Journal of Statistical Physics, Vol. 52, Nos. 1/2, 1988

# Lifshitz Tails and Long-Time Decay in Random Systems with Arbitrary Disorder

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*Received September 8, 1987; revision received February 9, 1988*

In random systems, the density of states of various linear problems, such as phonons, tight-binding electrons, or diffusion in a medium with traps, exhibits an exponentially small Liftshitz tail at band edges. When the distribution of the appropriate random variables (atomic masses, site energies, trap depths) has a delta function at its lower (upper) bound, the Lifshitz singularities are pure exponentials. We study in a quantitative way how these singularities are affected by a universal logarithmic correction for continuous distributions starting with a power law. We derive an asymptotic expansion of the Lifshitz tail to all orders in this logarithmic variable. For distributions starting with an essential singularity, the exponent of the Lifshitz singularity itself is modified. These results are obtained in the example of harmonic chains with random masses. It is argued that analogous results hold in higher dimensions. Their implications for other models, such as the long-time decay in trapping problems, are also discussed.

**KEY WORDS:** Random harmonic chains; Lifshitz singularities; trapping problems; density of states.

## 1. INTRODUCTION

Lifshitz noticed in 1964[1] that randomness strongly affects the band edges of the spectra of phonons, tight-binding electrons, etc., in solids: the usual Van Hove power-law singularities are replaced by exponentially small tails. Although much rigorous work has been devoted to Lifshitz singularities (see, e.g., ref. 2 and references therein), their precise analytical form is not easy to derive within specific models, even in one dimension.

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This paper will be mainly concerned with the Lifshitz tails in disordered harmonic chains. The equation of motion for the atomic displacements at frequency $\omega/2\pi$ reads

$$-m_n \omega^2 a_n = a_{n+1} + a_{n-1} - 2a_n \tag{1.1}$$

where the masses $m_n$ are independent random variables with a common distribution $\rho(m)\, dm$. The Lifshitz phenomenon occurs when the support of the mass distribution does not extend down to zero. We choose units such that this lower bound is $m = 1$.

The integrated density of states (IDS), denoted $H(\omega^2)$, is defined as being the fraction of eigenvalues of Eq. (1.1) less than some $\omega^2$. The maximal eigenvalue being $\omega^2_{\max} = 4$, the key question is: How does the IDS approach unity as $\omega^2 \to 4^-$? Lifshitz' original argument[1] is the following. The succession of a large number $N$ of light masses ($m = 1$) is needed to have an eigenmode at

$$\omega^2 = 4\cos^2(\varepsilon/2) \approx 4 - \varepsilon^2 \tag{1.2}$$

with $\varepsilon \approx \pi/N$. Hence, if $p$ denotes the probability to have $m = 1$, the IDS exhibits the following exponentially small "Lifshitz tail":

$$1 - H(\omega^2) \equiv H_c(\omega^2) \sim p^{\pi/\varepsilon} \tag{1.3}$$

This argument has been refined, and made rigorous in various instances, both for continuum and lattice models in any dimension $d$. The usual statement of those results reads[2]

$$\lim_{\varepsilon \to 0} \ln \frac{\ln H_c}{|\ln \varepsilon|} = d \tag{1.4}$$

Unfortunately, this regorous equality, involving two logs, does not provide a very precise description of the actual behavior of $H_c(\omega^2)$.

We have studied in refs. 3–6 *binary* mass distributions, where $m_n = 1$ or $M > 1$ with probabilities $p$ and $1 - p$, respectively. Our main result reads

$$H_c(\omega^2) \approx p^{\pi/\varepsilon} Q(\pi/\varepsilon) \tag{1.5}$$

The amplitude $Q$ is a periodic function of its argument $\pi/\varepsilon$ with unit period and depends on the mass ratio $M$. In the $M \to \infty$ limit, considered by Domb *et al.*,[7] the periodic amplitude assumes a very simple form: $Q(x) = (1 - p)\, p^{\mathrm{Int}(x) - x}$, where $\mathrm{Int}(x)$ denotes the integer part of $x$. It was argued in ref. 5 that Eq. (1.5) gives the asymptotic behavior of the IDS for any distribution in which the lightest mass $m = 1$ occurs with a nonzero weight $p$. This statement has been confirmed in ref. 6, where we studied in detail a family of exactly soluble models[8] (diluted exponential distribution). In this case, we gave an analytical derivation of Eq. (1.5) and expressed the Fourier coefficients of $Q$ in terms of the solution of a differential equation.

The aim of the present paper is to obtain an accurate, even though not rigorously proven, estimation of the IDS in cases where the mass distribution starts in a continuous way at $m=1$, with no delta function. The possible occurrence of a logarithmic correction to Eq. (1.3) in such cases was considered by previous authors.[9,10] In particular, a rigorous lower bound to $H_c(\omega^2)$ involving a logarithmic factor is given in ref. 10.

We obtain, using more quantitative but less rigorous tools, this leading logarithmic correction to the Lifshitz tail as well as a systematic expansion beyond it. We put special emphasis on distributions starting as a power law

$$\rho(m) \sim A\alpha\delta^{\alpha-1} \qquad (\delta \to 0) \tag{1.6}$$

with the notation

$$m_n = 1 + \delta_n \tag{1.7}$$

Our final result is given in Eq. (3.44).

Let us first present a rough heuristic estimate of the Lifshitz tail associated with such a mass distribution. Since the lhs of Eq. (1.1) reads approximately $-(4+4\delta_n-\varepsilon^2)a_n$, the highest eigenmode of a succession of $N$ light masses will be little sensitive to the actual values of the $\delta_n$, and hence stay around $\varepsilon \sim \pi/N$, independently of the boundary conditions inherited from the rest of the chain, as long as $4\delta_n < \varepsilon^2$. Since such a collective event occurs with a probability of the order of $\varepsilon^{2\alpha N}$, we get the following very crude approximation:

$$H_c \sim \exp\left(-\frac{2\pi\alpha}{\varepsilon}|\ln\varepsilon|\right) \tag{1.8}$$

A more accurate derivation of this result, including all subleading powers of $|\ln\varepsilon|$, is given in Section 3.

The general setup of this paper is a follows. Section 2 is devoted to an analogue of the Lifshitz phenomenon in a simpler model, namely the distribution of the random variable $z = 1 + x_1 + x_1x_2 + x_1x_2x_3 + \cdots$. We show how the exponential tail of the distribution of $z$, obtained in an exact way for a particular example, can indeed be derived in the general case. In Section 3, we apply the same techniques (exact solution + general case) to the Schmidt function and to the IDS of random harmonic chains. Our analytical results are compared to numerical data. Section 4 contains a generalization of the results to other mass distributions (essential singularities), to other models (localization, trapping problem), and to higher dimensions.

