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The distribution of the reflection phase of disordered conductors

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Abstract. The reflection coefficient of one-dimensional disordered conductors is asymptotically a pure phase, when the sample length is much larger than the localisation length. We study the stationary distribution of this reflection phase for tight-binding chains with diagonal disorder, i.e. random site potentials. We derive the Dyson integral equation obeyed by this distribution and relate it to the Lyapunov exponent and the integrated density of states. This general approach allows us to consider then more specifically two types of disorder. In the case of a binary alloy, where the potentials take two values, the distribution of the reflection phase is shown to have generically an infinity of power-law singularities related to the occurrence of periodic patterns of potentials. This phenomenon produces divergences in the distribution when the strength of disorder exceeds some energy-dependent threshold. We also obtain an exact expression for the distribution of the reflection phase for a symmetric exponential distribution of potentials. This non-trivial solvable model allows us to examine analytically various properties of the phase distribution, such as the anomalies which occur at weak disorder.

1. Introduction

The reflection phase of one-dimensional disordered conductors has been the subject of several recent works [1-4]. One of the main motivations of these studies was the need to understand how the phases average as the sample length gets larger, and whether their distribution becomes flat, i.e. uniform, in the limit of a very long conductor. Such a 'phase averaging' hypothesis has indeed often been made, at least in an implicit way, throughout the history of localisation theory [5-7] in the derivation of various scaling laws concerning e.g. the moments of the distribution of the resistance.

The first work which addresses the question of the distribution of a reflection phase is, to our knowledge, by Sulem [8] who dealt in fact with the propagation of waves in macroscopic random media. This author considered a continuum model and realised, both analytically and numerically, that the phase of the reflection coefficient approaches a non-trivial distribution in the limit of a large sample thickness, in this language, but that this limit distribution is far from being uniform in general. References [1-3] have dealt with similar questions in the specific problem of one-dimensional quantum conductors. Reference [1] considers the most general model, where each unit of the conductor brings three new random parameters, and shows by general arguments that

the limit distribution of the phases has no reason to be uniform. Reference [2] considers more specifically the one-dimensional tight-binding Anderson model. The authors show in particular, mostly through numerical work, that the phase distribution becomes uniform only in the weak disorder regime, except at the band centre, which plays a very special role. More recently, [3] provides analytical results on the distribution of the reflection phase for a continuum model in the weakly localised regime, where the sample length is less than the localisation length. Also in this case the distribution is found not to be uniform, and this effect has some consequences on the moments of the resistance distribution.

In a recent paper [4] one of us, in collaboration with J Pendry, has studied the problem by means of a systematic perturbation theory, which yields the Fourier coefficients of the phase distribution, through a novel formalism involving an infinite transfer matrix. This work has shown in particular that the distribution of the phases becomes generically uniform as the strength of the disorder vanishes. In the case of the tight-binding model this occurs for every energy, except at the band centre, where the distribution has a non-trivial limit for a vanishingly small disorder. This result of an infinitely degenerate perturbation theory is in fact related to the so-called 'anomalies', described by several authors [9–12], which affect the weak disorder expansion of quantities like the Lyapunov exponent and the density of states of the Anderson model, and other disordered systems in one dimension.

The present work aims at giving a more accurate and rigorous description of the distribution of the phase of the reflection coefficient. We have limited ourselves to the tight-binding model with diagonal disorder, i.e. random site potentials, in the strongly localised regime, where the length of the disordered region of the sample is by far larger than the localisation length. In this regime, the reflection phase reaches a non-trivial stationary, or invariant, distribution. We investigate in particular the regularity properties of this distribution, as well as its dependence both on energy and on the strength of disorder. The present approach is a global one, which does not rely on perturbation theory, nor on any approximation scheme.

The content of this paper is as follows. In section 2, we recall some general definitions and formalism for the tight-binding model. We show that the distribution of the reflection coefficient, and of related quantities, obeys a linear integral equation, of a type first studied by Dyson [13] in the context of one-dimensional random systems. We also derive expressions for the Lyapunov exponent and the integrated density of states of the problem in terms of the invariant phase distribution. Section 3 is devoted to the case of a binary distribution of the random site potentials. This case is very particular since the distribution of the reflection phase usually has an infinity of power-law singularities, which show up as infinitely high peaks as soon as the strength of disorder exceeds some energy-dependent threshold. This novel phenomenon is related to the occurrence of divergences in the density of states of e.g. harmonic chains with random masses, first described by Halperin [14]. By adapting an approach used by one of us, in collaboration with Th M Nieuwenhuizen [15], to study Halperin's 'island frequencies', we obtain a complete labelling and quantitative description of the power-law singularities in the present problem. Section 4 presents what is certainly the only non-trivial distribution of potentials for which the problem is exactly soluble. For this symmetric exponential distribution, with an arbitrary width, we can derive the distribution of the reflection phase in an exact way. Some of the various possible applications of this result are discussed. Section 5 presents a short summary and conclusion.

2. Generalities

In this section, we recall some general formalism for the tight-binding model of disordered one-dimensional conductors. Our main goal is the study of the distribution of the reflection coefficient of very long random chains. We derive an integral equation *à la* Dyson [13] for the invariant distribution of the reflection phase in this regime. This formalism will be used extensively in the next sections.

We consider an ensemble of disordered conductors described by the tight-binding Schrödinger equation

$$\Phi_{n+1} + \Phi_{n-1} + \varepsilon_n \Phi_n = E \Phi_n. \tag{2.1}$$

Each chain consists of a central disordered region of N atoms ($1 \leq n \leq N$), for which the site energies ε_n are independent random variables, with a common probability density $\rho(\varepsilon)$. This region is connected to two semi-infinite perfect leads, where the ε_n vanish.

