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Lifshitz Singularities in Random Harmonic Chains: Periodic Amplitudes near the Band Edge and near Special Frequencies

Th. M. Nieuwenhuizen[1] **and J. M. Luck**[2]

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We give a complete description of the scaling behavior of the integrated density of states of random harmonic chains with random masses near the band edge $\omega_{\max}$ and near special frequencies ω_s. There are four different situations: $\omega \uparrow \omega_{\max}$, $\omega \downarrow \omega_s$, $\omega \uparrow \omega_s$ (critical case), $\omega \uparrow \omega_s$ (general case). Our analytic results have the form of infinite sums involving Fourier coefficients of the scaling behavior of the Dyson–Schmidt function *at* the special frequency or the band edge. Binary mass distributions are considered in detail in the limit of a small fraction p of light masses. Our predictions are compared with extensive numerical data.

KEY WORDS: Integrated density of states; random chains; special frequencies; exponential singularities; periodic amplitudes.

1. INTRODUCTION

The study of random systems requires concepts and techniques that are unknown from studies of crystalline matter. Local quantities fluctuate from sample to sample, because of lack of translational invariance. Nevertheless, one still expects simple scaling laws to occur in the vicinity of continuous phase transitions.

The aim of this paper is to give a detailed analysis of such scaling behavior in a simple system. We shall consider the integrated density of states (IDS) of random harmonic chains. Our aim is to study frequencies around which the IDS is governed by collective behavior. In the ordered case, one has a van Hove power-law singularity near the band edge. In

[1] Institut für Theoretische Physik A, RWTH Aachen, 5100 Aachen, West Germany.
[2] Service de Physique Théorique, CEN Saclay, 91191 Gif-sur-Yvette, France.

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random systems, this is replaced by a Lifshitz (exponentially small) singularity.[1] We shall derive its precise scaling form in Section 3, and show that it is modulated by a periodic amplitude.

Oscillatory critical amplitudes are indeed common in binary random one-dimensional systems[2,3] and in systems that allow for an exact renormalization transformation.[4]

Restricting ourselves to binary random harmonic chains in Sections 4 and 5, we discuss related exponential singularities of the IDS near so-called special frequencies. We are able to predict numerically observed structures.

The very same problem has been studied before.[5] In that paper the exponents were derived, and properties of eigenfunctions were discussed. Independently the exponents have also been discussed by Endrullis and Englisch.[6] In the present paper, we aim to describe a method that yields the full scaling behavior. In particular, we obtain a detailed description of the structure of the oscillatory amplitude for small values of the concentration p of light masses.

Our setup is as follows. Section 2 is devoted to a brief survey of notations and of properties of the Schmidt function at a special frequency. In Section 3, we examine the Lifshitz singularity of the IDS at the upper band edge. The singularities near special frequencies ω_s are considered in Section 4, both for $\omega \downarrow \omega_s$ and for $\omega \uparrow \omega_s$ in the critical case ($M = M_c$). The most intricate case ($\omega \uparrow \omega_s$; $M > M_c$) is the subject of Section 5. Section 6 presents a short discussion.

2. BASIC DEFINITIONS. THE SCHMIDT FUNCTION

We first consider a binary random harmonic chain of masses $m_n = 1$ or $m_n = M$ ($M > 1$), which occur independently with probabilities p and $1 - p$, respectively. The equation for an eigenfunction with frequency ω is

$$-m_n \omega^2 a_n = a_{n+1} + a_{n-1} - 2a_n \tag{2.1}$$

We take fixed boundary conditions $a_0 = a_{L+1} = 0$. Equation (2.1) can be cast in the matrix form

$$\mathbf{A}_n = \begin{pmatrix} 2 - m_n \omega^2 & -1 \\ 1 & 0 \end{pmatrix} \mathbf{A}_{n-1} \equiv T_{m_n} \mathbf{A}_{n-1} \tag{2.2}$$

where

$$\mathbf{A}_n = \begin{pmatrix} a_{n+1} \\ a_n \end{pmatrix}$$

is the state vector, and T_{m_n} is the transfermatrix. It is useful to diagonalize the matrix of the light masses T_1. The upper bound of the spectrum is $\omega = 2$, which is the largest eigenfrequency of a chain with only light masses. We define an angle β (wavenumber) through

$$\omega = 2\sin(\tfrac{1}{2}\beta); \qquad 0 \leqslant \beta \leqslant \pi \tag{2.3}$$

Then the matrices

$$\begin{aligned} U &= (2i\sin\beta)^{-1/2}\begin{pmatrix} 1 & -1 \\ e^{-i\beta} & -e^{i\beta} \end{pmatrix} \\ U^{-1} &= (2i\sin\beta)^{-1/2}\begin{pmatrix} e^{i\beta} & -1 \\ e^{-i\beta} & -1 \end{pmatrix} \end{aligned} \tag{2.4}$$

diagonalize T_1. We give the results for T_1^{-1} and T_M^{-1}:

$$\tau_1^{-1} \equiv U^{-1}T_1^{-1}U = \begin{pmatrix} e^{-i\beta} & 0 \\ 0 & e^{i\beta} \end{pmatrix} \tag{2.5a}$$

$$\tau_M^{-1} \equiv U^{-1}T_M^{-1}U = Q_\beta \tag{2.5b}$$

where Q_β is given by

$$Q_\beta = \frac{1}{\cos\gamma}\begin{pmatrix} e^{-i\beta - i\gamma} & i\sin\gamma\, e^{i\beta} \\ -i\sin\gamma\, e^{-i\beta} & e^{i\beta + i\gamma} \end{pmatrix} \tag{2.5c}$$

The angle γ is defined by

$$\tan\gamma = (M-1)\tan(\tfrac{1}{2}\beta); \qquad 0 \leqslant \gamma < \pi/2 \tag{2.6}$$

One easily verifies the relation

$$Q_\beta(\tau_1^{-1})^{j-1} = Q_{j\beta} \tag{2.7}$$

The eigenvalue problem can be studied by considering the ratios $Y_n = a_{n+1}/a_n$ of the components of the vector $\mathbf{A}_n$. The ratio b_n^+/b_n^- of the two complex components of the vector $\mathbf{B}_n = U^{-1}\mathbf{A}_n$ has unit length, and defines an angle φ_n by

$$e^{i\varphi_n} = \frac{e^{i\beta}Y_n - 1}{e^{-i\beta}Y_n - 1} \qquad \left(Y_n = \frac{a_{n+1}}{a_n}\right) \tag{2.8}$$

So the real Y_n axis is mapped onto the unit circle. The action of the matrices (2.5) on φ_n reads

$$\varphi_{n-1} = \varphi_n - 2\beta \pmod{2\pi} \qquad \text{if} \quad m_n = 1 \tag{2.9a}$$

$$= R_\beta(\varphi_n) \qquad \text{if} \quad m_n = M \tag{2.9b}$$

where

$$e^{iR_\beta(\varphi)} \frac{e^{i\varphi - i\beta - i\gamma} + i \sin\gamma \, e^{i\beta}}{-i\sin\gamma \, e^{i\varphi - i\beta} + e^{i\gamma + i\beta}} \tag{2.10a}$$

In the following, we shall always use the notation $R(\varphi)$ for a Möbius transform like (2.10) related to a 2×2 matrix Q, as in (2.5c). We denote the Möbius transform attached to Q^N by R^N. In terms of R_β, Eq. (2.7) reads

$$R_{j\beta}(\varphi) = R_\beta(\varphi - 2(j-1)\beta) \tag{2.10b}$$

The boundary conditions $Y_0 = \infty$, $Y_{L+1} = 0$ are mapped onto

$$\varphi_0 = 2\beta, \qquad \varphi_{L+1} = 0 \tag{2.11}$$

In order to study the integrated spectral density, we now briefly derive the integral equation of Dyson[7] and Schmidt.[8] According to Eq. (2.1), the variable $Y_n = a_{n+1}/a_n$ satisfies the recurrence relation

$$Y_n = 2 - m_n\omega^2 - 1/Y_{n-1} \tag{2.12}$$

Its distribution function

$$Z_n(u) = \text{Prob}\{Y_n^{-1} < u\} \tag{2.13}$$

satisfies

$$\begin{aligned} Z_n(u) = {} & pZ_{n-1}(2 - \omega^2 - 1/u) + (1-p)\, Z_{n-1}(2 - M\omega^2 - 1/u) \\ & - \theta(-u) + Z_n(0) \end{aligned} \tag{2.14}$$

where θ is the Heaviside step function, defined by $\theta(x) = 1$ for $x > 0$ and 0 for $x \leqslant 0$. The integrated density of states $H(\omega^2)$ can be related to $Z(u)$ at given ω^2: for a large but finite chain, $H(\omega^2)$ is approximately equal to the number of changes of sign in the sequence a_n $(1 \leqslant n \leqslant L)$ divided by L. In terms of the ratios Y_n, $H(\omega^2)$ is just the fraction of negative Y_n. One therefore has, with probability one (or after averaging over the ensemble),

$$H(\omega^2) = \text{prob}\{Y < 0\} = Z(0) \tag{2.15}$$

where we already introduced the limit Schmidt function $Z = \lim_{n\to\infty} Z_n$. Combining (2.14) and (2.15), we find for $n \to \infty$

$$Z(u) = pZ(2-\omega^2-1/u) + (1-p)\,Z(2-M\omega^2-1/u) - \theta(-u) + H(\omega^2) \tag{2.16}$$

