(n+2)(n+3)(n+4)}{24} \delta_{m,n+4} - \frac{(n+1)(n+2)(n+3)(2n+3)}{6} \delta_{m,n+3} \right. \\
& + \frac{(n+1)(n+2)(7n^2+14n+9)}{6} \delta_{m,n+2} \\
& - \left[(n^2-1)(n+2)(2n+1) + \frac{(n+1)(2n^3+3n^2+37n+18)}{6} \right] \delta_{m,n+1} \\
& + \frac{5n^2(7n^2+5)}{12} \delta_{m,n} - \left[(n^2-1)(n-2)(2n-1) + \frac{(n-1)(2n^3-3n^2+37n-18)}{6} \right] \delta_{m,n-1} \\
& + \frac{(n-1)(n-2)(7n^2-14n+9)}{6} \delta_{m,n-2} - \frac{(n-1)(n-2)(n-3)(2n-3)}{6} \delta_{m,n-3} \\
& \left. + \frac{(n-1)(n-2)(n-3)(n-4)}{24} \delta_{m,n-4} \right\}. \tag{C6}
\end{aligned}$$

APPENDIX D: CALCULATION OF THE LYAPUNOV EXPONENT IN THE BAND

1. Calculation of $\text{Re } \gamma$

Defining $\Delta f(\phi) \equiv f(\phi - \theta) - f(\phi)$, Eq. (3.10) becomes

$$\mathcal{I}(f) \equiv \int_0^\pi \Delta f(\phi) \ln \sin \phi \, d\phi. \tag{D1}$$

Then, from (3.10),

$$\text{Re } \gamma(E) = \mathcal{I}(\Delta w) + \mathcal{I}(\Delta z). \tag{D2}$$

The following identities are used below

$$\mathcal{I}(\sin 2n\phi) = \int_0^\pi \sin 2n\phi \ln \sin \phi \, d\phi = 0, \tag{D3}$$

$$\mathcal{I}(\cos 2n\phi) = \int_0^\pi \cos 2n\phi \ln \sin \phi \, d\phi = -\frac{\pi}{2n}. \tag{D4}$$

We calculate below $\text{Re } \gamma(E)$ with remainder of order ϵ^4 . First we consider $\mathcal{I}(\Delta w)$ in two possible cases $q > 3$ and $q = 3$. If $q > 3$, then $w(\phi) = O(\eta^2)$ only if θ is sufficiently close to $\pi/4$, that is, if $q = 4$. Then

$$w(\phi) = w_0 + 2\text{Re}(w_4 e^{8i\phi}). \tag{D5}$$

Noting that $\Delta w_0 = 0$ and

$$\mathcal{I}(\Delta e^{2ni\phi}) = -\frac{\pi}{2n} (e^{-2ni\theta} - 1), \tag{D6}$$

one obtains from (D6)

$$\mathcal{I}(\Delta w) = -\frac{\pi}{4} \text{Re } w_4 (e^{-8i\theta} - 1). \tag{D7}$$

If $\theta = \pi/4 - y\eta^2$ with $y = O(1)$, then $w_4 = O(\eta^2)$ [see (5.21)] and $e^{\pm 8i\theta} - 1 = O(\eta^2)$, so that

$$\mathcal{I}(\Delta w) = O(\eta^4) \quad \text{for all } \theta \text{ in the band.} \tag{D8}$$

If $q = 3$ then using (D6) one obtains

$$\mathcal{I}(\Delta w) = \text{Re} \mathcal{I}(w_3 \Delta e^{6i\phi}) = -\frac{\pi}{3} \text{Re} [w_3 (e^{-6i\theta} - 1)]. \tag{D9}$$

As above, if $\theta = \pi/3 - y\eta^2$ with $y = O(1)$, then $w_3 = O(\eta)$ [see (5.13)] and $e^{-6i\theta} - 1 = O(\eta^2)$, so that $\mathcal{I}(\Delta w) = O(\eta^2)$ for all θ . Therefore we have to calculate the contribution at this order. We consider the two possible cases $|\theta - \pi/3| \gg \eta^2$ and $\theta = \pi/3 - y\eta^2$ with $y = O(1)$. In the first case we get from (5.13)

$$w_3 = w_0 \eta^3 \frac{i \langle \xi^3 \rangle}{16} \frac{2e^{6i\theta} - 1}{6 \sin^2 3\theta - i \sin 6\theta} + o(\eta^3), \tag{D10}$$

and it is easy to see from (D9) that $\mathcal{I}(\Delta w) = 0$ in this case.

When $\theta = \pi/3 - y\eta^2$ with $y = O(1)$, (5.17) must be used rather than (D10). Defining the constant

$$K \equiv \frac{w_0 \langle \xi^3 \rangle}{3(64y^2 + 81)}, \tag{D11}$$

one obtains

$$\begin{aligned}
\mathcal{I}(\Delta w_3 e^{6i\phi} + \Delta w_{-3} e^{-6i\phi}) \\
= \frac{\eta\pi K \sin 3\theta}{3} [8y \sin 3\theta + 9 \cos 3\theta] \\
= -9\pi K y \eta^3 + O(\eta^5). \tag{D12}
\end{aligned}$$

Equation (D12) is the $O(\epsilon^3)$ contribution of $w(\phi)$ to $\text{Re } \gamma(E)$.