Let R_N and T_N denote the reflection and transmission coefficients (amplitudes) for an electron beam incident from the right, with wavevector $(-k)$, and hence energy

$$E = 2 \cos k \quad 0 < k < \pi. \tag{2.2}$$

This means that we have by definition

$$\Phi_n = \begin{cases} e^{-ik(n-N)} + R_N e^{ik(n-N)} & \text{for } n \geq N \\ T_N e^{-ikn} & \text{for } n \leq 1. \end{cases} \tag{2.3}$$

Let us now introduce the usual transfer-matrix formalism, which will also be used hereafter. Equation (2.1) can be recast in the following form

$$\begin{pmatrix} \Phi_{n+1} \\ \Phi_n \end{pmatrix} = M_n \begin{pmatrix} \Phi_n \\ \Phi_{n-1} \end{pmatrix} \tag{2.4}$$

where the transfer matrix M_n reads

$$M_n = \begin{pmatrix} E - \varepsilon_n & -1 \\ 1 & 0 \end{pmatrix}. \tag{2.5}$$

Hence the propagation of the wavefunction along the chain is described by a product of non-commuting 2×2 transfer matrices. We also define the Riccati variable Y_n through

$$Y_n = \frac{\Phi_{n+1}}{\Phi_n}. \tag{2.6}$$

The tight-binding equation (2.1) is then equivalent to the recursion relation

$$Y_n = E - \varepsilon_n - \frac{1}{Y_{n-1}}. \tag{2.7}$$

We now show that the reflection coefficient R_N is related in a simple way to the Riccati variable Y_N at the last site N of the disordered section of the chain, and therefore that the R_N also obey a recursion formula. To do so, we compare the chain defined above, with N impurities, and the chain with $(N - 1)$ impurities obtained by removing the last random site energy ($\varepsilon_N = 0$). Let R_N and R_{N-1} denote the reflection coefficients of these two conductors. Equation (2.3) implies that both chains have the

same $Y_0 = e^{-ik}$ and therefore the same Y_1, \dots, Y_{N-1} , but different values of Y_N . According to the same relations, the Y_N of the chain with N impurities is related to R_N by

$$Y_N = \frac{e^{-ik} + R_N e^{ik}}{1 + R_N}. \quad (2.8)$$

Equation (2.7) then yields the following recursion relation

$$R_N = \frac{e^{2ik} R_{N-1} + i\delta_N (1 + e^{2ik} R_{N-1})}{1 - i\delta_N (1 + e^{2ik} R_{N-1})} \quad (2.9)$$

with the notation

$$\delta_N = \frac{\varepsilon_N}{2 \sin k}. \quad (2.10)$$

Equation (2.9) expresses how the reflection coefficient of a disordered chain evolves when an extra impurity is added to it. The initial condition to this recursion is clearly $R_0 = 0$, since no random region is present in this case. When N increases, the transmission T_N decays to zero because of localisation effects. More quantitatively, it is well known that $|T_N| \sim e^{-\gamma N}$, where γ denotes the Lyapunov exponent, or inverse localisation length, to be discussed below. As a consequence, the unitarity relation $|R_N|^2 + |T_N|^2 = 1$ implies that R_N has asymptotically unit modulus for large N : it is a pure phase.

Throughout the following, we assume that the random conductors are long enough to be deeply in the localised regime. This condition reads $N\gamma \gg 1$. We define the reflection phase θ_N by

$$R_N = e^{i\theta_N} \quad -\pi < \theta_N < \pi. \quad (2.11)$$

We also introduce the following variable, which will be convenient in the technical developments

$$t_N = \tan \frac{\theta_N}{2} = -i \frac{R_N - 1}{R_N + 1} = \frac{\cos k - Y_N}{\sin k}. \quad (2.12)$$

In terms of this quantity, the recursion formulae (2.7) and (2.9) assume the form

$$t_N = 2\delta_N + \frac{t_{N-1} + \tau}{1 - t_{N-1}\tau} \quad (2.13)$$

with the notation

$$\tau = \tan k. \quad (2.14)$$

The main advantage of (2.13) is that it involves only real quantities in a natural way.

When the sample length N becomes large, the reflection phase θ_N is asymptotically distributed according to a probability density $P(\theta)$, which is stationary, i.e. independent of N , and hence invariant under the random recursion relation (2.9). This invariant probability measure can be alternatively described in terms of the Riccati Y -variable or the t -variable. Let $S(Y)$ and $Q(t)$ denote the corresponding densities. Equation (2.12) implies that these quantities are simply related through

$$Q(t) = (1 + \cos \theta) P(\theta) = \sin k S(Y). \quad (2.15)$$

The existence of an invariant measure for the one-dimensional Anderson model, as well as some of its regularity properties, have been investigated rigorously in [16]. The present work clearly does not pretend at any mathematical rigour on this point.

We will use the t -variable in the technical developments throughout the following in order to avoid dealing with complex numbers and to benefit from the simplicity of the transform (2.13). The distribution $Q(t)$ obeys an integral equation, of the type first derived by Dyson [13], which expresses its invariance under the random transformation (2.13). This property reads

$$Q(t) = \int \rho(\varepsilon) d\varepsilon \int Q(u) du \delta_D\left(t - 2\delta - \frac{u + \tau}{1 - u\tau}\right) \tag{2.16}$$

where t and u represent t_N and t_{N-1} respectively and δ_D denotes the Dirac delta function, which enforces the condition

$$u = g_\delta(t) = \frac{t - 2\delta - \tau}{1 + (t - 2\delta)\tau} \tag{2.17}$$

and we are left with

$$Q(t) = \int \rho(\varepsilon) d\varepsilon |g'_\delta(t)| Q[g_\delta(t)] \tag{2.18}$$

where the prime denotes differentiation w.r.t t , and δ and ε are related by (2.10). Equation (2.18) will be referred to as the Dyson equation of the problem, and used extensively in the next two sections.

It will be shown in section 3 that the probability densities $P(\theta)$ and $Q(t)$ are very singular quantities when the site potentials have a binary distribution. We prefer therefore to introduce now the following integrated densities, or distribution functions

$$W_P(\theta) = \int_{-\pi}^{\theta} P(\varphi) d\varphi \quad W_Q(t) = \int_{-\infty}^t Q(u) du. \tag{2.19}$$

These quantities are continuous functions in any circumstance. They are not differentiable when the densities themselves are divergent.

We end this section by discussing the relationship between the probability density $P(\theta)$, or its equivalent formulations $Q(t)$ and $S(Y)$, and two other quantities of much physical interest, namely the Lyapunov exponent and the integrated density of states. To do so it is advantageous to define, for a complex energy E , a characteristic function (or complex Lyapunov exponent) $\Omega(E)$ [17] through

$$\Omega(E) = \lim_{M \rightarrow \infty} \frac{1}{M} \sum_{N=1}^M \ln Y_N \tag{2.20}$$

where the principal branch of the complex logarithm is used. It can be shown (see e.g. [17]) that the limit of this quantity as E goes to the real axis reads

$$\Omega(E \pm i0) = \gamma(E) \pm i\pi H(E) \tag{2.21}$$

where $\gamma(E)$ is the above mentioned Lyapunov exponent (inverse localisation length) of the problem, and $H(E)$ denotes its integrated density of states (IDOS), i.e. the fraction of energy eigenvalues in the spectrum which are larger than some E . This rather unconventional definition is required by the fact that the off-diagonal terms in (2.1) have a positive sign.