This equation can also be mapped onto the unit circle. The variables φ and u are related by [see Eqs. (2.8), (2.13)]

$$e^{i\varphi} = \frac{e^{i\beta}-u}{e^{-i\beta}-u}; \qquad u = \frac{e^{i\beta}-e^{i\varphi-i\beta}}{1-e^{i\varphi}} \tag{2.17}$$

and the quantity

$$V(\varphi) \equiv Z(u(\varphi)) \tag{2.18}$$

is a monotonic function on $[0; 2\pi]$ satisfying $V(0)=0$, $V(2\pi)=1$. It obeys the relation

$$V(\varphi) = pV(\varphi-2\beta) + (1-p)\,V(R_\beta(\varphi)) - I(0<\varphi<2\beta) + H(\omega^2) \tag{2.19}$$

Here I is the characteristic function of an interval:

$$\begin{aligned} I(\varphi_0<\varphi<\varphi_1) &= 1, \qquad \varphi_0<\varphi \ (\mathrm{mod}\ 2\pi)<\varphi_1 \\ &= 0, \qquad \text{elsewhere} \end{aligned} \tag{2.20}$$

Iterating Eq. (2.19) l times, one has

$$\begin{aligned} V(\varphi) = {} & p^l V(\varphi-2l\beta) + \sum_{j=1}^{l} (1-p)\,p^{j-1}\,V(R_{j\beta}(\varphi)) \\ & - \sum_{j=1}^{l} p^{j-1} I(-2\beta<\varphi-2j\beta<0) + (1-p^l)\,H(\omega^2)/(1-p) \end{aligned} \tag{2.21}$$

At the special frequency one will have $\beta=(l-k)\pi/l$. Then this equation reduces to

$$\begin{aligned} V(\varphi) = {} & \sum_{j=1}^{l} r_j V(R_{j\beta}(\varphi)) - (1-p)^{-1} \sum_{j=1}^{l} r_j I(-2\beta<\varphi-2j\beta<0) \\ & + (1-p)^{-1}\,H(\omega^2) \end{aligned} \tag{2.22}$$

where

$$r_j = (1-p)\,p^{j-1}/(1-p^l), \qquad j=1,\dots,l \tag{2.23}$$

The fixed points of $R_\delta(\varphi)$ for arbitrary δ are given by

$$\psi_\pm(\delta) = \delta \pm v(\delta) \tag{2.24a}$$

where $0 < v(\delta) < \pi$ is defined by

$$\cos v(\delta) = \sin(\gamma + \delta)/\sin \gamma \tag{2.24b}$$

and satisfies $0 < v(\delta) < \delta$ if $0 < \delta < \pi$. The fixed point will be real if and only if $|\sin(\gamma + \delta)| \leqslant \sin \gamma$.

3. THE LIFSHITZ SINGULARITY NEAR THE BAND EDGE

We first consider binary chains. Let ω be given by

$$\omega = 2\sin(\tfrac{1}{2}\beta), \qquad \beta = \pi - \varepsilon \tag{3.1}$$

In order to find an eigenfrequency near $\omega = 2$ ($\beta = \pi$), one needs a segment in the chain with a large number of consecutive light masses. Hence we assume that there are N such light masses, on (relabeled) sites $j = 1, \ldots, N$, and that there are heavy masses at sites $j = 0$ and $j = N + 1$. The probability to find such a succession is

$$(1-p)^2 p^N$$

which is exponentially small in N. As soon as N has been related to the frequency variable ε, we will obtain an exponentially small behavior in frequency.

In order to do so, boundary conditions have to be specified. The main point of our method will be to first fix boundary conditions and solve the highest eigenfrequency of the island of N light masses and then finally average over the boundary conditions. Hence we set

$$a_0 = c_L a_1, \qquad a_{N+1} = c_R a_N \tag{3.2}$$

where c_L and c_R are fixed real numbers. The highest excitation of the island has the amplitude

$$a_n = A e^{i\beta n} + B e^{-i\beta n} \tag{3.3}$$

Fixing A and B according to Eq. (3.2), one finds for large N

$$\varepsilon = \pi\{N - 1 + (1 + c_L)^{-1} + (1 + c_R)^{-1}\}^{-1}$$

or, equivalently, for small ε

$$N=\frac{\pi}{\varepsilon}-1+\frac{c_L}{1+c_L}+\frac{c_R}{1+c_R}+O(\varepsilon) \tag{3.4}$$

Let us denote by $W_H(c_L;\ \varepsilon)$ the integrated probability to find the boundary condition c_L. Obviously it is governed by the semi-infinite part of the chain to the left of zero . But in Section 2 we introduced the Dyson–Schmidt function $Z(u, \omega^2)$ just as the distribution function of the ratio of two successive amplitudes on the right end of a semi-infinite chain. The function W_H differs from it in the sense that there is an extra heavy mass at site 0:

$$W_H(c_L)=Z(2-M\omega^2-1/c_L)-\theta(-c_L)+\text{const}$$

Using the Dyson–Schmidt equation (2.16), we can write this as

$$W_H(c_L)=(1-p)^{-1}\{Z(c_L)-pZ(2-\omega^2-1/c_L)+p\theta(-c_L)\}+\text{const} \tag{3.5}$$

Finally, by symmetry, c_R is governed by the semi-infinite part of the chain to the right of $n=N+1$, and brings the same distribution.

Now that we have discussed all individual probabilities, the integrated density of states can be constructed. Given the values of ε, c_L, and c_R, we define N by Eq. (3.4). It is no longer an integer; we denote its integer part by $[N]$. To leading order in $p^{\pi/\varepsilon}$, only segments with $[N]+1$, $[N]+2$, $[N]+3$,..., will produce an eigenmode with frequency between $\omega^2=2+2\cos\varepsilon$ and $\omega^2=4$. Hence, to leading order, the increase of the integrated density of states is given by

$$1-H(\omega^2)=\int dW_H(c_L)\int dW_H(c_R)\sum_{j=1}^{\infty}(1-p)^2\ p^{[N]+j} \tag{3.6}$$

The following relation will often be employed, for real values of N

$$p^{[N]}=\frac{1-p}{p}\sum_{n=-\infty}^{\infty}\frac{-1}{\ln p+2\pi in}(pe^{2\pi in})^N \tag{3.7}$$

It can be verified easily by equating the Fourier coefficients of the periodic function $p^{[N]-N}$. Performing the sum in Eq. (3.6) and inserting Eqs. (3.7) and (3.4), we then derive

$$1-H(\omega^2)=\frac{(1-p)^2}{p}\sum_{n=-\infty}^{\infty}\frac{-1}{\ln p+2\pi in}Q_{1,n}^2(pe^{2\pi in})^{\pi/\varepsilon} \tag{3.8a}$$

$$\equiv p^{\pi/\varepsilon}Q_1\left(\frac{\pi}{\varepsilon}\right) \tag{3.8b}$$

So we have deduced that $1-H(\omega^2)$ indeed is exponentially small in frequency, in agreement with the original work of Lifshitz. Moreover, one sees that it has a periodic amplitude $Q_1(\pi/\varepsilon)$. The function Q_1 has coefficients

$$\begin{aligned} Q_{1,n} &= \int dW_H(c;\varepsilon)(pe^{2\pi in})^{-c(1+c)^{-1}} \\ &= \int dW_H(-1+1/v;\varepsilon)(pe^{2\pi in})^{1-v} \end{aligned} \tag{3.9}$$

which weakly depend on ε. Since we are only interested in the asymptotic behavior, we set $\varepsilon=0$ in Eq. (3.9) and denote $Z(u,\omega^2=4)$ by $Z_s(u)$. In Ref. 5 it was discussed that $Z_s(-1+1/v)$ vanishes for $v<0$ and equals unity for $0<v<v_- \equiv \frac{1}{2}\{1-M+(M^2-M)^{1/2}\}^{-1}$. Hence, for $v>v_+ \equiv 1+[4(M-1)]^{-1}$, Eq. (2.7) reduces to

$$Z_s(-1+1/v) = pZ_s(-1+1/(v-1)) \tag{3.10}$$

and has the solution

$$Z_s(-1+1/v) = p^v P_1(v), \qquad v \geqslant \{4(M-1)\}^{-1} \tag{3.11}$$

where P_1 is a periodic function with unit period. It can be expanded in a Fourier series as

$$P_1(v) = \frac{1-p}{p} \sum_{n=-\infty}^{\infty} \frac{-1}{\ln p + 2\pi in} P_{1,n} e^{2\pi inv} \tag{3.12}$$

The function P_1 and its coefficients $P_{1,n}$ are determined by the Dyson–Schmidt equation for Z_s. An iterative solution for small values of p will be discussed later [see below (3.16)].

Combining Eqs. (3.9) and (3.5), we find

$$\begin{aligned} Q_{1,n} &= (1-p)^{-1} \int d\{Z_s(-1+1/v) - pZ_s(-1+1/(v-1))\}(pe^{2\pi in})^{1-v} \\ &= (1-p)^{-1} \int_{v_+-1}^{v_+} dZ_s(-1+1/v)(pe^{2\pi in})^{1-v} \end{aligned} \tag{3.13}$$

Inserting Eqs. (3.11) and (3.12), we discover the remarkable result

$$Q_{1,n} = P_{1,n} \tag{3.14}$$

Equations (3.14) and (3.8) constitute our final result. They express that, if (the scaling behavior of) *the Schmidt function at the band edge* has been determinded, *the scaling behavior of the integrated density of states near the band edge* is also known.