## 2. A SIMPLE MODEL

### 2.1. Preliminaries

Before studying the Lifshitz tail of random harmonic chains, we consider a simpler disordered model which exhibits a very analogous behavior. Consider an infinite sequence of independent random variables $x_n$ with a common probability distribution $\rho(x)\,dx$, and define the variable

$$z=\sum_{n\geqslant 0}\prod_{i=1}^{n}x_i=1+x_1+x_1x_2+x_1x_2x_3+\cdots \tag{2.1}$$

This quantity has been met in probability theory[11] and in different examples of one-dimensional disordered physical systems, such as the Ising chain in a random field[12] or random walk in a random medium.[13-15]

Let $R(z)$ be the probability density of the random variable $z$. The large-$z$ behavior of $R(z)$ strongly depends on the distribution of the $x_n$.[16] To be more specific, let $b$ denote the upper bound of $\rho(x)$. If $b<1$, $z$ has a finite upper bound $B=(1-b)^{-1}$. If $b>1$, but $\int \ln x\rho(x)\,dx<0$, then $R(z)\sim z^{-(\alpha+1)}$, where the exponent $\alpha$ is given by $\int x^{\alpha}\rho(x)\,dx=1$.

The marginal case $b=1$ is reminiscent of the Lifshitz phenomenon. A large number $N$ of consecutive $x_n$ close to unity are indeed necessary to build up a value $z\approx N$. Hence, the situation is analogous to that of random harmonic chains, described in the introduction. In the $x_n$ take their largest value $b=1$ with a nonzero probability $p$, then $R(z)\sim p^z$. This exponential decay is very similar to the Lifshitz tail of the IDS (1.3), where $p$ is the probability of occurrence of the lightest mass. The rest of this section is devoted to the more subtle situation where $p$ vanishes, $\rho(x)$ ending up at $b=1$ with no delta function.

### 2.2. An Exactly Soluble Example

We have shown in ref. 16 that the probability density $R(z)$ can be obtained in an exact way for a particular class of power-law distributions $\rho(x)\,dx$. This family of exactly soluble cases contains one example of interest for the present purpose, namely

$$\rho(x)=\sigma x^{\sigma-1}\qquad(0\leqslant x\leqslant 1) \tag{2.2}$$

where $\sigma > 0$ is an arbitrary parameter. It has indeed been shown in ref. 16 that $R(z)$ obeys the following differential-difference equation:

$$(z-1)\,R'(z)+(1-\sigma)\,R(z)+\sigma R(z-1)=0 \tag{2.3}$$

This relation yields a closed-form expression for the Laplace transform $F(s)=\int e^{-sz}R(z)\,dz$ of the distribution of $z$,

$$F(s)=\exp[-s+\sigma G(s)], \qquad G(s)=\int_0^s \frac{e^{-t}-1}{t}\,dt \tag{2.4}$$

The density $R(z)$ is given by the inverse Laplace formula

$$R(z)=\int \frac{ds}{2\pi i}\exp[s(z-1)+\sigma G(s)] \tag{2.5}$$

and the large-$z$ behavior of this exact expression can be obtained by applying the steepest descent method to the integral. The saddle point (negative) value $s_c$ of $s$ is given by the transcendental equation

$$-s_c=\ln\left[(-s_c)\frac{z-1}{\sigma}+1\right] \tag{2.6}$$

and we get the following estimate:

$$R(z)\approx[2\pi G''(s_c)]^{-1/2}\exp[s_c(z-1)+G(s_c)] \tag{2.7}$$

We will discuss the large-$z$ behavior of this result in the next subsection, after having derived an asymptotic expression for $R(z)$ valid for any power-law distribution.

## 2.3. The General Case

Our aim is now to obtain an estimate of the large-$z$ behavior of the density $R(z)$ for an arbitrary distribution of the $x_n$ ending up as a power law at $b=1$. Let us define

$$x_n=1-\delta_n \tag{2.8}$$

and assume that the probability density of $\delta_n$ reads

$$\tilde{\rho}(\delta)\approx A\alpha\delta^{\alpha-1} \qquad (\delta\to 0) \tag{2.9}$$

so that the probability that $\delta_n$ is less than some $\delta$ reads

$$\tilde{h}(\delta)\approx A\delta^{\alpha} \qquad (\delta\to 0) \tag{2.10}$$

The density $R(z)$ of the variable $z$ defined in Eq. (2.1) is the limit of the densities of an infinite sequence of variables $z_n$, defined through the recursion

$$z_n = 1 + x_n z_{n-1} \tag{2.11}$$

where the $x_n$ have the common probability density $\rho(x)$. Hence, the distribution $R(z)\,dz$ is invariant under the transformation (2.11). This property is expressed by an integral equation[16]

$$R(z) = \int \frac{\rho(x)\,dx}{x} R\left(\frac{z-1}{x}\right) \tag{2.12}$$

of the type of those introduced by Dyson[17] and Schmidt.[18] We will therefore refer to Eq. (2.12) as the Dyson–Schmidt equation of the problem.

The large-$z$ behavior of $R(z)$ can be extracted from Eq. (2.12) as follows. Since $R(z)$ is rapidly decreasing, the integral is dominated by values of $x$ close to unity, i.e., small values of $\delta$. It is therefore legitimate to approximate Eq. (2.12) as

$$R(z+1) \approx \int \tilde{\rho}(\delta)\,d\delta\,R(z+z\delta) \tag{2.13}$$

We then set $R(z) = \exp[-\alpha\Phi(z)]$, expand the integrand as

$$R(z+z\delta) \approx \exp[-\alpha\Phi(z) - \alpha\Phi'(z)\,z\delta]$$

and perform the integral with the distribution (2.9). We end up with an implicit equation for $\Phi'(z)$

$$\Phi'(z) = \lambda - \mu + \ln\Phi'(z) \tag{2.14}$$

with the notation

$$\lambda = \ln z \tag{2.15}$$

$$\mu = (1/\alpha)\ln[A\Gamma(\alpha+1)] - \ln\alpha \tag{2.16}$$

Hence we have $\Phi'(z) \sim \ln z$, and $\Phi(z) \sim z\ln z$, up to subleading powers of $\ln z$. This suggests the change of variable

$$\Phi(z) = zg(\lambda) \tag{2.17}$$

Then Eq. (2.14) yields

$$g(\lambda) + g'(\lambda) = f(\lambda) = \lambda - \mu + \ln f(\lambda) \tag{2.18}$$

Let us show that Eq. (2.18) is equivalent to Eq. (2.7) in the case of exactly soluble distributions (2.2), up to terms of relative order $1/z$ in $\Phi(z)$, i.e., terms of order $e^{-\lambda}$ in $g(\lambda)$. Since the present case corresponds to $\alpha = 1$ and $\mu = \ln \sigma$, the second equality of (2.18) is equivalent to Eq. (2.6) with $-s_c = f(\lambda)$. We also have to identify $\sigma G(s) = -z[s_c + g(\lambda)]$. The first equality of Eq. (2.18) is then a consequence of the stationarity condition $z = -\sigma G'(s_c)$ for the integrand in Eq. (2.5) at the saddle point. Of course, Eq. (2.5) contains the whole analytic structure of $R(z)$, whereas Eq. (2.18) only yields its asymptotic form for large $z$. In particular, since Eq. (2.18) is the result of a *local* analysis of the Dyson–Schmidt equation (2.12), it cannot predict the absolute normalization of the Lifshitz tail of $R(z)$, which depends on the mass distribution in a *global* way.