The above relations between the variables Y_N , R_N , θ_N , and t_N yield the following expressions

$$\begin{aligned}\Omega(E) &= \int \ln Y S(Y) dY \\ &= \int \ln \frac{e^{-ik} + e^{ik+i\theta}}{1 + e^{i\theta}} P(\theta) d\theta \\ &= \int \ln(\cos k - t \sin k) Q(t) dt\end{aligned}\tag{2.22}$$

where it is understood that the invariant probability densities are evaluated for an energy E with an infinitesimal imaginary part.

3. The binary alloy

In this section we study the distribution $P(\theta)$ of the reflection phase in the case of a binary symmetric distribution of the site potentials: every ε_n is either $+\varepsilon$ or $-\varepsilon$, with equal probabilities $1/2$.

It will turn out that $P(\theta)$ is a very singular quantity in this case, with an infinity of power-law singularities under generic circumstances. As we shall see below, the mechanism responsible for this novel singular behaviour is closely related to the following phenomenon, first discussed by Halperin [14], who considered binary random harmonic chains, made of light and heavy atoms. The density of states of this system becomes infinite at the eigenfrequencies of finite clusters or 'islands' of light masses in a 'sea' of heavy ones. These singularities occur at high frequency, where heavy masses damp excitations, and only yield divergences of the density of states when the disorder strength (here, the mass difference) exceeds some threshold.

A similar effect occurs in the present problem, where the two different site energies $\pm\varepsilon$ play in some sense the part of the atomic masses. We will first present a heuristic and descriptive study of the phenomenon, before going to a more rigorous analysis, based on the Dyson equation (2.18).

Consider the periodic chain $+-+-+\dots$ made of an infinite repetition of the simple cell or pattern $(+-)$. Throughout this section, the symbols $+$ and $-$ will denote the signs of the site potentials ε_n . This simplest example of a pattern with period 2 will turn out to be physically the most important one. Provided the energy E lies in a gap of this periodic structure, the infinite periodic chain exhibits only two well defined reflection angles, namely θ_+ and θ_- , corresponding to both types of atoms at which the reflection coefficient can be measured. These phases are entirely determined by the structure of the basic pattern, and by the energy E .

The simplest way of realising this is to consider the transfer matrix M of the cell, defined as the product of the two elementary transfer matrices of the form (2.5) associated with the atoms of the cell. In the present case we have

$$M = \begin{pmatrix} E^2 - \varepsilon^2 - 1 & \varepsilon - E \\ \varepsilon + E & -1 \end{pmatrix}.\tag{3.1}$$

Since M has unit determinant, its eigenvalues are determined by its trace: $\text{tr } M = E^2 - \varepsilon^2 - 2$. If the energy is such that $|\text{tr } M| > 2$, the eigenvalues of M read $\exp(\pm K)$,

up to a sign, where K is defined by

$$|\text{tr } M| = 2 \cosh K. \tag{3.2}$$

Hence the wavefunction grows essentially like $\Phi_n \sim \exp(nK)$, with two different amplitudes, according to the parity of the site label n . The Riccati variable defined in (2.6) admits therefore two limit values, namely Y_+ and Y_- , which are related to the values θ_{\pm} of the reflection phase by (2.8), (2.11) and (2.12).

Consider now all chains for which the disordered region ends up with the repetition of any finite number L of contiguous cells $(+-)$. It is expected that, for L large enough, the reflection phase θ of such a chain will be very close to either θ_+ or θ_- . In a more quantitative way, since the eigenfunction inside the segment made of the L cells $(+-)$ is a linear combination of $\exp(nK)$ and $\exp(-nK)$, it can be argued that the difference $|\theta - \theta_{\pm}|$ is of the order of the ratio of both solutions taken at the end of the segment, namely $\exp(-2KL)$. On the other hand, the probability of having such a configuration is proportional to 2^{-2L} . By eliminating the number L of cells between the above estimates, we predict that the distribution function $W_p(\theta)$, defined by (2.19), has a power-law singularity

$$W_{p,\text{sg}}(\theta) \sim |\theta - \theta_{\pm}|^{\alpha} \quad \text{with } \alpha = \frac{\ln 2}{K}. \tag{3.3}$$

Such a singularity corresponds, via a formal differentiation, to a power-law behaviour $|\theta - \theta_{\pm}|^{\alpha-1}$ for $P(\theta)$ itself. Hence the probability density exhibits a divergency, an infinitely high peak, only when we have $\alpha < 1$, i.e. $K > \ln 2$. Since the magnitude of K is a measure of randomness, this means that there is a threshold in the disorder strength for peaks to appear. When the exponent α is larger than unity, only some derivative of $P(\theta)$ diverges at $\theta = \theta_{\pm}$.

The heuristic argument just described also predicts that the distribution of the phase exhibits similar but weaker singularities, characterised by the same exponent α , at all the values of the phase corresponding to adding one, two, etc atoms of any type at the end of the large region made of $(+-)$ cells. We will also come back to this point in a more detailed way later in this section.

Moreover, periodic arrangements of larger patterns, such as for instance $(+--)$ and $(++-)$, which have period $p = 3$, up to a cyclic permutation, also produce their own sets of singularities whenever the energy lies in a gap of the associated spectra. These are also power-law singularities, with an exponent α given by

$$\alpha = \frac{p \ln 2}{2K} \tag{3.4}$$

where p denotes the period of the cell, and K is still related to the trace of the associated product of p transfer matrices through (3.2). It is nevertheless expected on physical grounds that the singularities connected with the $(+-)$ cell will be the most important ones. The numerical work presented below fully confirms this assertion.

We now turn to a more accurate analysis, based on the Dyson equation (2.18), of the singularities in the distribution $P(\theta)$, or equivalently $Q(t)$ or $S(Y)$. Here again, we prefer to use the language of the t -variable, for the sake of simplicity. The present study is an adaptation of the work by Nieuwenhuizen and Luck [15] on the density of states of harmonic chains. We will present the full derivation in the case of the $(+-)$ cell, which is both the simplest and the most important case.