We have defined $Q_{1,n}$ and $P_{1,n}$ in such a way that $P_{1,n} = Q_{1,n} = 1$ in the limit $M \to \infty$. Indeed, one verifies by explicit calculation from the exact solution derived by Domb *et al*.[9]

$$\begin{aligned} Z_s(-1+1/v) &= p^{[v]}, \qquad v>0 \\ &= 0, \qquad v<0 \end{aligned} \tag{3.15}$$

$$1 - H(\omega^2) = (1-p)\, p^{[\pi/\varepsilon]}, \qquad \varepsilon \downarrow 0; \quad M = \infty \tag{3.16}$$

The second result was given, for instance, in Ref. 3. Comparing with Eq. (3.8), one sees that $Q_1(x) = (1-p)\, p^{[x]-x}$ in this limiting situation.

A slightly different behavior is present for small values of p. In our numerical work we always found that, for small p, the function $Z_s(-1+1/v)$ is close to making one step per period. (It is not a discontinuous function for finite p, but the smaller the value of p, the more it looks like it; see Section 6). The positions of these "steps" are determined by heavy masses only, as can be seen from the following argument, which was discovered numerically in a related model.[2] One starts with the solution for $p = 0$:

$$Z_s(-1+1/v) = \theta(v^{-1}(1-\bar{v}-v)), \qquad p=0 \tag{3.17}$$

where

$$\bar{v} = \tfrac{1}{2}\{1 - (M/(M-1))^{1/2}\} \tag{3.18}$$

is negative. Substituting this in the second term of the right-hand side of Eq. (2.7) and iterating, one obtains

$$\begin{aligned} Z_s(-1+1/v) &= (1-p) \sum_{k=0}^{\infty} p^k \theta(v^{-1}(k+1-\bar{v}-v)) \\ &= p^{[v+\bar{v}]}, \qquad v > -\bar{v} \\ &= 0, \qquad v < -\bar{v} \end{aligned} \tag{3.19}$$

A better approximation can be obtained by repeating this procedure. Steps will be reduced by at least another factor $(1-p)$. We will not elaborate on this, however. Instead, we investigate the consequences of Eq. (3.19). Using Eq. (3.7), we can compare with Eq. (3.12) and find

$$Q_{1,n} = (pe^{2\pi i n})^{\bar{v}}, \qquad p \to 0 \tag{3.20}$$

Inserting this into (3.8) and using (3.7) again, we find

$$1 - H(\omega^2) = (1-p)\, p^{[\pi/\varepsilon + 2\bar{v}]}, \qquad p \to 0 \tag{3.21}$$

with $\bar{v}$ given in (3.18). Hence, if Z_s is close to making one step per period, so is $H(\omega^2)$. The prediction $2\bar{v}$ for the shift in (3.21) as compared to (3.16) has been verified numerically for systems with a small value of p, e.g., $p = 10^{-1}$. We had to restrict ourselves to such values to have a clearly visible scaling region.

Subdominant structures in Z_s will show up as smaller "steps." Due to the quadratic behavior in (3.8), they will cause more "small steps" in $H(\omega^2)$. We shall consider an analogous behavior in Section 4.2, where the same "proliferation mechanism" explains the dominant behavior of $H(\omega^2)$.

We already reported the result (3.8),[3] with another relation to the Schmidt function, which was conjectured to take the value given in (3.17). However, if we insert the present prediction (3.19) for the Schmidt function into Eq. (5.15) of Ref. 3, we immediately recover Eq. (3.21)! This explains why we could observe good agreement with numerical results in the small-p region.

Finally we note that Eq. (3.8) is valid for more general mass distributions. In fact, it holds whenever the lightest mass $m = 1$ occurs with nonzero probability p, the heavier masses having any distribution $R_H(m)$. Then Eq. (3.11) will again hold, with M denoting the one-but-lightest mass. And, if there is no mass gap at $m = 1$, one has $M = 1$, $v_+ = \infty$, and Eq. (3.11) will only be valid in the limit $v \to \infty$. Nevertheless, Eq. (3.8) still holds.

We discuss elsewhere[10] an example of such a situation, where an exact solution is available.[11,12] Equation (3.8) and its generalization for the two-point Green's function can then be derived in an independent manner. Moreover, coefficients like $Q_{1,n}$ can be found by solving second-order differential equations.

4. LIFSHITZ SINGULARITIES NEAR SPECIAL FREQUENCIES

Although the spectrum of a harmonic chain with random masses has no gaps, a behavior similar to that near the band edge also occur inside the spectrum. A frequency where this happens is called a "special frequency." The condition for occurrence of a special frequency is that there is a large enough gap in the mass distribution at $m = 1$. If we denote the one-but-lightest mass by M and if

$$\omega = 2\sin(\tfrac{1}{2}\beta), \qquad \beta \equiv \beta_s = \pi(l-k)/l \tag{4.1}$$

with $1 \leqslant k < l$ integers and mutual prime, then $\omega \equiv \omega_s$ is a "special frequency" if M satisfies

$$M \geqslant M_c(k, l) = 1 + \tan(k\pi/2l) \operatorname{cotan}(\pi/2l) \tag{4.2}$$

In such a situation $\omega = \omega_s$ is not an eigenfrequency of any chain in the ensemble.[13,14] The very same situation exists near the band edge. Hence also in the present case one expects essential singularities: again a large succession of a certain small sequence of light and heavy masses is needed for having an eigenmode with ω close to ω_s.

A lengthy discussion of properties of binary chains for frequencies near special frequencies was given recently.[5] We refer the reader to that paper for more details. Here we aim to give a more accurate description of the behavior of $H(\omega^2)$ for $\omega \to \omega_s$. It was already noted in Ref. 5 that one has to distinguish three cases: $\omega \downarrow \omega_s$ (Section 4.1); $\omega \uparrow \omega_s$, $M = M_c$ (Section 4.2), $\omega \uparrow \omega_s$, $M > M_c$ (Section 5). Here we recall that at the special frequency

$$H(\omega_s^2) = \sum_{n=1}^{l-1} r_{f(n)} \tag{4.3}$$

where $f(n)$ is defined by $f(n) \cdot (l - k) = n (\bmod l)$. This result is independent of $M \geqslant M_c(k, l)$.

As in Section 3, we shall restrict ourselves for simplicity to binary distributions. Our results expressing $H(\omega^2)$ as an infinite sum involving the squares of amplitudes of the scaling behavior of the Schmidt function will be valid in the general case if the conditions (4.1), (4.2) are satisfied.

4.1. To the Right of a Special Frequency

In this section, the role of the light mass in Section 3 is played by a succession of one heavy and $l - 1$ light masses, denoted by HL^{l-1}.[5,6] We mean that the Möbius transformation $Q_{l\beta}$ [cf. Eq. (2.7)], which is parabolic at ω_s, becomes elliptic when

$$\omega = 2 \sin(\tfrac{1}{2}\beta), \qquad \beta = \beta_s + \varepsilon, \quad \varepsilon > 0 \tag{4.4}$$

Then, for φ close to zero, and going from site n to site $n + 1$, the phase is transformed by $Q_{l\beta}^{-1}$:

$$HL^{l-1}\colon \quad \varphi \to R_{l\beta}^{-1}(\varphi) = \varphi + \tan\gamma\, \varphi^2 + 2l\varepsilon + O(\varphi^3) \tag{4.5a}$$

On the other hand, also the transformation connected to light masses is elliptic. One has of course

$$L^l: \quad \varphi \to \varphi + 2l\varepsilon \tag{4.5b}$$

We conclude that the central part of the chain may consist of an arbitrary sequence of successions of HL^{l-1} and L^l. Although L^l is close to the identity for $|\varphi| \simeq \sqrt{\varepsilon}$, there is not much difference between HL^{l-1} and L^l for φ close to zero. Since we have not been able to solve this full problem, we restrict ourselves to small values of p. Then the probability

$$q_l = (1-p)\, p^{l-1} \tag{4.6}$$

for finding HL^{l-1} is much larger than the probability p^l for finding L^l. Consequently, the central part of the chain will only contain successions of HL^{l-1}.

For reasons of symmetry we consider the eigenfrequencies of an island $(HL^{l-1})^N H$, which has (relabeled) site indices $i = 1, 2, \ldots, Nl+1$. The boundary conditions $a_0 = c_L a_1$, $a_{Nl+2} = c_R a_{Nl+1}$ determine phases φ_L and φ_R through Eq. (2.8). The phase φ_{Nl+1} is also defined by (2.8) and related to φ_R as

$$\varphi_{Nl+1} = 2\beta - \varphi_R \tag{4.7}$$

The difference between these two phases is that φ_{Nl+1} is "read off from the left" and φ_R "from the right." Writing $(HL^{l-1})^N H = (HL^{l-1})^{N+1} L^{1-l}$, we can relate φ_L to φ_R, using the definitions of Section 2,

$$\varphi_L = R_{l\beta}^{N+1}(2l\varepsilon - \varphi_R) \tag{4.8a}$$

This is compact notation of

$$\begin{aligned} e^{i\varphi_L} = {} & \{\sin\mu \cos\gamma \cos(N\mu + \mu) e^{2il\varepsilon - i\varphi_R} \\ & + i \sin(N\mu+\mu)(-\sin(\gamma + l\varepsilon)\, e^{2il\varepsilon - i\varphi_R} + \sin\gamma e^{il\varepsilon})\} \\ & \times \{\sin\mu\cos\gamma\cos(N\mu+\mu) \\ & + i\sin(N\mu+\mu)(-\sin\gamma\, e^{il\varepsilon - i\varphi_R} + \sin(\gamma + l\varepsilon))\}^{-1} \end{aligned} \tag{4.8b}$$

Here the parameter μ is defined by[5]

$$\cos\mu = \cos(\gamma + l\varepsilon)/\cos\gamma, \qquad 0 \leqslant \mu \leqslant \pi \tag{4.9}$$

For small ε one finds $\mu \simeq (2l\varepsilon \tan\gamma)^{1/2}$.