Equation (2.18) yields an asymptotic expansion of $\Phi(z)$ to all orders in $\lambda$. Indeed, since the relevant values of $\delta$ in the integral (2.13) are of order $(z \ln z)^{-1}$, our approach is correct up to terms of order $e^{-\lambda}$, which is also the order of the unknown integration constant in Eq. (2.18). We first expand $f(\lambda)$ for $\lambda \to +\infty$ as

$$f(\lambda) = \lambda + K + \frac{K}{\lambda} + \frac{1}{\lambda^2}\left(-\frac{1}{2}K^2 + K\right) + \frac{1}{\lambda^3}\left(\frac{1}{3}K^3 - \frac{3}{2}K^2 + K\right) + \frac{1}{\lambda^4}\left(-\frac{1}{4}K^4 + \frac{11}{6}K^3 - 3K^2 + K\right) + \cdots \tag{2.19}$$

with the notation

$$K = \ln \lambda - \mu \tag{2.20}$$

where $\lambda$ and $\mu$ have been defined in Eqs. (2.15)–(2.16). We then integrate this expansion term by term, according to Eq. (2.18), and we end up with

$$R(z) \approx \exp\left\{-\alpha z\left[\lambda + P_0(K) + \sum_{j \geq 1} \frac{P_j(K)}{\lambda^j}\right]\right\} \tag{2.21}$$

with

$$\begin{aligned}
P_0(K) &= P_1(K) = K - 1\\
P_2(K) &= -\tfrac{1}{2}K^2 + 2K - 2\\
P_3(K) &= \tfrac{1}{3}K^3 - \tfrac{5}{2}K^2 + 6K - 6\\
P_4(K) &= -\tfrac{1}{4}K^4 + \tfrac{17}{6}K^3 - \tfrac{23}{2}K^2 + 24K - 24\\
&\vdots
\end{aligned}$$

It can now be checked that the approximations that were needed to derive Eq. (2.14) from Eq. (2.12) are indeed correct in the $z \to \infty$ limit.

## 3. RANDOM HARMONIC CHAINS

### 3.1. Preliminaries

In this subsection, we recall briefly some useful definitions used in the study of the spectra of random harmonic chains. We introduce the ratio (Ricatti variable)

$$u_n = a_n/a_{n+1} \tag{3.1}$$

in terms of which the equation of motion (1.1) reads

$$u_n = (2 - m_n\omega^2 - u_{n-1})^{-1} \tag{3.2}$$

where the masses $m_n$ have the common probability density $\rho(m)$. The distribution of the random variables $u_n$ approaches, as $n \to \infty$, an invariant distribution $R(u)\,du$. The Dyson–Schmidt integral equation[17,18] expressing this invariance reads

$$R(u) = \frac{1}{u^2}\int \rho(m)\,dm\,R(2 - m\omega^2 - u^{-1}) \tag{3.3}$$

The IDS $H(\omega^2)$ is equal to the probability that $u$ is negative,

$$H(\omega^2) = \int_{-\infty}^{0} R(u)\,du; \qquad H_c(\omega^2) = \int_0^{+\infty} R(u)\,du \tag{3.4}$$

as a consequence of a well-known theorem by Sturm.

### 3.2. An Exactly Soluble Example

Just as we did in Section 2, we first present the exact evaluation of $H(\omega^2)$ for a particular mass distribution before studying the general case. Among those distributions already mentioned in the introduction, those of interest for the present purpose read

$$\tilde{\rho}(\delta) = (1/M)e^{-\delta/M} \tag{3.5}$$

with the notation (1.7): $m_n = 1 + \delta_n$. The associated IDS is given by[8]

$$H_c = (1/\pi)\{\varepsilon - \mathrm{Im}[\eta(1 - C_1)]\} \tag{3.6}$$

where $\varepsilon$ is as in Eq. (1.2), $\eta = iM\,\mathrm{cotan}(\varepsilon/2)$, and the complex sequence $C_k$ obeys the recursion relation

$$C_{k+1} + C_{k-1} - 2C_k = U_k C_k \tag{3.7}$$

with

$$U_k = \frac{1 - e^{2ik\varepsilon}}{k\eta} \tag{3.8}$$

together with the boundary conditions $C_0 = 1$; $\lim_{k \to \infty} C_k = 0$. The rather lengthly derivation of these results will not be repeated here. We just mention that the $C_k$ are related in a simple recursive way to the moments $\mu_k$ of the above-defined invariant measure $R(u)\,du$, and that Eq. (3.6) is a mere transcription of Eq. (3.4) in the language of the $C_k$.

In order to extract the Lifshitz tail of $H_c$ at $\varepsilon \to 0$ from the exact expression (3.7), we perform the same manipulations as we did in ref. 6 for the case where $\delta = 0$ occurs with a nonzero probability $p$. We end up with

$$\frac{dH}{d\omega^2} \approx \int \frac{w(x)\,dx}{4i\pi\varepsilon^2}\, e^{\pi x/\varepsilon} f(x)^2 \tag{3.9}$$

where $w(x) = (1 - e^{-x})/x + e^{-x}$. The idea beyond the derivation of Eq. (3.9) is the assumption that the sequence $C_k$ admits an analytic scaled limit $f(x)$ as $\varepsilon \to 0$ and $k \to +\infty$ simultaneously, the complex quantity $x = -2ik\varepsilon$ being kept fixed. Then $f(x)$ obeys the following difference equation:

$$\Delta_\varepsilon f(x) = f(x + 2i\varepsilon) + f(x - 2i\varepsilon) - 2f(x) = -4\varepsilon^2 V(x)\, f(x) \tag{3.10}$$