For the binary distribution of site potentials under consideration, (2.18) reads

$$2Q(t) = |g'_+(t)|Q[g_+(t)] + |g'_-(t)|Q[g_-(t)] \tag{3.5}$$

where $g_{\pm}(t)$ denote the function $g_{\delta}(t)$ defined in (2.17), with $\delta = \pm \varepsilon / (2 \sin k)$ according to (2.10). The transcription of the above heuristic argument goes as follows. The limit reflection angles θ_+ and θ_- correspond by definition via (2.12) to variables t_+ and t_- such that

$$t_+ = g_-(t_-) \quad t_- = g_+(t_+). \tag{3.6}$$

A direct evaluation yields in the present case

$$t_{\pm} = \pm \delta \pm \left(\frac{\tau \delta \pm 1}{\tau \delta \mp 1} (\delta^2 + 1) \right)^{1/2}. \tag{3.7}$$

Let us also introduce the notation

$$\lambda_+ = g'_+(t_+) \quad \lambda_- = g'_-(t_-). \tag{3.8}$$

Both of these quantities are positive. The occurrence of singularities in $Q(t)$ at $t = t_{\pm}$ appears clearly through the following argument, inspired by [15]. Since all values of the probability density $Q(t)$ are necessarily positive, the Dyson equation (3.5) implies that we have $2Q(t_+) \geq \lambda_- Q(t_-)$ and $2Q(t_-) \geq \lambda_+ Q(t_+)$, and hence $4Q(t_{\pm}) \geq \lambda_+ \lambda_- Q(t_{\pm})$. Therefore, if the product

$$\Lambda = \lambda_+ \lambda_- \tag{3.9}$$

is larger than 4, the only way out is that both values of Q are either zero or infinite!

A quantitative description of the actual behaviour of $Q(t)$ is obtained by linearising the Dyson equation around $t = t_{\pm}$ as follows. If $Q_{sg}(t)$ denotes the singular parts of $Q(t)$ around t_{\pm} , (3.5) implies that we have, up to first order in the variations x and y

$$2Q_{sg}(t_+ + x) \approx \lambda_+ Q_{sg}(t_- + \lambda_+ x) \quad 2Q_{sg}(t_- + y) \approx \lambda_- Q_{sg}(t_+ + \lambda_- y). \tag{3.10}$$

The general asymptotic solution of these equations has the form of a power law, modulated by periodic amplitudes, namely

$$Q_{sg}(t_+ + x) \approx |x|^{\alpha-1} A^{\pm} \left(\frac{\ln |x|}{\ln \Lambda} \right) \tag{3.11}$$

$$Q_{sg}(t_- + y) \approx \frac{1}{2} \lambda_-^{\alpha} |y|^{\alpha-1} A^{\pm} \left(\frac{\ln |\lambda_- y|}{\ln \Lambda} \right)$$

where the value of the exponent α

$$\alpha = \frac{2 \ln 2}{\ln \Lambda} \tag{3.12}$$

can be rewritten after a good deal of manipulation as

$$\alpha = \frac{\ln 2}{K} \quad \text{with } \varepsilon^2 - E^2 = 2(\cosh K - 1) = 4 \sinh^2(K/2) \tag{3.13}$$

in full agreement with the previous result (3.3).

The amplitudes A^{\pm} are two periodic functions of their argument, with unit period, and the superscript \pm denotes the sign of x or y . The occurrence of periodic amplitudes is a common feature of a large variety of disordered systems with a discrete, e.g. binary, distribution of the random couplings [15, 18-20]. As usual, the above linear analysis predicts their existence and their period, but not their specific form.

An integration of (3.11) shows that the distribution function $W_Q(t)$ of the t -variable, defined in (2.19), also has a power-law singular component around t_{\pm}

$$W_{Q,sg}(t_+ + x) \approx |x|^{\alpha} B^{\pm} \left(\frac{\ln |x|}{\ln \Lambda} \right)$$

$$W_{Q,sg}(t_- + y) \approx \frac{1}{2} |y|^{\alpha} B^{\pm} \left(\frac{\ln |\lambda_- y|}{\ln \Lambda} \right).$$
(3.14)

The B^{\pm} are two periodic amplitudes, with unit period, which are essentially primitives of the A^{\pm} . Hence the B^{\pm} are slightly more regular mathematical objects. It can indeed be argued, by analogy with [18], that they are always continuous functions, but they are nowhere differentiable when $\alpha < 1$. Some plots of these amplitudes will be presented later on.

The results (3.11) and (3.14) show that the distribution $Q(t)$ is never a smooth function, even at weak disorder ($\varepsilon \rightarrow 0$). Indeed, for any small value ε of the site potentials, the energy interval $|E| < \varepsilon$ around the band centre lies in a gap of the infinite $(+-)$ structure. In this whole range, (3.12) and (3.13) predict a finite value of the exponent α . Hence the distribution functions $W_P(\theta)$ and $W_Q(t)$ are not $n(\alpha)$ times differentiable, where $n(\alpha)$ denotes the integer part of $\alpha + 1$. The derivatives of that order are indeed infinite at t_{\pm} . In particular, at the band centre ($E = 0$), (3.13) reads $\varepsilon = 2 \sinh(K/2)$. Hence the order $n(\alpha)$ of the singularities blows up at weak disorder as $(\ln 2)/\varepsilon$.

As mentioned previously, the distribution $P(\theta)$ and $Q(t)$ exhibit a divergence, or a 'peak', only when $\alpha < 1$. This condition can be recast in the form of a threshold value for the disorder ε , namely $\varepsilon > \varepsilon_0$, with $\varepsilon_0^2 = E^2 + 1/2$. At the band centre, we have thus a threshold $\varepsilon_0 = 1/\sqrt{2}$.

Let us now show how 'secondary peaks' arise. There are actually an infinity of values of t , besides t_{\pm} , where the distribution $Q(t)$ has singularities with the same exponent α , modulated by similar periodic amplitudes. Indeed, by inserting the singular behaviour (3.11) into the RHS of the Dyson equation (3.5), we can show that a similar singular component is present at $t = t_{++} = f_+(t_+)$ and $t = t_{--} = f_-(t_-)$, where the f_{\pm} denote the inverses of the g_{\pm}

$$f_{\pm}(t) = \pm 2\delta + \frac{t + \tau}{1 - t\tau}.$$
(3.15)

These functions coincide, as they should, with the transforms entering the recursion relation (2.13). The singularities at these two values are caused by chains for which the disordered region ends up with $(+-)^L++$, and $(-+)^L--$, respectively, for large L , whence the notation. By iterating the procedure, we obtain analogous singularities at an infinity of values, such as $t_{---} = f_+(f_-(t_-))$, $t_{+++} = f_+[f_+(f_-(t_+))]$, etc. These values of t describe the reflection phases of patterns of the form $(+-)^{\infty}U$ or $(-+)^{\infty}V$, where U and V denote arbitrary finite 'binary words' made of the symbols $+$ and $-$.

We now compare the above analytical results with some numerical data. These have been obtained by the enumeration method already used extensively in [15, 18, 19]. This approach consists of enumerating in an exact way all the 2^N different configurations of a finite disordered chain with N sites, and of calculating the associated reflection phase by iterating (2.13). We start from an arbitrary initial condition, not necessarily the 'physical' one. This choice is indeed fully irrelevant. The data can then be for

instance accumulated in a histogram. The only error of the method is a systematic one, due to the finiteness of the sample length N . Large computers allow us to handle $N = 20 - 22$.