The length N for which (4.8) has a solution at given values of φ_L, φ_R, and ε can be obtained for small ε:

$$N = \pi/\mu - 1 + \Delta + O(\mu) \tag{4.10}$$

with

$$\Delta = \tfrac{1}{2} \operatorname{cotan} \gamma \, (\operatorname{cotan} \tfrac{1}{2}\varphi_L + \operatorname{cotan} \tfrac{1}{2}\varphi_R) \tag{4.11}$$

Whenever N is an integer, an eigenfrequency will be present. Because chains with length $[N] + j$ ($j = 1, 2, ...$) have an eigenmode with frequency between ω_s and ω, we can already write down the equivalent of Eq. (3.6):

$$H(\omega^2) - H(\omega_s^2) = \sum_{j=1}^{\infty} \int dW_H(\varphi_L)\, dW_H(\varphi_R)(1-p) q_l^{[N]+j} \tag{4.12}$$

Here the integrals with respect to W again perform the average over the boundary conditions. Following the ideas of Section 3, we find

$$\begin{aligned} W_H(\varphi_L) &= V(R_\beta(\varphi_L)) + \text{const} \\ &= (1-p)^{-1}\{V(\varphi_L) - q_l V(R_{l\beta}(\varphi_L))\} \\ &\quad - (1-p)^{-1} \sum_{j=2}^{l-1} q_j V(R_{j\beta}(\varphi_L)) - p^l V(\varphi_L - 2l\varepsilon) + \text{const} \end{aligned} \tag{4.13}$$

where we made use of Eq. (2.15).

Inserting Eq. (3.7) into Eq. (4.12), we obtain the final result, valid for general mass distributions, for which ω_s is a special frequency

$$H(\omega^2) - H(\omega_s^2) = (q_l)^{\pi/\mu}\, Q_2(\pi/\mu), \qquad \omega \downarrow \omega_s \tag{4.14a}$$

where

$$Q_2(x) = \frac{1}{(1-p) q_l} \sum_{n=-\infty}^{\infty} \frac{1}{\ln q_l + 2\pi i n} Q_{2,n}^2 e^{2\pi i n x} \tag{4.14b}$$

The coefficients $Q_{2,n}$ have been defined as

$$Q_{2,n} = (1-p) \int (q_l e^{2\pi i n})^{(\operatorname{cotan} \varphi \operatorname{cotan} \gamma)/2}\, dW_H(\varphi) \tag{4.15}$$

and will again be approximated by their value at $\varepsilon = 0$. For φ_L close to 2π, the sum in (4.13) involves the function V for values of argument between 0 and $\varphi_+(a\beta)$, where it vanishes for $\varepsilon = 0$. We shall also omit the term proportional to p^l from (4.13). So only the first two terms remain. In Ref. 5 it was discussed that $V(\varphi, \varepsilon=0) \equiv V_s(\varphi)$ has the scaling behavior

$$1 - V_s(2\pi - \varphi) = (r_l)^x P_2(x), \qquad x \equiv \tfrac{1}{2}\operatorname{cotan}(\tfrac{1}{2}\varphi)\operatorname{cotan}\gamma_s \qquad (0 < \varphi < \varphi_+) \tag{4.16}$$

This is valid for

$$x \geqslant x_- \equiv \tfrac{1}{2}\operatorname{cotan}\{\pi - \tfrac{1}{2}R_{\pi(1-1/l)}(0)\}\operatorname{cotan}\gamma_s$$

Moreover,

$$r_l = q_l(1-p^l)^{-1} = (1-p)\,p^{l-1}(1-p^l)^{-1} \tag{4.17}$$

The function P_2 has the following Fourier series:

$$P_2(x) = \sum_{n=-\infty}^{\infty} \frac{-1}{\ln r_l + 2\pi i n} P_{2,n}\, e^{2\pi i n x} \tag{4.18}$$

Combining (4.15) with (4.16) and (4.18), we find

$$Q_{2,n} = \int_{x_-}^{x_-+1} (q_l\, e^{2\pi i n})^{-x}\, d\{r_l^x P_2(x)\} = P_{2,n} \tag{4.19}$$

where we used that $r_l \simeq q_l$ in our approximation $p^l \ll 1$. In fact, the form of (4.19) suggests that for arbitrary p indeed r_l instead of q_l should enter Eq. (4.14). Therefore, it is tempting to think that the solution for finite p is obtained by making (only) this replacement in (4.14). It would be interesting to have a direct proof of this point.

Equations (4.14) and (4.19) constitute our result for $\omega \downarrow \omega_s$. Again there is an essential singularity, multiplied by a periodic amplitude. It has been derived for binary distributions, but is valid in general.

Restricting ourselves again to the binary case, we can make more concrete predictions by studying the coefficients $Q_{2,n} = P_{2,n}$. First of all, in the case $M = \infty$, one picks up the weight of the modes with frequency ω_s,[9]

$$H(\omega_s^2 + 0) - H(\omega_s^2) = (1-p) r_l = (1-p)^2 p^{l-1}(1-p^l)^{-1}, \qquad M = \infty \tag{4.20}$$

It cannot be obtained from our previous approach because of the interchange of the limits $M \to \infty$ and $\varepsilon \to 0$.

More interesting is the behavior for finite M and small p. As in the preceding section, we can provide an iterative solution starting from the value for $p=0$:

$$V_s(\varphi)=\theta(\varphi-\psi_+(\beta_s)) \tag{4.21}$$

where $\psi_+(\beta_s)$ is defined by (2.24). Equation (4.21) states that for $p=0$ there is only one chain in the ensemble. It has only heavy masses and produces a phase $\psi_+(\beta_s)$. In order to find the low-p behavior, we insert (4.21) into all terms in the rhs of Eq. (2.22), except for the term with $R_{l\beta_s}(\varphi)=R_0(\varphi)$. To leading order in p, this equation then takes the form

$$V_s(\varphi)=r_l V(R_0(\varphi))+r_1\theta(\varphi-\psi_+(\beta_s)) \tag{4.22}$$

It has the solution

$$1-V_s(\varphi)=r_1\sum_{j=0}^{\infty} r^j\theta(\varphi-R_0^{-j}(\psi_+(\beta_s)) \tag{4.23}$$

where it can be checked that

$$\begin{aligned}&\tfrac{1}{2}\operatorname{cotan} R_0^{-j}\{\psi_+(\beta_s)\}\operatorname{cotan}\gamma_s\\ &\quad=-j+\tfrac{1}{2}\operatorname{cotan}\psi_+(\beta_s)\operatorname{cotan}\gamma_s\end{aligned} \tag{4.24}$$

Hence the sum can be carried out and one finds, for $\varphi\downarrow 0$,

$$1-V_s(2\pi-\varphi)=\frac{r_1}{1-r_l}\,r_l^{[x+1+\{\operatorname{cotan}(\psi_+(\beta_s)/2)\operatorname{cotan}\gamma_s\}/2]} \tag{4.25}$$

with x defined in (4.6). Hence, in this first approximation, V_s indeed has the expected scaling behavior and makes one step per period. Using Eq. (3.7), one can read off the coefficients $P_{2,n}$ defined in (4.18). Inserting the result into (4.14) and performing the sum, we end up with

$$H(\omega^2)-H(\omega_s^2)=\frac{1-p}{1-q_l}\,q_l^{[\pi/\mu+\operatorname{cotan}(\psi_\mp(\beta_s)/2)\operatorname{cotan}\gamma_s]} \tag{4.26}$$

As in Section 3, one finds that the shift in the expression for $H(\omega^2)$ is twice as large as the one in V_s. We have verified this leading small-p behavior numerically, and indeed found the correct shifts in V_s and $H(\omega^2)$.

In Fig. 1, we present a plot of numerical data for $\Delta H=H(\omega^2)-H(\omega_s^2)$ in a typical case. The data plotted in all the figures of the present paper have been obtained by an exact enumeration of mass configuration of finite systems of length $N\leqslant 18$ ($N=18$ has $2^{18}\approx 2\times 10^5$ configurations). This very efficient method has already been described.[2,3,5]

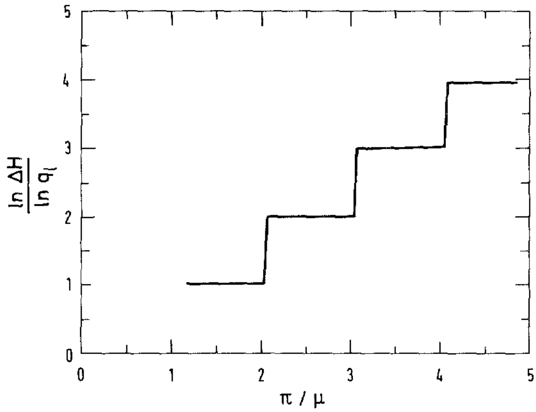

Fig. 1. Plot of $\ln \Delta H / \ln q_l$ (where ΔH is the IDS difference) versus the variable π/μ of Eq. (4.9), for $\omega^2 \downarrow \omega_s^2$ and $k=1$, $l=4$, $M=10$, $p=0.1$.