with

$$V(x) = \frac{1 - e^{-x}}{4Mx}$$

which is just the scaled limit of Eq. (3.7). As long as the complex variable $x$ remains bounded, Eq. (3.10) becomes the differential equation $f''(x) = V(x)\, f(x)$ in the $\varepsilon \to 0$ limit. This procedure was indeed used in ref. 6, where we only needed the values of $f(x)$ for $\operatorname{Re} x = \ln p$ (finite). It turns out that $f(x)$ is needed for $\operatorname{Re} x \to -\infty$ in the present situation, and that the $\varepsilon \to 0$ limit of Eq. (3.10) is less trivial, since the potential $V(x)$ becomes large. The rapid increase of $V(x)$ can be taken into account as follows. If we assume that there exists a "renormalized potential" $V_R(x)$ such that

$$f''(x) = V_R(x)\, f(x) \tag{3.11}$$

then we have $f^{(2n)}(x) \approx V_R(x)^n f(x)$ for $\operatorname{Re} x \to \infty$, and the action of the difference operator $\Delta_\varepsilon$ can be resummed as

$$\begin{aligned}\Delta_\varepsilon f(x) &= 2 \sum_{n \geqslant 1} \frac{(2i\varepsilon)^{2n}}{(2n)!} f^{(2n)}(x) \\ &\approx 2\left[\sum_{n \geqslant 1} \frac{(2i\varepsilon)^{2n}}{(2n)!} V_R(x)^n\right] f(x) \\ &\approx 2\{\cos[2\varepsilon V_R(x)^{1/2}] - 1\} f(x)\end{aligned} \tag{3.12}$$

A comparison with Eq. (3.10) then gives the relationship between both potentials

$$q(x) = \varepsilon V_R(x)^{1/2} = \sin^{-1}[\varepsilon V(x)^{1/2}] \tag{3.13}$$

The last steps of the analysis are now simple, since both the WKB method for Eq. (3.11) and the steepest descent method for the integral (3.9) become exact in the $\varepsilon \to 0$ limit. The WKB expression for $f(x)$ reads

$$f(x) \approx \exp\left[-\frac{1}{\varepsilon}\int_0^x q(y)\, dy\right] \tag{3.14}$$

The saddle point of the integrand $e^{\pi x/\varepsilon} f(x)^2$ then corresponds to $q = \pi/2$, i.e., $x = x_c$, where $x_c$ is the solution of

$$V(x_c) = \frac{1 - e^{-x_c}}{4Mx_c} = \frac{1}{\varepsilon^2} \tag{3.15}$$

and we end up with the estimate

$$\frac{dH}{d\omega^2} \approx H_c \approx \exp\left\{\frac{1}{\varepsilon}\left[\pi x_c - 2\int_0^{x_c} q(y)\, dy\right]\right\} \tag{3.16}$$

As we did in Section 2, we postpone the discussion of the small-$\varepsilon$ behavior of this expression to the next subsection.

### 3.3. The Schmidt Function at the Band Edge

The subsection is devoted to the asymptotic behavior, for $\varepsilon = 0$, of the invariant probability density $R(u)$ defined in Section 3.1. The integrated density $Z(u) = \int_{-\infty}^{u} R(u')\, du'$ is often referred to as the Schmidt function of the problem. We consider mass distributions starting with an arbitrary power law (1.6)

$$\tilde{\rho}(\delta) \sim A\alpha\delta^{\alpha-1} \tag{3.17}$$

with the notation (1.7): $m = 1 + \delta$. The support of $R(u)$ is then $-1 \leqslant u \leqslant 0$. We perform the change of variable

$$u_n = -1 + 1/v_n \tag{3.18}$$

and we introduce the invariant density $S(v)$ such that $R(u)\,du = S(v)\,dv$. Equation (3.2), for $\varepsilon = 0$, i.e., $\omega^2 = 4$, now reads

$$v_n = \frac{(1 + 4\delta_n)v_{n-1} + 1}{1 + 4\delta_n v_{n-1}} \tag{3.19}$$

and the Dyson–Schmidt equation (3.3) becomes

$$S(v) = \int \frac{\tilde{\rho}(\delta)\,d\delta}{[1 - 4\delta(v-1)]^2}\,S\left[\frac{v-1}{1 - 4\delta(v-1)}\right] \tag{3.20}$$

The large-$v$ behavior of $S(v)$ can be estimated as follows. Since this function is expected to decrease very rapidly, we approximate Eq. (3.20) for small $\delta$ as

$$S(v+1) \approx \int \tilde{\rho}(\delta)\,d\delta\,S(v + 4v^2\delta) \tag{3.21}$$

This equation is very similar to Eq. (2.13), and so is the way to solve it. We define

$$S(v) = \exp[-\alpha v g(\lambda)] \tag{3.22}$$

with

$$\lambda = \ln v \tag{3.23}$$

and we obtain

$$g(\lambda) + g'(\lambda) = f(\lambda) = 2\lambda - \mu + \ln f(\lambda) \tag{3.24}$$

with the notation

$$\mu = (1/\alpha)\ln[A\Gamma(\alpha+1)] - \ln(4\alpha) \tag{3.25}$$

The following expansion of $S(v)$ for large $v$ then follows, along the very same lines as in Section 2.3:

$$S(v) = \exp\left\{-\alpha v\left[2\lambda + Q_0(K) + \sum_{j \geqslant 1} \frac{Q_j(K)}{(2\lambda)^j}\right]\right\} \tag{3.26}$$

with

$$Q_0(K) = Q_1(K) = K - 2$$
$$Q_2(K) = -\tfrac{1}{2}K^2 + 3K - 6$$
$$Q_3(K) = \tfrac{1}{3}K^3 - \tfrac{7}{2}K^2 + 15K - 30$$
$$Q_4(K) = -\tfrac{1}{4}K^4 + \tfrac{23}{6}K^3 - 26K^2 + 105K - 210$$

and with the notation

$$K = \ln(2\lambda) - \mu \tag{3.27}$$

where $\lambda$ and $\mu$ are as in Eqs. (3.23)–(3.25).

### 3.4. The Schmidt Function Close to the Band Edge

We now generalize the results of the previous subsection to the vicinity of the band edge, i.e., to small, nonzero values of $\varepsilon$. The support of the invariant distribution $R(u)\,du$ is then the whole real line, and it is advantageous to map the $u$ axis onto the unit circle through[5]

$$u = \frac{z-1}{e^{i\varepsilon} - ze^{-i\varepsilon}} \tag{3.28}$$

and to parametrize the circle by

$$z = e^{-2i\varphi} \qquad (0 \leqslant \varphi \leqslant \pi) \tag{3.29}$$

In terms of this angle, the transformation (3.2) becomes, up to first order in $\delta_n$,

$$\varphi_n = \varphi_{n-1} + \varepsilon - \frac{4\delta_n}{\varepsilon}\sin^2(\varphi_{n-1} + \varepsilon) \tag{3.30}$$

Let $T_\varepsilon(\varphi)$ denote the invariant density such that $R(u)\,du = T_\varepsilon(\varphi)\,d\varphi$. It follows from Eq. (3.4) and from the definition of $\varphi$ that the IDS is given by

$$H(\omega^2) = \int_0^{\pi-\varepsilon} T_\varepsilon(\varphi)\,d\varphi; \qquad H_c(\omega^2) = \int_{\pi-\varepsilon}^{\pi} T_\varepsilon(\varphi)\,d\varphi \tag{3.31}$$

Notice that the Lifshitz mechanism now appears very clearly: a large number $N \approx \pi/\varepsilon$ of light atoms, with $\delta_n < \varepsilon^2$, is needed for $\varphi$ to be close to $\pi$, and hence to get a contribution to $H_c$.