Figure 1 shows a histogram of the distribution $P(\theta)$ of the reflection phase in a typical case with an exponent α smaller than unity. The values $k/\pi = 0.45$ and $\varepsilon = 1$ indeed yield $\alpha = 0.7556$. A large number of deeply pronounced peaks are clearly visible: besides the largest two peaks corresponding to θ_+ and θ_- , all of them are 'secondary peaks' as defined previously. We have labelled the largest of them according to the notation explained above.

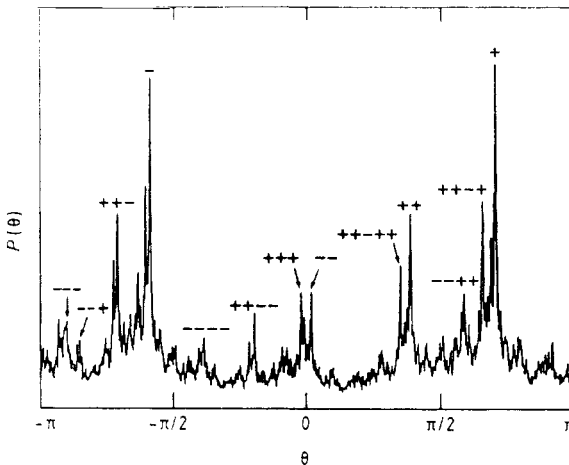


Figure 1. Histogram of the distribution $P(\theta)$ of the reflection phase, obtained from the exact enumeration method, for the binary potential distribution with $\varepsilon = 1$, and $k/\pi = 0.45$, so that the exponent α equals 0.7556. The histogram contains 1000 bins; units along the vertical axis are arbitrary. The labelling of the most visible 'secondary peaks' is described in the text.

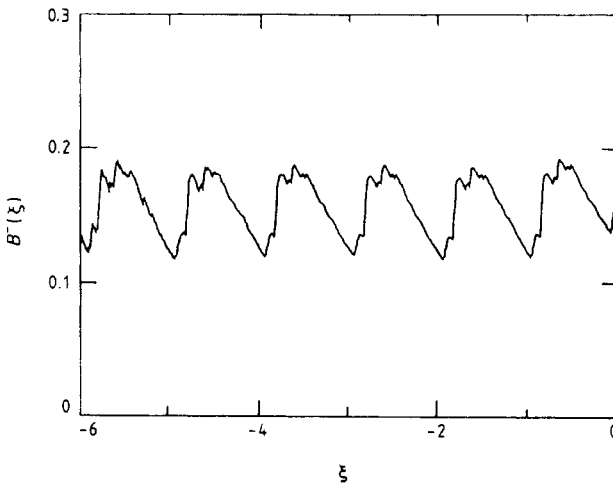


Figure 2. Plot of the periodic amplitude B^- , against its argument $\xi = \ln(-x)/\ln \Lambda$. The parameters $k/\pi = 0.45$, and $\varepsilon = 1.4$, are such that $\alpha = 0.5431$.

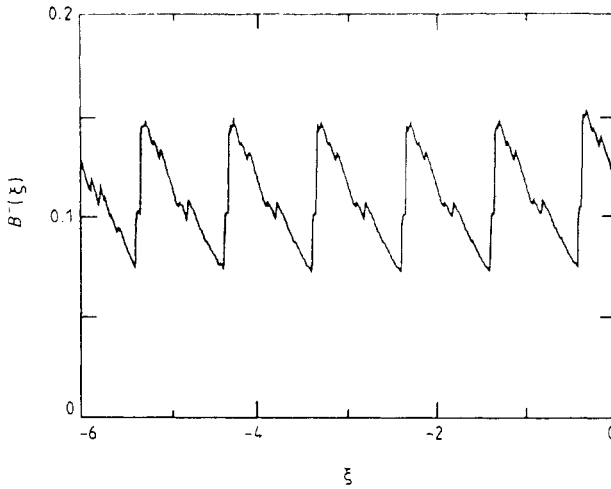


Figure 3. Same as figure 2, for $k/\pi = 0.27$, and $\epsilon = 1.7$, so that $\alpha = 0.6777$.

Figures 2 and 3 show plots of the periodic amplitude B^- of the singularity of the integrated distribution function $W_Q(t)$, defined in (3.14), against its argument $\xi = \ln(-x)/\ln \Lambda$, extracted from data for t around t_* . In both cases we have $\alpha < 1$, in such a way that the plotted functions are continuous but nowhere differentiable. Such curves always seem aesthetically appealing, at least to the authors.

4. An exactly solvable model

This section is devoted to the case where the site energies ϵ_N have a symmetric exponential distribution of width W

$$\rho(\epsilon) = \frac{1}{2W} e^{-|\epsilon|/W}. \tag{4.1}$$

The remarkable property of this distribution is that all the quantities of interest: the distribution of the reflection phase $P(\theta)$, the Lyapunov exponent $\gamma(E)$ and the IDOS $H(E)$, can be evaluated exactly following a technique introduced by Nieuwenhuizen [21], which consists of an exact integration over the given random variables (here, the site energies). This powerful method has been applied to a large variety of disordered physical systems in one dimension (see e.g. [22–25]).

For reasons that will become clear in the following, it turns out to be advantageous to introduce the logarithmic transform

$$D(z) = \int Q(t) dt \ln(z - t) \tag{4.2}$$

of $Q(t)$, the invariant probability density introduced in section 2. Here again, the principal branch of the complex logarithm is used. This definition ensures that $D(z)$ is analytic in the upper half plane ($\text{Im } z > 0$), and continuous as z approaches the real axis. Furthermore, as a direct consequence of (2.16), we have

$$D(z) = \int \rho(\epsilon) d\epsilon \int Q(t) dt \ln\left(z - 2\delta - \frac{t + \tau}{1 - t\tau}\right). \tag{4.3}$$

By rewriting the differential element $\rho(\varepsilon) d\varepsilon = r(\delta) d\delta$, with

$$r(\delta) = \frac{\beta}{2} e^{-\beta|\delta i} \quad \beta = \frac{2 \sin k}{W} \tag{4.4}$$

and reshuffling the argument of the logarithm, we obtain the following integral equation for the function $D(z)$

$$D(z) + D(1/\tau) = \int r(\delta) d\delta \left[D\left(\frac{z - 2\delta - \tau}{1 + (z - 2\delta)\tau}\right) + \ln(z - 2\delta + 1/\tau) \right]. \tag{4.5}$$