4.2. To the Left of a Special Frequency: Critical Mass Ratio

This situation is very close to (but more interesting than) the behavior to the right of a special frequency, discussed in the previous section. Also, in the present case, there is a transformation, which is parabolic at the special frequency and becomes the leading elliptic one away from ω_s. It is connected to a succession of one heavy mass and $a-1$ light masses, where the integer a is defined by

$$(l-k)a = 1 \ (\mathrm{mod}\ l), \qquad 1 \leqslant a \leqslant l-1 \tag{4.27}$$

An extensive discussion of this point is given in Ref. 5. Here we first repeat the argument of Section 4.1, which leads to a more complete description of the phenomenon:

$$\omega = 2\sin(\tfrac{1}{2}\beta), \qquad \beta = \beta_s - \varepsilon \tag{4.28}$$

and introduce the variable μ by

$$\cos\mu = (-1)^\eta \cos(\gamma + a\beta)/\cos\gamma \tag{4.29}$$

Here $\eta = 0$ or 1, in such a way that $\mu \to 0$ when $\varepsilon \to 0$. Hence μ is of order $\sqrt{\varepsilon}$ for small ε; see Ref. 5 for the prefactor. As in Section 4.1, we take p small ($p^l \ll 1$) and arrive at a result analogous to (4.14):

$$H(\omega_s^2) - H(\omega^2) = (q_a)^{\pi/\mu}\, Q_3(\pi/\mu) \tag{4.30a}$$

with

$$Q_3(x) = \frac{1}{(1-p)q_a} \sum_{n=-\infty}^{\infty} \frac{-1}{\ln q_a + 2\pi i n} P_{3,n}^2 \, e^{2\pi i n x} \tag{4.30b}$$

and

$$q_a = (1-p)\, p^{a-1} \tag{4.31}$$

As before, the coefficients $P_{3,n}$ come from the scaling behavior of the Schmidt function at ω_s to the right of the fixed point π/l of the relevant parabolic transformtion,

$$V_s(\pi/l + \theta) = (r_a)^x \, P_3(x); \qquad x = \tfrac{1}{2} \operatorname{cotan}(\tfrac{1}{2}\theta) \operatorname{cotan} \gamma_c \tag{4.32}$$

where $\gamma_c = \frac{1}{2}\pi(1 - 1/l)$ is the value in the critical case and P_3 is periodic with the expansion

$$P_3(x) = \sum_{-\infty}^{\infty} \frac{-1}{\ln r_a + 2\pi i n} P_{3,n} \, e^{2\pi i n x} \tag{4.33}$$

where

$$r_a = q_a(1-p^l)^{-1} = (1-p)\, p^{a-1}(1-p^l)^{-1} \tag{4.34}$$

The result (4.30), (4.33) is also valid for more general mass distributions. In the binary case we can apply the ideas of the previous sections and obtain by iteration of the Schmidt equation (2.22) a result valid for small p:

$$V_s\left(\frac{\pi}{l} + \theta\right) = \frac{r_a}{1 - r_a} \sum_{\substack{j=1 \\ j \neq a}}^{l} r_j r_a^{[x - x_j]} \tag{4.35a}$$

where

$$x_j = \tfrac{1}{2} \operatorname{cotan}\{\tfrac{1}{2}\psi_+(\beta_s) + (j-1)\beta_s - \pi/2l\} \operatorname{cotan} \gamma_c \tag{4.35b}$$

From this one derives, using Eq. (3.7),

$$P_{3,n} = \sum_{\substack{j=1 \\ j \neq a}}^{l} r_j (r_a e^{2\pi i n})^{-x_j} \tag{4.36}$$

We first assume that $a \geqslant 2$. Then to leading order in p only the terms $1 \leqslant j \leqslant a-1$ are important, because for these terms $r_j/r_a = p^{j-a} \gg 1$. In other words, only the steps in (4.35) with $1 \leqslant j \leqslant a-1$ are leading for $p \downarrow 0$.

In fact we find $a-1$ essentially equal steps of strength $1/(a-1)$ per period in the quantity $\ln V_s(\varphi+\pi/2l)/\ln r_a$. Thus, for $a=2$ there is essentially one step per period and we are back in the situation of Section 4.1.

More interesting is the situation where $a \geqslant 3$. In Fig. 2 we present numerical data for the case $a=3$, where two "steps" are observed per period. To a high accuracy they are equal to 1/2 and complete agreement with Eq. (4.35) is found.

Because Eq. (4.30) is quadratic in $P_{3,n}$, the two leading terms from (4.36) for the case $a=3$ produce three terms in (4.30). Hence, we predict for this case three leading "steps" per period in $H(\omega^2)$. Performing some algebra, we deduce the following "steps" for the case $x_1 < x_2$:

$$\begin{aligned}
\Delta &\frac{\ln[H(\omega_s^2)-H(\omega^2)]}{\ln r_3} \\
&=\frac{1}{\ln r_3} \ln \frac{r_3 r_1^2+2r_1r_2+r_2^2}{r_1^2+2r_1r^2+r_2^2} \approx \frac{1}{2}+\frac{\ln 2}{2\ln p} \\
&=\frac{1}{\ln r_3} \ln \frac{r_3(r_1^2+2r_1r_2)+r_2^2}{r_3r_1^2+2r_1r_2+r_2^2} \approx \frac{1}{2} \\
&=\frac{1}{\ln r_3} \ln \frac{r_3(r_1^2+2r_1r_2+r_2^2)}{r_3(r_1^2+2r_1r_2)+r_2^2} \approx -\frac{\ln 2}{2\ln p}
\end{aligned} \tag{4.37}$$

at the points $\pi/\mu = 2x_1,\ x_1+x_2,\ 2x_2 \pmod 1$, respectively. We note that the steps in (4.37) sum to unity, as they should. In Fig. 3 we present numerical data, which fully confirm the behavior predicted by (4.37).

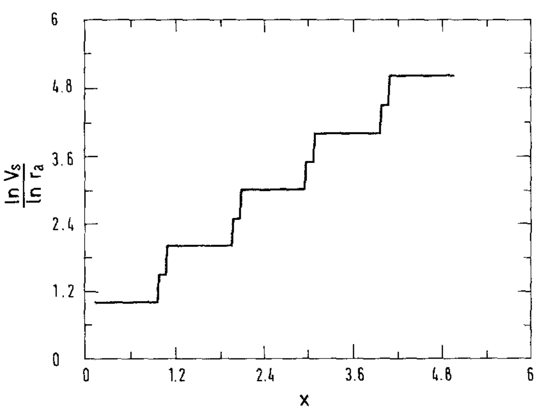

Fig. 2. Plot of $\ln V_s/\ln r_a$ (where V_s is the Schmidt function) versus the variable x of Eq. (4.32) for $k=2$, $l=7$, $(a=3)$, $p=0.1$, and $M=M_c=3.110$.

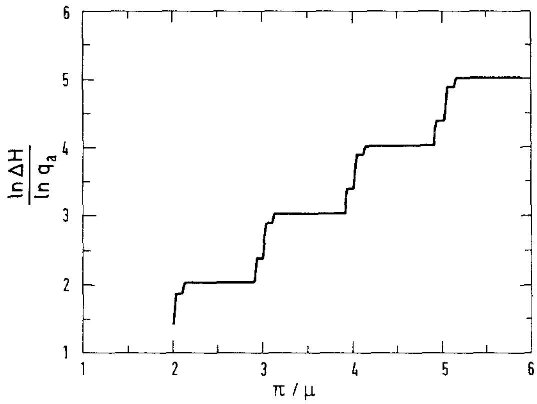

Fig. 3. Plot of $\ln \Delta H / \ln q_a$ (where ΔH is the IDS difference) versus the variable π/μ of Eq. (4.29), for $\omega^2 \uparrow \omega_s^2$, in the same model as Fig. 2.

Finally there remains the case $a = 1$, which occurs when $k = l - 1$. It is a "very special" frequency, because the important succession HL^{a-1} consists of one heavy mass only. This was already noticed in Ref. 5, where an eigenfunction with such a behavior was presented.