Next we calculate the contribution of $\mathcal{I}(\Delta z)$ to $\text{Re } \gamma(E)$. Using the expression (5.28) for $z^2(\phi)$ one finds that

$$\Delta z^2(\phi) = \frac{w_0}{2} (\cos 4\phi - \cos 2\phi), \tag{D13}$$

yielding

$$\mathcal{I}[\Delta z^2(\phi)] = \frac{\pi w_0}{8}. \tag{D14}$$

Now the contribution of $z^3(\phi)$ is calculated in the two cases $q > 3$ and $q = 3$. If $q > 3$, then (5.34) and (5.33)

imply that $\mathcal{I}[\Delta Z^3(\phi)] = 0$. If $q = 3$, then from (5.36) one obtains

$$z_1^3 = Z_1^3 + \eta^3 w_0 \frac{i\langle \xi^3 \rangle}{64} \frac{1}{1 - e^{-2i\theta}} \frac{1}{27\langle \xi^2 \rangle/4 - 6iy}, \quad (\text{D15})$$

and so on. After some algebra one obtains

$$\mathcal{I}[\Delta z^3(\phi)] = 9\pi Ky\eta^3 + O(\eta^5). \quad (\text{D16})$$

Note that the $O(\eta^3)$ contributions of (D12) and (D16) sum to zero.

Finally $w_0 = 1/\pi$ to normalize the probability distribution function. Combining the contributions of orders less than ϵ^4 one obtains

$$\text{Re } \gamma(E) = \frac{1}{8}\eta^2 + O(\epsilon^4) = \frac{\epsilon^2}{8\sin^2\theta} + O(\epsilon^4). \quad (\text{D17})$$

2. Calculation of $\text{Im } \gamma$

We have to calculate

$$\begin{aligned} \text{Im } \gamma(E) &= \pi \int_{\pi-\theta}^{\pi} p(\phi) d\phi \\ &= \pi \int_{\pi-\theta}^{\pi} [w(\phi) + z(\phi)] d\phi. \end{aligned} \quad (\text{D18})$$

First we evaluate the integral of $w(\phi)$. If $q > 3$, then $w(\phi)$ is given by (D5), so that

$$\pi \int_{\pi-\theta}^{\pi} w(\phi) d\phi = \theta + \frac{\pi}{4} \text{Im} [w_4(1 - e^{-8i\theta})]. \quad (\text{D19})$$

As above, we find that

$$\pi \int_{\pi-\theta}^{\pi} w(\phi) d\phi = \theta + O(\eta^2) \quad \text{for all } \theta \text{ in the band} \quad (\text{D20})$$

[compare with (D7)]. If $q = 3$, the contribution of order

ϵ^3 comes from

$$\pi \int_{\pi-\theta}^{\pi} \left[\frac{1}{\pi} + 2\text{Re}(w_3 e^{6i\phi}) \right] d\phi. \quad (\text{D21})$$

We consider separately $|\theta - \pi/3| \gg \eta^2$ and $\theta = \pi/3 - y\eta^2$ with $y = O(1)$. In the former case we use the expression (D10) and obtain

$$\pi \int_{\pi-\theta}^{\pi} \left[\frac{1}{\pi} + 2\text{Re}(w_3 e^{6i\phi}) \right] d\phi = \theta - \frac{\langle \xi^3 \rangle}{24}. \quad (\text{D22})$$

In the latter case we use (5.17) and obtain

$$\pi \int_{\pi-\theta}^{\pi} \left[\frac{1}{\pi} + 2\text{Re}(w_3 e^{6i\phi}) \right] d\phi = \theta - 8Ky^2. \quad (\text{D23})$$

Next we calculate the integral of $z(\phi)$. For all θ we have

$$\pi \int_{\pi-\theta}^{\pi} z^2(\phi) d\phi = 0. \quad (\text{D24})$$

The contribution of $z^3(\phi)$ depends on q . If $q > 3$, we use (5.33) to obtain

$$\pi \int_{\pi-\theta}^{\pi} z^3(\phi) d\phi = -\frac{\langle \xi^3 \rangle}{24}. \quad (\text{D25})$$

If $q = 3$ and $|\theta - \pi/3| \gg \eta^2$, we use (5.36) to obtain

$$\pi \int_{\pi-\theta}^{\pi} z^3(\phi) d\phi = O(\eta^4). \quad (\text{D26})$$

and for $\theta = \pi/3 - y\eta^2$ (D15) yields

$$\pi \int_{\pi-\theta}^{\pi} z^3(\phi) d\phi = -\frac{81K}{8}. \quad (\text{D27})$$

The final result is

$$\text{Im } \gamma(E) = \theta - \frac{\langle \xi^3 \rangle}{24} \frac{\epsilon^3}{\sin^3\theta} + O(\epsilon^4), \quad (\text{D28})$$

and is valid for all θ in the band, both near and far from $\pi/3$.

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