The key point which allows an exact solution is as follows. δ only enters the integrand through the combination $z - 2\delta$. Hence, if we evaluate $D'(z)$ from (4.5), the differentiation WRT z can be converted into a differentiation WRT δ inside the integral, which can in turn be compensated by an integration by parts. More explicitly, if we define the partial integral over positive values of δ

$$D_+(z) = \int_0^{+\infty} \beta e^{-\beta\delta} d\delta \left[D\left(\frac{z - 2\delta - \tau}{1 + (z - 2\delta)\tau}\right) + \ln(z - 2\delta + 1/\tau) \right] \tag{4.6}$$

the procedure just described leads to

$$D'_+(z) = \frac{\beta}{2} \left[D\left(\frac{z - \tau}{1 + z\tau}\right) + \ln(z + 1/\tau) - D_+(z) \right]. \tag{4.7}$$

This equation can be iterated to get an expression for $D''_+(z)$. A very analogous formula holds for the integral $D_-(z)$ over negative values of δ . We end up with the second-order differential-difference equation for $D(z)$

$$D''(z) = \frac{\beta^2}{4} \left[D(z) - D\left(\frac{z - \tau}{1 + z\tau}\right) + D(1/\tau) - \ln(z + 1/\tau) \right]. \tag{4.8}$$

We have thus reduced the whole problem of the determination of the distribution $P(\theta)$ to that of solving (4.8). Fortunately enough, this equation can be further simplified as follows. Since it relates values of the unknown function D at z and at $z_1 = (z - \tau)/(1 + z\tau)$, we are led to perform the change of variable

$$y = \frac{z - i}{z + i} \quad z = i \frac{1 + y}{1 - y} \tag{4.9}$$

which maps the upper half plane ($\text{Im } z > 0$) onto the unit disc ($|y| < 1$), and maps z_1 onto $y_1 = e^{-2ik}y$, where k is the wavevector. We also define a new unknown function $E(y)$ by

$$D(z) = E(y) - \ln(1 - y) - \ln \frac{1 - e^{-2ik}}{2i}. \tag{4.10}$$

The asymptotic behaviour $D(z) = \ln z + \mathcal{O}(1/z)$ for large z leads to

$$E(1) = \ln(2i \sin k) - ik. \tag{4.11}$$

On the other hand, (2.22) implies

$$\Omega = D(1/\tau) - \ln \sin k = E(e^{-2ik}) - \ln(2i \sin k) + 2ik. \tag{4.12}$$

Equations (4.11) and (4.12) allow us to show that (4.8) is fully equivalent to

$$(1 - y)^4 E''(y) - 2(1 - y)^3 E'(y) - (1 - y)^2 = -\beta^2 [E(y) - E(e^{-2ik}y) + \Omega_r] \tag{4.13}$$

where

$$\Omega_r = \Omega - ik \tag{4.14}$$

denotes the ‘random part’ of the characteristic function Ω , i.e. the difference between Ω and its value $\Omega_0 = ik$ in the absence of disordered site potentials.

The requirement that $E(y)$ is analytic in the unit disc and continuous at its boundary determines in a unique way both the function E and the complex constant Ω_r . If we insert into (4.13) the, necessarily convergent, series expansion

$$E(y) = E(0) + \sum_{n \geq 1} \frac{1}{n} c_n y^n \tag{4.15}$$

we obtain the following recursion relation

$$\Delta c_n = (1 - \beta^2 \Omega_r) \delta_{n,0} - 2\delta_{n,1} + \delta_{n,2} - \beta^2 \frac{1 - e^{-2ink}}{n} c_n. \tag{4.16}$$

Here $\delta_{m,n}$ is the Kronecker symbol, and Δc_n denotes the following five-term difference operator acting on the c_n

$$\Delta c_n = (n + 1)c_{n+2} + (n - 1)c_{n-2} - 2(2n + 1)c_{n+1} - 2(2n - 1)c_{n-1} + 6nc_n \tag{4.17}$$

with the convention that $c_n = 0$ for $n \leq 0$.

Four boundary conditions are therefore necessary to specify the c_n entirely. Equation (4.16) taken for $n = 0, 1$, and 2 , the three cases where the equation is not homogeneous, provides two boundary conditions and determines Ω_r as well. The two missing conditions come from considering the behaviour of c_n for $n \rightarrow \infty$. Indeed, assuming that c_n is a slowly varying function of n for large n , and forgetting about oscillatory terms proportional to e^{-2ink} , we approximate (4.16) and (4.17) as

$$n\Delta c_n \approx n^2 \frac{d^4 c_n}{dn^4} \approx -\beta^2 c_n. \tag{4.18}$$

Four independent solutions of this homogeneous equation read asymptotically

$$c_n \sim \exp(\omega\sqrt{n}) \quad \omega = (\pm 1 \pm i)\sqrt{2\beta} \tag{4.19}$$

where both \pm signs are independent of each other. The two values of ω with a positive real part yield a growing solution, and have to be discarded. The requirement of regularity at infinity thus fixes the last two boundary conditions.

We have therefore shown that (4.16) and (4.17) determine the function E in a unique way. We now have to express the quantity of main interest, namely the distribution of the reflection phase, in terms of $E(y)$. The definition (4.2) of $D(z)$ implies that the distribution $Q(t)$ is given by the following boundary value

$$-\pi Q(t) = \text{Im } D'(z = t + i0). \tag{4.20}$$

This value of z corresponds to $y = -e^{i\theta}$. Expressing $Q(t)$ in terms of $P(\theta)$ according to (2.15) and $D(z)$ in terms of $E(y)$ according to (4.10), we obtain the final result

$$2\pi P(\theta) = 1 + 2 \sum_{n \geq 1} (-1)^{n-1} \text{Re}(c_n e^{in\theta}). \tag{4.21}$$

Hence the c_n are essentially the Fourier coefficients of the distribution of the reflection phase. These complex quantities are defined as the unique solution of (4.16) and (4.17), with the appropriate boundary conditions, as discussed above. We shall now examine analytically some properties of this exact solution, and present some numerical illustrations of it.