Now the approximation (4.35) essentially makes one step per period for small p, coming from the leading $j = 2$ term. Numerically a richer structure can be observed. Figure 4 shows the "first" special frequency ($\omega_s^2 = 2$; $k = 1$, $l = 2$, $a = 1$). A better approximation is obtained by iterating the Schmidt equation (2.22) once more. Here one substitutes (4.35) in all terms of the right-hand side of Eq. (2.22), except in the term with $j = a$. One then needs

$$X_j(x) = \tfrac{1}{2} \operatorname{cotan} \gamma_c \operatorname{cotan} \tfrac{1}{2}\{R_j(\varphi) - \pi/l\} \tag{4.38}$$

where x and φ are related by (4.32). It can be shown that

$$\begin{aligned} X_j(x) = &-1 - \tfrac{1}{2} \operatorname{cotan} \gamma_c \,\{\tfrac{1}{2} \operatorname{cotan} \gamma_c + x \operatorname{cotan}(j\beta - \pi/l)\} \\ &\times \{x - \tfrac{1}{2} \operatorname{cotan} \gamma \operatorname{cotan}(j\beta - \pi/l)\}^{-1} \end{aligned} \tag{4.39}$$

Iterating this equation, one finds

$$V_s(\varphi) = \sum_{\substack{j,j'=1 \\ j,j' \neq a}}^{l} \sum_{k=k(j')}^{\infty} (1 - r_a)^{-1} r_j r_{j'} r_a^{k+1+[X_{j'}(x-k) - x_j]} \tag{4.40}$$

where

$$k(j') = [x - \tfrac{1}{2} \operatorname{cotan} \gamma_c \operatorname{cotan}(j'\beta_s - \pi/l)] + 1$$

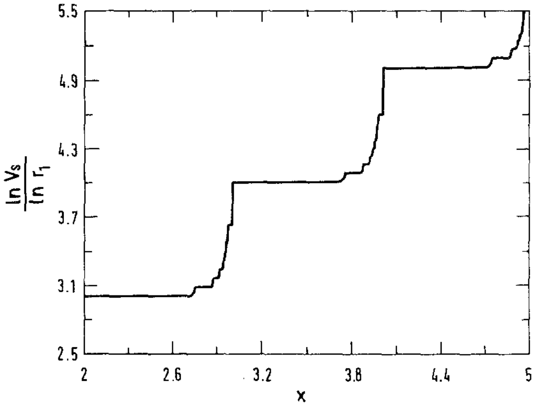

Fig. 4. Same as Fig. 2, for the "first" special frequency ($k=1$, $l=2$, $a=1$, $p=0.1$, and $M=M_c=2$).

In the case $k=1$, $l=2$ the sum simplifies. Then $a=1$, $j=j'=2$, $\beta_s=\pi/2$, $\gamma_c=\pi/4$, $x_2=0$, $r_2=1-r_1$. Hence our second iterate reads

$$V_s(\varphi)=r_2 \sum_{k=[x+1]}^{\infty} r_1^{k+[1/(4k-4x)]} \tag{4.41}$$

This is to be compared with the first iterate $V_s(\varphi)=r_1^{1+[x]}$ from (4.35). The values of $V_s(\varphi)$ given by Eq. (4.41) already present the leading sequence of structures of Fig. 4.

Since we could not obtain reliable numerical data for $H(\omega^2)$, we shall not work out the implications of the rich structure of $V_s(\varphi)$. It is expected that $H(\omega^2)$ has a much richer structure.

5. TO THE LEFT OF A SPECIAL FREQUENCY: GENERAL MASS RATIO

This case has proved to be more subtle than previous ones. Our result (5.29) is more complicated than an exponential times a periodic amplitude. Nevertheless, we are able to describe numerical data precisely (see Section 5.2).

5.1. Relation between $H(\omega^2)$ and $V_s(\varphi)$

We again set

$$\omega=2\sin\tfrac{1}{2}\beta, \qquad \beta=\pi(l-k)/l-\varepsilon\equiv\beta_s-\varepsilon \tag{5.1}$$

For small enough ε, all transformations $R_{j\beta}$ $(j=1,\dots,l)$ connected to successions HL^{j-1} are hyperbolic. The only elliptic one is related to a sequence of l light particles (L^l: $\varphi \to \varphi + 2l\beta$). So, a succession of $Nl+j+1$ light masses shifts the phase:

$$\varphi_{Nl+j+1} = \varphi_0 + 2(Nl+j+1)\beta, \qquad 1 \leqslant j \leqslant l \tag{5.2}$$

Inserting boundary values φ_L and φ_R by $\varphi_0 \equiv \varphi_L$ and $\varphi_{Nl+j+1} \equiv 2\beta - \varphi_R$, one has

$$\varphi_L + \varphi_R = 2(N+j)\varepsilon - 2j\beta_s \pmod{2\pi} \tag{5.3}$$

In Ref. 5, it was discussed in more heuristic terms that φ_L and φ_R should be larger than or equal to $\psi_+(a\beta)$, the fixed point connected to the relevant sequence HL^{a-1}. Here a $(1 \leqslant a \leqslant l)$ is defined by $a \cdot \beta_s = \pi/l \pmod{\pi}$. The fact that at the special frequency the Schmidt function $V_s(\varphi)$ vanishes for $\varphi \leqslant \psi_+(a\beta_s)$ means that for $\varepsilon \to 0$, phases are always larger that $\psi_+(a\beta_s)$. We define

$$\delta = a\beta \pmod{\pi} = \pi/l - a\varepsilon \tag{5.4}$$

and introduce the following decomposition:

$$\varphi_{L,R} = \psi_+(a\beta) + \theta_{L,R} \equiv \pi/l - a\varepsilon + \nu(\delta) + \theta_{L,R} \tag{5.5}$$

where $\nu(\delta)$ is defined in (2.24). Next we calculate N from Eq. (5.3). For small ε, assuming small $\theta_{L,R}$ and using $\nu(\delta) < \delta$, it is found that by far the smallest value is taken if $j = l - a$:

$$N = (2\nu + \theta_L + \theta_R)/2l\varepsilon - 1, \qquad j = l - a \tag{5.6}$$

Here the argument of ν has been omitted. Following the arguments of Sections 3 and 4, one finds that only islands $HL^{l[N]+il+l-a+1}H$ contribute to the leading behavior of the IDS. Hence, one arrives at

$$\begin{aligned} H(\omega_s^2) - H(\omega^2) = \sum_{i=1}^{\infty} \int dW_H(\theta_L)\, dW_H(\theta_R)(1-p)^2 \\ \times p^{l[(2\nu+\theta_L+\theta_R)/2l\varepsilon]+il-a+1} \end{aligned} \tag{5.7}$$

Using (3.7), one can write this as

$$H(\omega_s^2) - H(\omega^2) = \sum_{n=-\infty}^{\infty} \frac{-p^{1-a}}{\ln p^l + 2\pi i n} (p^l e^{2\pi i n})^{\nu(\delta)/l\varepsilon}\, \Gamma_n^2(\varepsilon) \tag{5.8}$$

with

$$I_n(\varepsilon) = (1-p) \int dW_H(\theta)\, (p^l e^{2\pi i n})^{\theta/2l\varepsilon} \tag{5.9}$$

In Eqs. (5.7) and (5.9), $W_H(\theta)$ is the integrated probability that the phase at the right end of a semi-infinite chain ending with a heavy mass takes the value $\varphi = \psi_+(a\beta) + \theta$:

$$W_H(\theta) = V(R_\beta(\varphi)), \qquad \varphi \equiv \psi_+(\delta) + \theta \tag{5.10}$$

From Eq. (2.19) it can be deduced that

$$W_H(\theta) = (1-p)^{-1} \Big\{ V(\varphi) - p^l V(\varphi - 2l\beta) \\ - (1-p) \sum_{j=2}^{l} p^{j-1} V(R_{j\beta}(\varphi)) \Big\} \tag{5.11}$$

Due to the strong ε dependence in (5.9) we have to solve $V(\varphi)$ for ε small but finite. We set

$$\tilde{V}(\theta) = V(\psi_+(a\beta) + \theta) - V(\psi_+(a\beta)) \tag{5.12}$$

Expanding Eq. (2.21) about $\theta = 0$, we have

$$\tilde{V}(\theta) = p^l \tilde{V}(\theta + 2l\varepsilon) + (1-p)\, p^{a-1}\, \tilde{V}(\alpha\theta) - p^l\, \tilde{V}(2l\varepsilon) \tag{5.13}$$

with

$$\alpha = \frac{d}{d\theta} R_{a\beta}(\psi_+(a\beta) + \theta) \Big|_{\theta=0} \\ = \frac{-\sin\gamma \sin\nu(\delta) + \cos(\gamma+\delta)}{\sin\gamma \sin\nu(\delta) + \cos(\gamma+\delta)} > 1 \tag{5.14}$$

Here we have omitted terms of the form $V(R_{j\beta}(\varphi))$ for $j \neq a$. Because we shall only consider (5.13) for $-2\nu(\delta) < \theta \ll 1$ and we will find exponential decay for $\theta/\varepsilon \ll -1$, such terms indeed are exponentially small. For the same reason it is not important that $R_{\alpha\beta}(\varphi)$ should only be linearized near its fixed point: in the region where the linearization is not allowed, $V(R_{a\beta}(\varphi))$ is exponentially small anyhow.