In order to determine the small-$\varepsilon$ behavior of $T_\varepsilon(\varphi)$, let us rewrite Eq. (3.3) in terms of the angle $\varphi$, and for small $\delta$, as

$$T_\varepsilon(\varphi+\varepsilon) \approx \int \tilde{\rho}(\delta)\, d\delta\, T_\varepsilon\left(\varphi + \frac{4\delta}{\varepsilon}\sin^2\varphi\right) \tag{3.32}$$

This equation is analogous to Eqs. (2.13) and (3.21), and the way to solve it will also be very similar to what we did previously.

We still consider the power-law mass distributions (1.6). We set $T_\varepsilon(\varphi) = \exp[-\Phi(\varphi)]$, linearize the integrand in Eq. (3.32), and perform the integration. We obtain

$$\varepsilon\Phi'(\varphi) = \alpha \ln[(4/\varepsilon)\sin^2\varphi\, \Phi'(\varphi)] - \ln[A\Gamma(\alpha+1)] \tag{3.33}$$

The change of function $\Phi(\varphi) = (\alpha/\varepsilon)\, X(\varphi)$ then yields

$$X'(\varphi) - \ln X'(\varphi) = 2\Lambda - \mu + 2\ln\sin\varphi \tag{3.34}$$

where $\mu$ is as in Eq. (3.25), and with

$$\Lambda = |\ln\varepsilon| \tag{3.35}$$

In analogy with Eqs. (2.18) and (3.24), Eq. (3.34) yields an asymptotic expansion of $\ln T_\varepsilon(\varphi)$ for fixed $\varphi$ in the $\varepsilon \to 0$ limit. We first derive the expansion

$$X'(\varphi) = 2\Lambda + J + \frac{J}{2\Lambda} + \frac{1}{8\Lambda^2}(-J^2+2J) + \frac{1}{48\Lambda^3}(2J^3 - 9J^2 + 6J)$$
$$+ \frac{1}{192\Lambda^4}(-3J^4 + 22J^3 - 36J^2 + 12J) + \cdots \tag{3.36}$$

with

$$J = K + 2\ln\sin\varphi, \qquad K = \ln(2\Lambda) - \mu \tag{3.37}$$

A term-by-term integration then yields

$$T_\varepsilon(\varphi) \approx \exp\left\{-\frac{\alpha\varphi}{\varepsilon}\left[2\Lambda + R_0(\varphi) + \sum_{j\geq 1}\frac{R_j(\varphi)}{(2\Lambda)^j}\right]\right\} \tag{3.38}$$

with

$$R_0(\varphi) = R_1(\varphi) = L_1 + K$$

$$R_2(\varphi) = \tfrac{1}{2}[-L_2 + 2(1-K)L_1 + 2K - K^2]$$

$$R_3(\varphi) = \tfrac{1}{6}[2L_3 + 3(2K-3)L_2 + 6(K^2 - 3K + 1)L_1 + 2K^3 - 9K^2 + 6K]$$

$$R_4(\varphi) = \tfrac{1}{12}[-3L_4 + 2(-6K+11)L_3 + 6(-3K^2 + 11K - 6)L_2$$
$$+ 6(-2K^3 + 11K^2 - 12K + 2)L_1 - 3K^4 + 22K^3 - 36K^2 + 12K]$$

where the functions $L_j(\varphi)$ are defined through

$$L_j(\varphi)=\frac{1}{\varphi}\int_0^{\varphi} dt\,(2\ln\sin t)^j \tag{3.39}$$

## 3.5. The Integrated Density of States

We are now able to obtain an asymptotic expansion for the logarithm of the IDS associated with any mass distribution starting with a power law (1.6). In virtue of Eq. (3.31), we have

$$H_c\approx T_\varepsilon(\pi) \tag{3.40}$$

and we can therefore use the result (3.38). We still have to evaluate the integrals $I_j=L_j(\pi)$. This is readily done by noticing that

$$I_j=\left(\frac{d}{dx}\right)^j_{x=0}\frac{1}{\pi}\int_0^{\pi} dt\,(\sin t)^{2x}=\left(\frac{d}{dx}\right)^j_{x=0}\frac{\Gamma(x+1/2)}{\pi^{1/2}\Gamma(x+1)} \tag{3.41}$$

This equation relates in a recursive way the $I_j$ to the differences

$$\begin{aligned}\Delta_j&=\psi^{(j-1)}(\tfrac{1}{2})-\psi^{(j-1)}(1)\\&=\begin{cases}(-1)^j(2^j-2)(j-1)!\,\zeta(j), & j\geqslant 2\\ -2\ln 2, & j=1\end{cases}\end{aligned} \tag{3.42}$$

We thus obtain

$$\begin{aligned}I_1&=\Delta_1=-2\ln 2\\ I_2&=\Delta_1^2+\Delta_2=4\ln^2 2+\pi^2/3\\ I_3&=\Delta_1^3+3\Delta_1\Delta_2+\Delta_3=-8\ln^3 2-2\pi^2\ln 2-12\zeta(3)\\ I_4&=\Delta_1^4+4\Delta_1\Delta_3+3\Delta_2^2+6\Delta_1^2\Delta_2+\Delta_4\\ &=16\ln^4 2+8\pi^2\ln^2 2+96\ln 2\,\zeta(3)+19\pi^4/15\end{aligned} \tag{3.43}$$

and out final result reads

$$H_c=\exp\left\{-\frac{2\pi\alpha}{\varepsilon}\left[\Lambda+S_0(v)+\sum_{j\geqslant 1}\frac{S_j(v)}{(2\Lambda)^j}\right]\right\} \tag{3.44}$$

with

$$\begin{aligned}S_0(v)&=S_1(v)=v/2\\ S_2(v)&=(1/4)(-v^2+2v-\pi^2/3)\\ S_3(v)&=(1/12)[2v^3-9v^2+2(\pi^2+3)v-3\pi^2-24\zeta(3)]\\ S_4(v)&=(1/24)\{-3v^4+22v^3-6(\pi^2+6)v^2\\ &\quad+[22\pi^2+144\zeta(3)+12]v-12\pi^2-264\zeta(3)-(19/5)\pi^4\}\end{aligned}$$

with the notation

$$\nu = K - 2\ln 2 = \ln(\Lambda/2) - \mu \tag{3.45}$$

where $\Lambda$, $\mu$, and $K$ are defined in Eqs. (3.35), (3.25), and (3.37), respectively.