Our exact solution provides an analytical form for the fall-off of the c_n , and hence of the regularity properties of the probability density $P(\theta)$. The behaviour of the c_n at large n is given by (4.19) where, as explained above, only the two decreasing solutions have to be considered. Hence the c_n decay more rapidly than any power of the index n , and the distribution $P(\theta)$ is very smooth (differentiable infinitely many times), in strong contrast with the case of the binary alloy studied in section 3. To be complete, let us mention that $P(\theta)$ is not an analytic function at $\theta = \pm\pi$. It can indeed be shown, e.g. by inserting the estimate (4.19) into (4.21) and evaluating the sum by the saddle-point method, that the distribution of the reflection phase has the following singular part around $\theta = \pm\pi$

$$P_{\text{sg}}(\theta) \sim \exp\left(-\frac{2 \sin k}{|\theta \pm \pi| W}\right). \quad (4.22)$$

This exponentially small singularity lies 'on top of' a very smooth background. The mechanism responsible for this singular contribution is in fact quite simple. If the N th atom has a very large site energy ε_N , either positive or negative, then the reflection phase θ_N differs from $\pm\pi$ only by a small amount $(2 \sin k)/|\varepsilon_N|$; such an event occurs at any site with probability $\exp(-|\varepsilon_N|/W)$. Equation (4.22) is recovered by eliminating ε_N between these two estimates. We are therefore led to expect an analytic distribution of the reflection phase whenever the site energies are bounded, and have a rather smooth (e.g. continuous) probability distribution.

The exact solution derived above also permits to study the distribution $P(\theta)$ in the weak disorder limit ($W \rightarrow 0$) in a simple and systematic way. This regime has already been studied in [4], using perturbation theory. Because of the prefactors $(1 - e^{-2ink})$ in the RHS of (4.16), the values of the wavevector k which are rational multiples of π have to be considered separately. These are the cases where the wavefunction in absence of randomness is commensurate to the lattice.

Consider first a generic value of the wavevector not rationally related to π . It can easily be shown from (4.16) and (4.17) that c_1 and c_2 are proportional to W^2

$$\begin{aligned} c_1 &\approx \frac{-2}{\beta^2(1 - e^{-2ik})} = \frac{i e^{ik} W^2}{4 \sin^3 k} \\ c_2 &\approx \frac{2}{\beta^2(1 - e^{-4ik})} = \frac{-i e^{2ik} W^2}{8 \sin^3 k \cos k} \end{aligned} \quad (4.23)$$

that c_3 and c_4 are proportional to W^4 , and more generally c_{2m-1} and c_{2m} are proportional to W^{2m} for a small disorder width W . These results were already obtained in [4].

This simple behaviour at weak disorder is modified for resonant values of the wavevector, rationally related to π . It is already known that the Lyapunov exponent and the density of states present anomalies [9-12] in their weak disorder expansion in such cases. The perturbative treatment of the present problem also has to be modified [4].

The strongest anomaly occurs at the band centre ($E = 0, k = \pi/2$). It is indeed clear from (4.23) that the expansion of c_2 is singular at that point. The band centre is actually the only case for which the c_n do not vanish in the $W \rightarrow 0$ limit. Thus the distribution $P(\theta)$ does not become trivial (uniform) at weak disorder. More precisely, it can be derived from (4.16) and (4.17) that the c_n are proportional to W^2 for odd values of n , but have non-vanishing limits for even n . These non-trivial values are

given by the following three-term recursion

$$(n + 1)c_{n+2} + (n - 1)c_{n-2} + 6nc_n = \delta_{n,2} \tag{4.24}$$

with $c_n = 0$ for $n \leq 0$, as previously. The solution of (4.24) gives the universal distribution

$$2\pi P_0(\theta) = 1 - 2 \sum_{n \geq 2} c_n \cos n\theta \tag{4.25}$$

of the reflection phase at the band centre for any weak disorder. The first few values of the c_n read

$$c_2 = 8.6107 \times 10^{-2} \quad c_4 = -1.1094 \times 10^{-2} \quad c_6 = 1.5872 \times 10^{-3}. \tag{4.26}$$

The c_n fall off as $(-1)^{n/2}(1 + \sqrt{2})^{-n}$ for large n , implying in particular that $P_0(\theta)$ is an analytic function. The present derivation, starting from an exact solution, is by far shorter than those using perturbative approaches [4, 9].

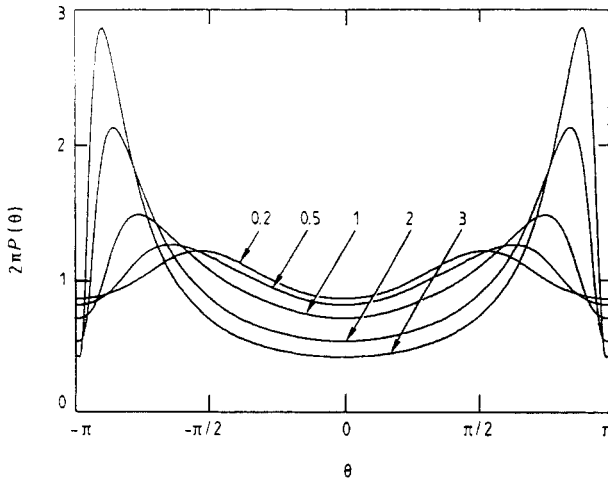


Figure 4. Plot of the distribution of the reflection phase, for the exactly soluble model, at the band centre, for different values of the disorder width W , indicated on the curves.

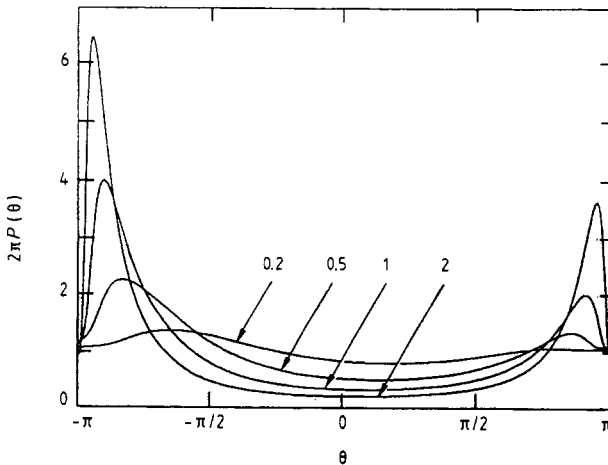


Figure 5. Same as figure 4, for a generic point of the spectrum: $k/\pi = 0.13$.

For other resonant values $k = \pi p/q$ of the wavevector, where p and q are two coprime integers, some of the coefficients c_n vanish as a smaller power of W than generically. This anomalous behaviour is also most easily studied from the exact solution. The smallest index which exhibits an anomaly is $n = q$: the leading power of W^2 in c_q is less by one unit than generically, in agreement with a recent systematic study of anomalies [12].