The interesting point is that Eq. (5.13) can be solved exactly, so that a closed expression for $I_n(\varepsilon)$ in Eq. (5.9) can be derived. Formally extending its region of validity to the whole real axis, we define

$$F(s)=\int_{-\infty}^{\infty} e^{-is\theta}\, d\tilde{V}(\theta) \tag{5.15}$$

It satisfies the equation

$$F(s)=(1-p^l)(1-p^l e^{2il\varepsilon s})^{-1}\, r_a F(s/\alpha) \tag{5.16}$$

where $r_a=(1-p)\,p^{a-1}/(1-p^l)$. The solution is

$$F(s)=\sum_{k=-\infty}^{\infty} c_k(is)^{-\zeta+ik\Omega}\prod_{j=0}^{\infty}\{(1-p^l)(1-p^l e^{2il\varepsilon s\alpha^{-j}})^{-1}\} \tag{5.17}$$

with cuts of powers taken along the negative real axis and

$$\zeta=-\ln r_a/\ln\alpha=-{}^{\alpha}\log r_a; \qquad \Omega=2\pi/\ln\alpha \tag{5.18}$$

The coefficients c_k can once more be determined from the Schmidt function $V_s(\varphi=\psi_+(a\beta)+\theta)$ *at* the special frequency. Here one starts from the inverse of Eq. (5.15):

$$\tilde{V}(\theta)=\int_{-\infty}^{\infty}\frac{ds}{2\pi is}(e^{is\theta}-1)\,F(s) \tag{5.19}$$

and takes θ positive and ε small ($\varepsilon\ll\theta\ll 1$). Closing the integral in the upper half-plane, one can neglect the ε dependence and obtains scaling behavior of the form already discussed in Ref. 5:

$$V_s(\psi_+(a\beta_s)+\theta)=\sum_{k=-\infty}^{\infty}\frac{-1}{\ln r_a+2\pi ik}P_{4,k}\theta^{\zeta-ik\Omega}, \qquad \theta\downarrow 0 \tag{5.20}$$

where $P_{4,k}$ are related to c_k by

$$c_k=-(\ln r_a+2\pi ik)^{-1}\,\Gamma(1+\zeta-ik\Omega)\,P_{4,k} \tag{5.21}$$

Note that the c_k decay much faster for large k than the $P_{4,k}$.

Next we determine $I_n(\varepsilon)$. The integral (5.9) is dominated by values $\theta/2l\varepsilon\ll -1$. Evaluating Eq. (5.19) for this situation, we can close the contour downward and find leading poles from the term with $j=0$,

$$s=s_n=(2il\varepsilon)^{-1}\sigma_n \tag{5.22}$$

where

$$\sigma_n = -\ln p^l - 2\pi i n \tag{5.23}$$

Summing the residues, we obtain

$$\tilde{V}(\theta) = (1-p^l) \sum_{k,n=-\infty}^{\infty} \frac{c_k}{\sigma_n} \left(\frac{2l\varepsilon}{\sigma_n}\right)^{\zeta - ik\Omega} \{p^l \exp(2\pi i n)\}^{-\theta/2l\varepsilon}$$
$$\times \prod_{j=1}^{\infty} \{(1-p^l)(1-p^l \exp(\alpha^{-j}\sigma_n))^{-1}\} \tag{5.24}$$

Indeed, it decays exponentially in the following way:

$$\tilde{V}(\theta) = p^{-\theta/2\varepsilon} (2l\varepsilon)^{\zeta} P(\theta/2l\varepsilon; {}^{\alpha}\log(2l\varepsilon)) \tag{5.25}$$

where P is periodic in both variables with unit periods. The result (5.24) has to be inserted into Eqs. (5.9), (5.11). The integral is dominated by the scaling region $1 \ll -\theta/2l\varepsilon \ll v(\delta)/l\varepsilon$. In that region only the first two terms of Eq. (5.11) are leading. The resulting integral can be evaluated from (5.24). A slightly shorter method starts with noting that, by the same argument,

$$I_n(\varepsilon) = \lim_{\xi \downarrow 0} \int (p^l e^{2\pi i n} e^{\xi})^{\theta/2l\varepsilon}\, d\{\tilde{V}(\theta) - \tilde{V}(\theta + 2l\varepsilon)\} \tag{5.26}$$

Using (5.15) and (5.22), this may be written

$$I_n(\varepsilon) = \lim_{s \to s_n} (1 - p^l e^{2il\varepsilon s}) F(s) \tag{5.27}$$

From (5.17) one then obtains, using definition (5.23),

$$I_n(\varepsilon) = (1-p^l) \prod_{j=1}^{\infty} \frac{1-p^l}{1-p^l \exp(\alpha^{-j}\sigma_n)} \sum_{k=-\infty}^{\infty} c_k \left(\frac{2l\varepsilon}{\sigma_n}\right)^{\zeta - ik\Omega} \tag{5.28}$$

It has the form

$$I_n(\varepsilon) = (2l\varepsilon)^{\zeta} J_n({}^{\alpha}\log(2l\varepsilon))$$

where J_n is periodic with unit period. We note that the expression (5.28), without the infinite product, can be recovered by taking the limit $\varepsilon \to 0$ in Eq. (5.11). Indeed, inserting V_s from (5.20) into (5.11) and afterward performing the integral (5.9), one obtains (5.28) without the infinite product.

Equations (5.8), (5.28), and (5.21) consitute our final result. We recall that δ is defined in (5.4), $v(\delta)$ in (2.24), α in (5.14), σ_n in (5.23), and ζ and Ω in (5.18), and c_k are related by (5.21) to the coefficients $P_{4,k}$ of the scaling behavior (5.20) of the Schmidt function at the special frequency. Note that the final result may be written

$$H(\omega_s^2) - H(\omega^2) = p^{v(\delta)/\varepsilon}(2l\varepsilon)^{2\zeta}\, Q(v(\delta)/l\varepsilon;\ {}^{\alpha}\log(1/2l\varepsilon)) \qquad (5.29)$$

where $Q(x, y)$ is periodic in x and y, with unit periods. Contrary to previous cases, the combination (5.29) cannot be rewritten in the form of an exponential times a periodic function of one variable.

5.2. Application to Binary Distributions

Equation (5.29) is valid for any mass distribution for which $\omega = \sin\{\pi(l-k)/2l\}$ is a special frequency. We now investigate its predictions for binary cases and compare with numerical results. We shall show that a large proliferation of structure takes place: even when the Schmidt function is close to making one step per period, the IDS will make several steps.

We first take the infinite-mass case, $M = \infty$. Then it is easily seen that $V(\pi/l + 0) = r_a$, $V(\pi/l - 0) = 0$, with r_a given below (5.16). Combining this with the general equations (5.20) and (3.7), one derives $P_{4,k} = 1 - r_a$ and c_k in (5.21) follows by putting $\zeta = \Omega = 0$, due to the fact that $\alpha = \infty$. Inserting this into (5.28), one finds $I_n(\varepsilon) = (1-p)\,p^{a-1}$. Then, performing the sum (5.8), again using (3.7), one arrives at

$$H(\omega_s^2) - H(\omega^2) = \frac{(1-p)^2\ p^{l+a-1}}{1-p^l}\ p^{l[\pi/l^2\varepsilon - a/l]}, \qquad M = \infty \qquad (5.30)$$

Here it was also used that $v(\delta) = \delta = \pi/l - a\varepsilon$ for $M = \infty$. So it can be seen that $H(\omega^2)$ makes one step per period in this limit. A more direct computation of (5.30) is given in the Appendix.

Next we take M finite and p small and employ the iteration method of previous sections to obtain the coefficients of the Schmidt function. At $p = 0$ the solution for V_s is still given by (4.21). In a first approximation we substitute this result into all terms with $j \neq a$ of the right-hand side of (2.22). One can get by iteration

$$V_s(\varphi) = \sum_{\substack{j=1 \\ j \neq a}}^{l}\ \sum_{n=0}^{\infty} r_j r_a^n \theta(R_{j\beta_s} R_{a\beta_s}^n(\varphi) - \psi_+(\beta_s)) \qquad (5.31)$$

and moreover one has

$$\frac{\sin \frac{1}{2}\{R^n_{\alpha\beta}(\varphi)-\psi_+(\alpha\beta)\}}{\sin \frac{1}{2}\{R^n_{\alpha\beta}(\varphi)-\psi_-(\alpha\beta)\}}=\alpha^n\frac{\sin \frac{1}{2}\{\varphi-\psi_+(\alpha\beta)\}}{\sin \frac{1}{2}\{\varphi-\psi_-(\alpha\beta)\}} \tag{5.32}$$

where $\psi_\pm(\delta)=\delta\pm v(\delta)$, with v defined in (2.24). Performing the sum (5.31), we obtain

$$V_s(\varphi)=\sum_{\substack{j=1\\ j\neq a}}^{l} r_j r_a(1-r_a)^{-1}\, r_a^{[{}^\alpha\log\{S(\psi_j)/S(\varphi)\}]} \tag{5.33a}$$

where

$$S(\varphi)=2\sin v(\alpha\beta_s)\sin\tfrac{1}{2}\{\varphi-\psi_+(\alpha\beta_s)\}/\sin\tfrac{1}{2}\{\varphi-\psi_-(\alpha\beta_s)\} \tag{5.33b}$$

behaves as $S(\psi_+(\alpha\beta)+\theta)\simeq\theta$ for $\theta\to 0$. Also,

$$\psi_j\equiv R^{-1}_{j\beta}(\psi_+(\beta_s))=\psi_+(\beta_s)+2(j-1)\beta_s \tag{5.33c}$$

Using (3.7), we derive from (5.33), by comparison with (5.20) and (5.21),

$$c_k=-(\ln r_a+2\pi ik)^{-1}\,\Gamma(1+\zeta-ik\Omega)\sum_{\substack{j=1\\ j\neq a}}^{l} r_j(r_a\, e^{2\pi ik})^{{}^\alpha\log S(\psi_j)} \tag{5.34}$$