Let us now prove that the present approach is equivalent to the exact solution discussed in the previous subsection. To do so, we define, for $0 \leqslant q \leqslant \pi/2$, the function $x(q)$ as being the reciprocal of $q(x)$, introduced in Eq. (3.13), and the function

$$F(q) = qx(q) - \int_0^{x(q)} q(y)\,dy \tag{3.46}$$

A comparison with Eq. (3.16) shows that the result of the exact solution reads $H_c \approx \exp[(2/\varepsilon)\,F(\pi/2)]$, since $x(0) \to 0$ with $\varepsilon$, and $x(\pi/2) = x_c$. On the other hand, $F(q)$ clearly satisfies $dF/dq = x(q)$, and $x(q)$ is such that

$$V[x(q)] = \frac{1 - e^{-x(q)}}{4Mx(q)} = \frac{\sin^2 q}{\varepsilon^2} \tag{3.47}$$

This last equation is equivalent to Eq. (3.34), up to exponentially small terms in $x(q)$, with the identification $-x(q) = X'(\varphi)$, and $\mu = -\ln(4M)$. We have therefore $F(q) = -X(\varphi)_{\varphi = q}$ for $0 \leqslant q \leqslant \pi/2$. Since $X(\pi) = 2X(\pi/2)$, both methods are equivalent, up to all orders in a $1/\lambda$ expansion.

The method that has led us to the expansion (3.44) of the IDS also provides a useful tool to get a good numerical estimate of $H_c$ for reasonable values of $\varepsilon$. Let us go back to Eq. (3.34). For a small but finite $\varepsilon$, this equation only admits a solution when its rhs is larger than unity, i.e., for $\varphi_0 \leqslant \varphi \leqslant \pi - \varphi_0$, with $\sin\varphi_0 = e^{(\mu+1)/2}\varepsilon$. Since the excluded regions $0 \leqslant \varphi \leqslant \varphi_0$ and $\pi - \varphi_0 \leqslant \varphi \leqslant \pi$ have a length of order $\varepsilon$, the integral

$$H_c^{(I)} = \exp\left[-\frac{\alpha}{\varepsilon}\int_{\varphi_0}^{\pi - \varphi_0} X'(\varphi)\,d\varphi\right] \tag{3.48}$$

provides a faithful resummation of the asymptotic, but surely divergent, expansion (3.44).

We have performed some numerical tests of the efficiency of the integral resummation (3.48). We have obtained numerical values of the IDS of random chains by two means. The first method concerns the exactly soluble (exponential) mass distributions (3.5). It consists in solving the difference equation (3.7) through a complex continued fraction, and in extracting $H_c$ from Eq. (3.6). The second method consists in solving iteratively Eq. (3.2) for a very large sample of $N = 10^6$ atoms. The IDS is then given as being the fraction of negative ratios $u_n$. This technique has the advantage of being efficient for any mass distribution, but the drawback of the limitation $H_c > 1/N$. We have used it for pure power-law distributions

$$\tilde{\rho}(\delta) = A\alpha\delta^{\alpha-1} \qquad (0 \leqslant \delta \leqslant A^{-1/\alpha}) \tag{3.49}$$

Figures 1–4 present comparisons of numerical data obtained by both methods mentioned above with the estimate (3.48). The agreement is always satisfactory; remember that our analytical approach cannot predict the overall scale of Lifshitz tails, which corresponds to a vertical shift on these logarithmic plots.

## 4. GENERALIZATION AND DISCUSSION

We presented in Section 3 an analytical method that provides both a full asymptotic expansion (3.44) and a useful closed-form integral resummation (3.48) of the Lifshitz tail of the IDS of random harmonic chains with any mass distribution starting as a power law (1.6).

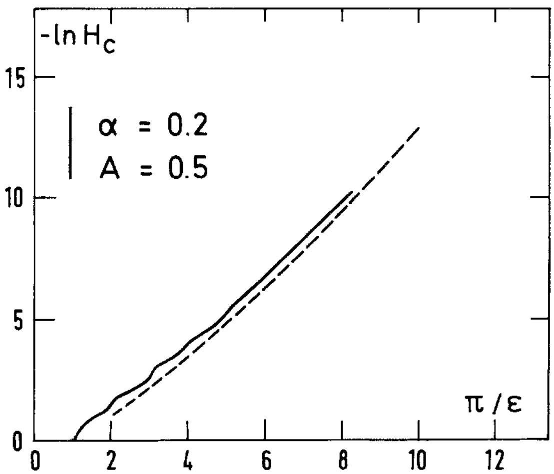


Fig. 1. Logarithmic plot of $H_c(\omega^2) = 1 - H(\omega^2)$ versus $\pi/\varepsilon$ for the pure power-law mass distribution (3.49) with $\alpha = 0.2$ and $A = 0.5$. (——) Numerical data obtained, as explained in the text, by iterating Eq. (3.2). (– –) Integral expression (3.48), resumming the asymptotic expansion (3.44). Note the damped oscillations at small integer values of $\pi/\varepsilon$, reminiscent of the periodic amplitude $Q$ of Eq. (1.3).

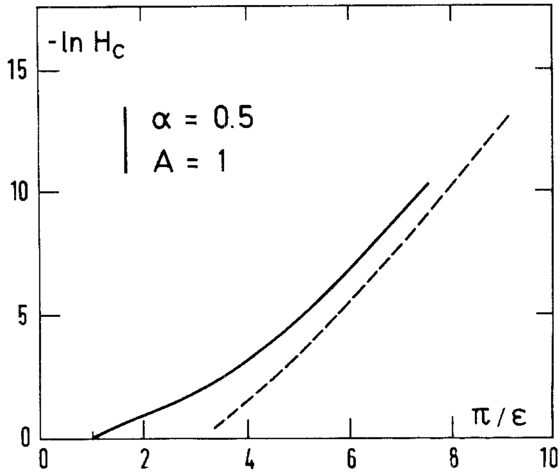


Fig. 2. Same as Fig. 1, with $\alpha = 0.5$ and $A = 1$.