We end up this section with some numerical illustrations of our exactly soluble model. It is indeed easy to solve the central equations (4.16) and (4.17) numerically. A first step consists of finding two independent general solutions, say $c_{n,1}$ and $c_{n,2}$, of the homogeneous equations (for all $n \geq 3$), which decay for $n \rightarrow \infty$. In a second step, one matches the amplitudes a_1 and a_2 so that the linear combination $c_n = a_1 c_{n,1} + a_2 c_{n,2}$ obeys (4.16) also in the inhomogeneous cases: $n = 0, 1$, and 2 . These are three equations for the three unknowns, namely a_1 , a_2 , and Ω_n , the 'random part' of the characteristic function. As explained in section 2, this last quantity yields, according to (2.21), the Lyapunov exponent and the integrated density of states of the problem as by-products of the computation, for any energy E in the spectrum $[-2, +2]$ of the perfect leads. Let us just mention that the characteristic function Ω for E outside this interval could also be obtained through a slight adaptation of the present analysis.

Figure 4 shows plots of the distribution $P(\theta)$ for different values of the disorder strength W , at the band centre ($E = 0$). In this case, the Fourier coefficients c_n are real, and $P(\theta)$ is an even function of θ . Figure 5 shows an analogous series of plots for a generic value of energy, corresponding to $k/\pi = 0.13$. As disorder becomes strong, the distribution is more and more peaked towards $\pm\pi$: this is indeed a general property, which would hold for any distribution of the site potentials.

In order to illustrate the phenomenon of the anomalies present in the weak disorder limit, Figure 6 presents plots of the first two (real) Fourier coefficients c_1 and c_2 , at the band centre, against the width W . In agreement with the above discussion of anomalies, c_1 vanishes as W^2 , whereas c_2 has a non-trivial anomalous $W \rightarrow 0$ limit, given by (4.26). Also note that this coefficient vanishes for some finite value of W .

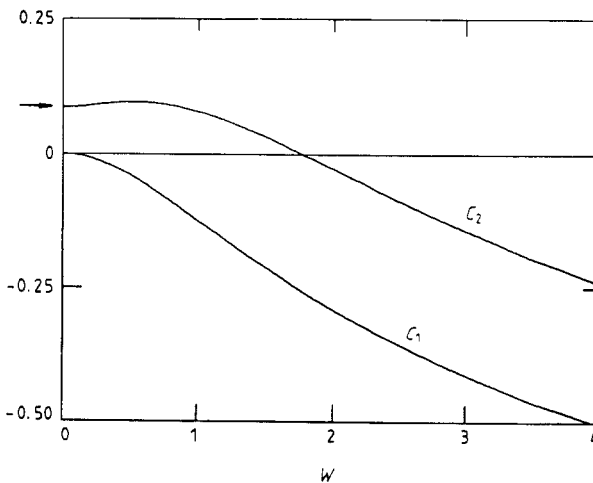


Figure 6. Plot of the first two Fourier coefficients c_1 and c_2 of the distribution of the reflection phase at the band centre. The arrow indicates the 'anomalous' limit of the second coefficient at a vanishing disorder.

5. Summary and conclusion

We have reported on the study of the distribution of the phase of the reflection coefficient of disordered conductors, described by the tight-binding model. The chains are made of a central region, with arbitrary diagonal disorder, connected to two semi-infinite perfect leads.

The formalism developed in section 2 for an arbitrary distribution of the site potentials shows how the reflection phase is simply related to the Riccati variable, defined in (2.6), which has been extensively used in analytical studies of one-dimensional disordered systems. This approach shows in a natural way that the reflection phase possesses a non-trivial stationary distribution $P(\theta)$, in the regime where the sample length is much larger than the localisation length $1/\gamma(E)$. This distribution, or rather an equivalent quantity $Q(t)$, obeys a linear integral equation (2.18), of a type studied first by Dyson [13]. Another consequence is that the Lyapunov exponent $\gamma(E)$ and the integrated density of states $H(E)$ of the problem have simple expressions in terms of $P(\theta)$, provided the energy E is in the spectrum of the perfect leads.

We have then proceeded to examine the distribution $P(\theta)$ of the reflection phase for two special types of disorder, namely the binary alloy, with site potentials $\pm\varepsilon$, and an exactly soluble model, with a symmetric exponential distribution of potentials.

The case of the binary alloy, where the site potentials assume the values $\pm\varepsilon$, with probability $1/2$, is considered in section 3. We have shown that long repetitions of periodic patterns of potentials are responsible for the existence of an infinity of power-law singularities in the reflection phase distribution. This effect is similar to the phenomenon, first described by Halperin [14], which affects the density of states of random harmonic chains, with light and heavy atomic masses. The predominant singularities are associated with repetitions $+-+--\dots$ of the pattern $(+-)$ with period two. Patterns with higher periods produce much weaker singular contributions. The exponent α which characterises these sets of singularities is obtained in an exact way. It depends both on the disorder strength ε and on energy, so that divergences, 'peaks', in $P(\theta)$ are actually observed only when disorder exceeds some energy-dependent threshold. The numerical results of an enumeration procedure show that the positions of all the most visible peaks present in this data are explained by the analytic approach. We also present plots of the periodic amplitudes, which modulate the power-law singularities. Such a singular behaviour of $P(\theta)$ will generally occur whenever the distribution of the site potentials contains some discrete component.

We consider in section 4 a special class of distributions of the site potentials, namely the symmetric exponentials, for which the whole problem is exactly soluble. The solution, namely the determination of the Fourier coefficients of the distribution $P(\theta)$, as well as $\gamma(E)$ and $H(E)$, follows a method introduced by Nieuwenhuizen [21]. This method, which reduces the problem to solving a difference equation (4.16), (4.17) can in principle be extended to a wider class of potential distributions $\rho(\varepsilon)$, symmetric or not, where a polynomial in ε multiplies the exponential of (4.1).

This exact solution allows a detailed investigation of various properties of the phase distribution. We find that $P(\theta)$ is differentiable infinitely many times, and fails to be analytic only because of an essential singularity at $\theta = \pm\pi$, related to the occurrence of arbitrarily large site potentials. It is therefore expected that $P(\theta)$ is analytic for any bounded and continuous distribution of the site potentials. We also investigate the behaviour of the Fourier coefficients c_n of $P(\theta)$ at weak disorder, and show how the

peculiarities of their perturbative expansion at the band centre, described in [4], are related to the anomalies which are known [9–12] to affect the weak disorder expansion of quantities such as the Lyapunov exponent for any commensurate wavevector, namely any value of k rationally related to π .

We finally want to mention that it would be worthwhile to generalise some of the present results to multichannel quasi-one-dimensional systems. In the strongly localised regime in such a geometry, there is total reflection, and hence a unitary reflection matrix. The eigenvalues of that matrix are therefore pure phases, and the object of interest is the distribution of these phases.

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