The method can be extended to other mass distributions. We illustrate its generality by considering distributions that have themselves an exponential singularity at their lower bound $m = 1$,

$$\tilde{\rho}(\delta) \sim \exp(-B\delta^{-\beta}) \qquad (\delta \to 0) \tag{4.1}$$

We go back to Eq. (3.32), set $T_\varepsilon(\varphi) = \exp[-\Phi(\varphi)]$, and again linearize the integrand, to obtain

$$\Phi(\varphi) - \Phi(\varphi + \varepsilon) \approx \ln \int d\delta \exp\left[-B\delta^{-\beta} - \frac{4\delta}{\varepsilon} \sin^2 \varphi \; \Phi'(\varphi)\right] \tag{4.2}$$

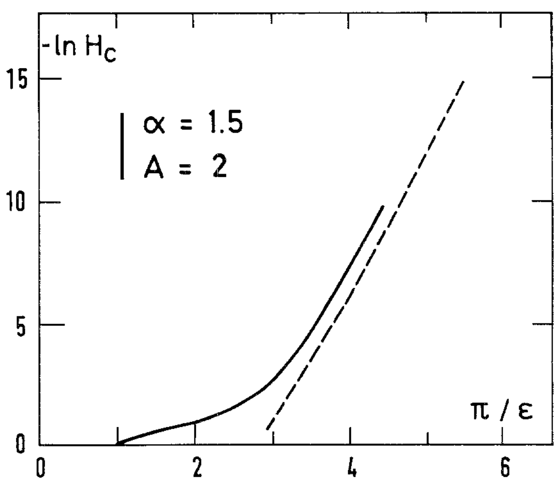


Fig. 3. Same as Fig. 1, with $\alpha = 1.5$ and $A = 2$.

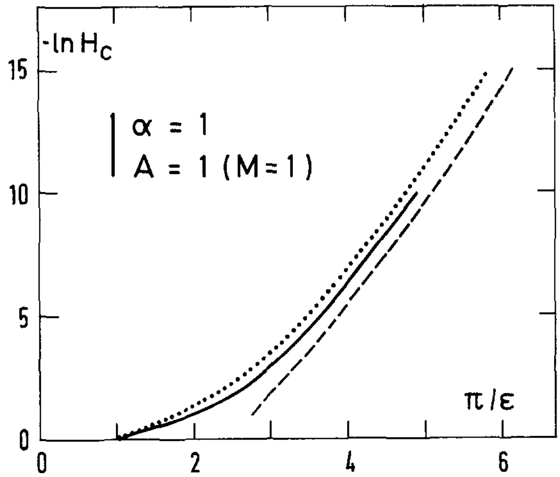


Fig. 4. Same as Fig. 1, with $\alpha = 1$ and $A = 1$. (·····) The IDS of the exactly soluble exponential distribution with $M = A^{-1} = 1$, obtained according to Eqs. (3.6)–(3.7).

In the $\varepsilon \to 0$ limit, the integral can be estimated through the steepest descent method. By approximating the difference in the lhs by a derivative, we obtain

$$\Phi'(\varphi) = C\varepsilon^{-(2\beta+1)}(\sin\varphi)^{2\beta}, \qquad \text{with} \quad C = B\beta 4^{\beta}(1+\beta^{-1})^{\beta+1} \tag{4.3}$$

and an integration leads to

$$T_\varepsilon(\varphi) \approx \exp\left[-C\varepsilon^{-(2\beta+1)}\int_0^{\varphi}(\sin t)^{2\beta}\,dt\right] \tag{4.4}$$

Hence, the terms that have been neglected in replacing the lhs of Eq. (4.2) by a derivative would give a contribution of relative order $\varepsilon$ in the square brackets. Even with the very singular distribution (4.1), the approximations needed by the present approach are legitimate. For $\varphi = \pi$, the integral in Eq. (4.4) is elementary, and we obtain, in virtue of Eq. (3.31),

$$H_c \approx \exp\left[-C\frac{\pi^{1/2}\Gamma(\beta+1/2)}{\Gamma(\beta+1)}\varepsilon^{-(2\beta+1)}\right] \tag{4.5}$$

This result is especially interesting, since it does not obey Eq. (1.4); exceptional distributions such as (4.1) were indeed excluded in ref. 2.

The results of the present paper can be adapted, *mutatis mutandis*, to other linear problems in disordered systems. Let us first mention the tight-binding Schrödinger equation in a random site potential

$$-\psi_{n+1}-\psi_{n-1}+V_n\psi_n=E\psi_n \tag{4.6}$$

If the distribution $\rho(V)\,dV$ of the potentials $V_n$ has a bounded support $a\leqslant V\leqslant b$, then the results of Section 3 hold for the Lifshitz tails of the IDS of the problem (4.6) at the top (resp. the bottom) of its spectrum. More precisely, when $E\to(b+2)^-$ [resp. $E\to(a-2)^+$], the parameters have to be identified as $\varepsilon^2=b+2-E$ and $4\delta_n=b-V_n$ (resp. $\varepsilon^2=E-a+2$ and $4\delta_n=V_n-a$). In a recent work on this problem,[19] the authors give Eq. (1.8) *without* the value $2\pi\alpha$ of the prefactor, and present numerical results for a uniform potential distribution. They extract a value $s\approx3.7$ for half the $\alpha=1$ prefactor of (1.8), while the correct result is $\pi+O(\ln|\ln\varepsilon|/|\ln\varepsilon|)$. Notice that the integral (3.48) reproduces their data with remarkable accuracy. Such logarithmic corrections are indeed a genuine obstacle to extracting the correct prefactor of Eq. (1.8) from numerical data for accessible values of $\varepsilon$.

Let us now discuss the implications of the present results for trapping problems. The motion of particles on a one-dimensional lattice with random traps is usually modeled by a master equation of the form (see, e.g., refs. 20 and 21)

$$dP_n/dt=P_{n+1}+P_{n-1}-2P_n-\omega_nP_n=-\lambda P_n \tag{4.7}$$

$P_n(t)$ denotes the probability for a particle to be at the $n$th site at time $t$, and the positive trap depths $\omega_n$ have a common distribution $\rho(\omega)\,d\omega$. The IDS $H(\lambda)$ of Eq. (4.7) also has a Lifshitz tail at $\lambda\to0^+$, which is described by the above results after identification $\varepsilon^2=\lambda$, $4\delta_n=\omega_n$. The quantities of interest are the probability $R(t)$ for a particle to return to its starting point, given by

$$R(t)=\int_0^\infty e^{-\lambda t}\,dH(\lambda) \tag{4.8}$$

and the survival probability $S(t)$, given by

$$S(t)=\int_0^\infty e^{-\lambda t}\,dH(q=0;\lambda) \tag{4.9}$$

where $H(q;\lambda)$ is the IDS at a fixed wavevector (momentum) $q$. As far as exponential factors are concerned, both IDS have the same Lifshitz singularity.

The case where the sites have $\omega=0$ (i.e., absence of a trap) with a finite probability $p$ is well understood.[20-22] It exhibits a stretched exponential behavior

$$R(t)\sim S(t)\sim \exp\{-\tfrac{3}{2}[2(\pi \ln p)^2 t]^{1/3}\} \tag{4.10}$$

For trap depth distribution starting as a power law, $\rho(\omega)\sim\omega^{\alpha-1}$, the results of Section 3 imply

$$R(t)\sim S(t)\sim \exp\left\{-3\left[\pi^2\alpha^2 t\left(\ln\frac{t}{\tau}\right)^2\right]^{1/3}\right\} \tag{4.11}$$

The "stretching" exponent 1/3 is affected by a universal $(\ln t)^{2/3}$ correction, independently of $\alpha$. The scale $\tau$ itself contains a logarithmic $t$ dependence. For distributions starting with an exponential singularity of the type (4.1), our result (4.5) implies

$$R(t)\sim S(t)\sim \exp(-Kt^{(2\beta+1)/(2\beta+3)}) \tag{4.12}$$

We finally want to mention the plausible form of the extension of the above results to an arbitrary dimension $d$. Since the heuristic argument that led to Eq. (1.8) has been confirmed by the more careful analysis of Section 3 in one dimension, its validity can indeed be expected to be quite general. Hence the following considerations are meant as reasonable, although not rigorous, conjectures.

For harmonic spectra of random alloys, where light atoms ($m=1$) occur with a probability $p$, the Lifshitz tail is known to have the form[2,20,21]

$$H_c\sim \exp(-\gamma_d|\ln p|\,\varepsilon^{-d}) \tag{4.13}$$

with $\varepsilon^2\approx\omega_{\max}^2-\omega^2$ and $\gamma_d=\Omega_d\lambda_d^{d/2}$, where $\Omega_d$ and $\lambda_d$ denote the volume of the unit sphere and the lowest eigenvalue of Laplace–Dirichlet operator in it, respectively. For mass distributions starting with a power law (1.6), in analogy with the one-dimensional case, the probability $p$ is replaced by the appropriate power of $\varepsilon$,

$$H_c\sim \exp(-2\alpha\gamma_d\varepsilon^{-d}\,|\ln \varepsilon|) \tag{4.14}$$

For mass distributions with an essential singularity of the type (4.1) we predict

$$H_c\sim \exp(-kB\varepsilon^{-(d+2\beta)}) \tag{4.15}$$

The translation of these results into the language of trapping problems in any dimension $d$ is

$$(4.13) \Rightarrow R(t) \sim S(t) \sim \exp[-C_1 \, |\ln p|^{2/(d+2)} \, t^{d/(d+2)}] \qquad (4.16)$$

$$(4.14) \Rightarrow R(t) \sim S(t) \sim \exp\left[-C_2 \left(\ln \frac{t}{\tau}\right)^{2/(d+2)} t^{d/(d+2)}\right] \qquad (4.17)$$

$$(4.15) \Rightarrow R(t) \sim S(t) \sim \exp[-C_3 \, t^{(d+2\beta)/(d+2\beta+2)}] \qquad (4.18)$$

Equations (4.15) and (4.18) show that, for exceptional distributions starting with an exponential singularity, the Lifshitz tail is governed by a nonuniversal effective dimensionality

$$d' = d + 2\beta \qquad (4.19)$$

which is always larger than the Euclidean dimension $d$. An analogous modification of the Lifshitz exponent has been recently described[9] for the Schrödinger equation in a potential with a periodic component and a *long-ranged* random component. Trapping problems on fractal structures[23] present a similar effect: the role of $d'$ is then played by the spectral dimension $d_s$, which is usually smaller than $d$.

## ACKNOWLEDGMENT

One of us (Th. M. N.) wishes to thank the members of the SPhT of the CEN Saclay, where part of this work was done, for their hospitality.

## REFERENCES

1. I. M. Lifshitz, *Adv. Phys.* **13**:483 (1964).
2. B. Simon, *J. Stat. Phys.* **38**:65 (1985).
3. Th. M. Nieuwenhuizen and J. M. Luck, *J. Stat. Phys.* **41**:745 (1985).
4. Th. M. Nieuwenhuizen, J. M. Luck, J. Canisius, J. L. van Hemmen, and W. J. Ventevogel, *J. Stat. Phys.* **45**:395 (1986).
5. Th. M. Nieuwenhuizen and J. M. Luck, *J. Stat. Phys.* **48**:393 (1987).
6. Th. M. Nieuwenhuizen and J. M. Luck, *Physica* **145A**:161 (1987).
7. C. Domb, A. A. Maradudin, E. W. Montroll, and G. H. Weiss, *Phys. Rev.* **115**:24 (1959).
8. Th. M. Nieuwenhuizen, *Phys. Lett.* **103A**:333 (1984); *Physica* **125A**:197 (1984).
9. W. Kirsch and B. Simon, *J. Stat. Phys.* **42**:799 (1986).
10. G. A. Mezincescu, *Commun. Math. Phys.* **103**:167 (1987).
11. H. Kesten, *Acta Math.* **131**:208 (1973); H. Kesten, M. V. Kozlov, and F. Spitzer, *Compositio Math.* **30**:145 (1975); W. Vervaat, *Adv. Appl. Prob.* **11**:750 (1979).
12. B. Derrida and H. J. Hilhorst, *J. Phys. A* **16**:2641 (1983).
13. B. Derrida and Y. Pomeau, *Phys. Rev. Lett.* **48**:627 (1982).
14. J. Bernasconi and W. R. Schneider, *J. Phys. A* **15**:L729 (1983).

15. Ya. G. Sinai, in *Lecture Notes in Physics*, Vol. 153 (Springer, Berlin, 1982), p. 12.
16. C. de Calan, J. M. Luck, Th. M. Nieuwenhuizen, and D. Petritis, *J. Phys. A* **18**:501 (1985).
17. F. J. Dyson, *Phys. Rev.* **92**:1331 (1953).
18. H. Schmidt, *Phys. Rev.* **105**:425 (1957).
19. A. Politi and T. Schneider, *Europhys. Lett.* **5**:715 (1988).
20. P. Grassberger and I. Procaccia, *J. Chem. Phys.* **77**:6281 (1982).
21. J. W. Haus and K. W. Kehr, *Phys. Rep.* **150**:263 (1987).
22. M. D. Donsker and S. Varadhan, *Commun. Pure Appl. Math.* **32**:721 (1979).
23. J. Klafter, G. Zumofen, and A. Blumen, *J. Phys. Lett. (Paris)* **45**:L49 (1984).