This has to be inserted in Eq. (5.28) in order to obtain $I_n(\varepsilon)$. Writing

$$\Gamma(1+\zeta-ik\Omega)=\ln\alpha\int_{-\infty}^{\infty}\exp(-\alpha^{-y})\,\alpha^{-y}(r_a\, e^{2\pi ik})^y\, dy \tag{5.35}$$

and making the shift $y\to y-{}^\alpha\log(\sigma_n S/2l\varepsilon)$, we can first perform the sum using (3.7) and then the integral. The result becomes

$$\begin{aligned} I_n(\varepsilon)=&(1-p^l)\prod_{m=1}^{\infty}\{(1-p^l)(1-p^l\exp(\alpha^{-m}\sigma_n))^{-1}\}\\ &\times\sum_{\substack{j=1\\ j\neq a}}^{l}\sum_{i=-\infty}^{\infty} r_j r_a^i(p^l e^{2\pi in})^{\alpha^{-i}S(\psi_j)/2l\varepsilon} \end{aligned} \tag{5.36}$$

Finally, this result has to be inserted into Eq. (5.8) for $H(\omega^2)$. We first set the infinite product equal to unity, which is its value for $M=\infty$. We then find a result, which may be written in the form (5.29), with Q replaced by Q_0, where

$$Q_0(x, y) = p^{l+1-a-lx}(1-p^l) \sum_{\substack{j,j'=1 \\ j,j' \neq a}}^{l} \sum_{m,m'=-\infty}^{\infty} r_j r_{j'} r_a^{m+m'-2y} \times p^{l[x+\alpha^{y-m} S(\psi_j) + \alpha^{y-m'} S(\psi_{j'})]} \tag{5.37}$$

It is clear that $Q_0(x, y)$ is separately periodic in its two variables. In the examples we consider, we will again take p small. Then, to leading order, only the values $1 \leqslant j,\ j' \leqslant a-1$ are relevant. In particular, when $a=2$, $j=j'=1$. It was already discussed in the closely related situation at $M=M_c$ (see Section 4.2) that $V_s(\varphi)$ is then close to making one step per period, implying again that only $S(\psi_1)$ should matter. Nevertheless, the infinite sum (5.36) over m and m' causes more structure in Q_0. We now argue that in the case $a=2$ this sum is often dominated by three terms. We shall present data for cases where $\alpha^y S(\psi_1)$ is of order unity, whereas α^{-1} ranges between 2×10^{-2} and 10^{-1}. Therefore, negative values of m and m' will give very small contributions, and because $p^l \ll r_a$, also terms where $m=0$ or $m'=0$ are small. The next terms are $(m, m')=(1, 1)$; $(1, 2)$ or $(2, 1)$; $(2, 2)$. These three terms are the dominant ones; the others have too many factors r_a. We conclude that, for such cases with $a=2$, *the leading step in the Schmidt function causes three leading steps in the IDS.* In Figs. 5 and 6 we present plots of $\ln[H(\omega_s^2) - H(\omega^2)]/\ln p^l$ versus $v(\delta)/l\varepsilon$ in two typical examples. We have tested the agreement with Eqs. (5.29) and (5.30). It is satisfactory, although the values of ε that we have used are not much

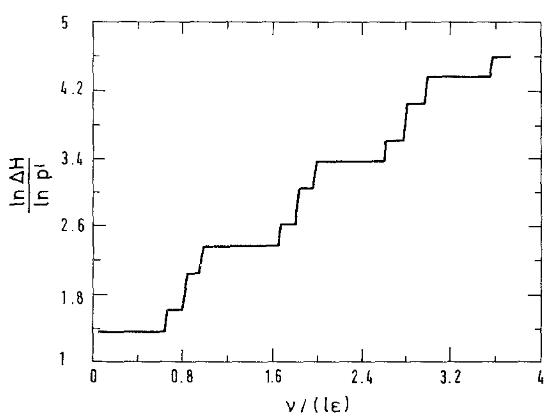

Fig. 5. Plot of $\ln \Delta H/\ln p^l$ (where ΔH is the IDS difference) versus the variable $v/l\varepsilon$, for $\omega^2 \uparrow \omega_s^2$, and $k=1$, $l=3$ $(a=2)$, $M=3$ $(M_c=2)$, $p=0.1$.

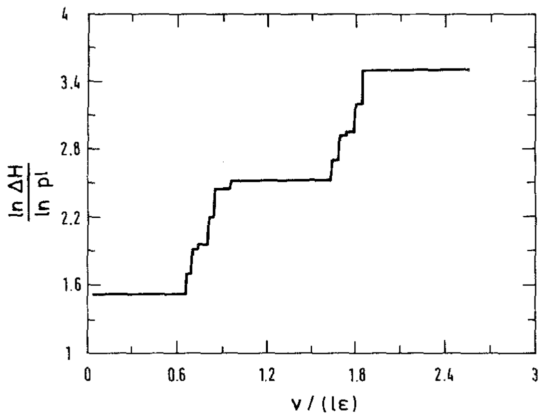

Fig. 6. Same as Fig. 5, for $k=1$, $l=4$ $(a=3)$, $M=3$ $(M_c=2)$, $p=0.1$.

smaller than unity. It has been checked that the influence of the infinite product in (5.36) on $H(\omega^2)$ is negligible, mainly because $\alpha^{-1} \ll 1$ and $p \ll 1$. Hence, we shall omit it.

6. DISCUSSION

We have introduced a powerful method to describe the periodic amplitudes of the Lifshitz (exponential) singularities in the integrated density of states (IDS) of harmonic chains with random masses. These singularities occur near the high-frequency band edge and near "special frequencies." The latter exist if the mass gap between the lightest particle (mass $m_- \equiv 1$) and the one-but-lightest particle (mass M) is large enough. It occurs first when $M=2$. The special frequencies are denumerable and accumulate at the band edge.

Special frequencies have the property that they are not an eigenfrequency of any chain of the ensemble.[13,14] This point is responsible for the very small probability (essential singularity) of finding an eigenfrequency close to a special frequency. In Refs. 5 and 6 it is explained that such eigenfrequencies are related to eigenfunctions that "live" on islands that are large repetitions of a certain unit group of light and heavy masses. In the present paper we employ this notion and solve the eigenfrequencies of the islands given the boundary conditions on the left and right ends. Since these boundary conditions are determined by the semi-infinite parts of the chain to the left and to the right of the island, their distribution is expressed in terms of the distribution function of Dyson and Schmidt. The latter function is a Cantor function *at* the special frequency. It is shown that its scaling behavior near relevant points determines the IDS for frequencies close to the special frequency.

We have also applied our general results to binary mass distributions. We introduce a method for explaining the detailed structure of the IDS near special frequencies for small concentrations p of the light masses. The main point is that when $p \ll 1$, the semi-infinite side parts of the central island are dominated by heavy masses. Corrections due to insertion of one, two, three, etc., light masses can successively be calculated in a small-p expansion. It is then found that this method predicts "steps" in $H(\omega^2)$, which become the smaller, the more times the iteration is pursued. Numerical calculations with reasonable but not extremely high resolution confirm this behavior.

The occurrence of "steps" in $H(\omega^2)$ for small p is not unexpected. In a previous paper[3] we extended an argument of Halperin[15] concerning the behavior of $H(\omega^2)$ near the eigenmodes of a small island containing light (and possibly also heavy) masses, emerging from a sea of only heavy masses. The result of Ref. 3 reads

$$H(\omega_0^2 \pm \varepsilon) - H(\omega_0^2) = \varepsilon^{2\alpha} R_{\pm}(\ln \varepsilon / \ln \mu), \qquad \varepsilon \downarrow 0 \tag{6.1}$$

where $R_{\pm}$ are two periodic functions with unit periods. The exponent $\alpha = \ln(1-p)/\ln|u_0|$ and the scale $\mu = u_0^{-2}$ are determined by

$$u_0 = \tfrac{1}{2}M\omega^2 - 1 + (\tfrac{1}{4}M^2\omega^4 - M\omega^2)^{1/2} \tag{6.2}$$

For small p, $\alpha \simeq -p/\ln |u_0|$ goes to zero, so that the structures in $H(\omega^2)$ look like "steps." Our approach of the excitations in the neighborhood of special frequencies also rests on the picture of a central island containing several light (and possibly also heavy) masses in the middle of a sea of heavy masses. This implies that all structure present in $H(\omega^2)$ will satisfy the scaling behavior (6.1). But when p is small and the resolution is not extremely high, it looks very much like a function making steps.

It was already discussed in Refs. 5 and 6 that four different cases have to be distinguished:

(i) Behavior near the band edge ($\omega \uparrow \omega_{\max}$) (Section 3). This is the case originally considered by Lifshitz. The central island consists of light masses only. Our final result for several mass distributions is given by Eqs. (3.8), (3.14), and (3.12). In binary cases this has been worked out to give (3.21).

(ii) To the right of a special frequency (Section 4.1). The central island is a repetition of units of one heavy and $l-1$ light masses (HL^{l-1}).

The result for general cases is given by (4.14), (4.19), and (4.18). Its application to binary distributions is given in (4.26).

(iii) To the left of a special frequency at critical mass ratio. The central island is a sequence of units HL^{a-1}, where a $(1 \leqslant a \leqslant l-1)$ is defined by $(l-k)a = 1$ (mod l), Our general result is given by (4.30), (4.33). The application to binary situations is discussed afterward. An application is given in (4.37).

(iv) To the left of a special frequency at general mass ratio (Section 5.1). The central island consists of light particles only. This is the most complicated case. The general result follows from (5.8), (5.28), (5.21), and (5.20). Application to binary distributions is discussed in Section 5.2; see Eqs. (5.29) and (5.37) for specific results.

The first three cases are very similar. One has a decay like $\Delta H(\omega^2) \sim \exp(-\mathrm{const} \cdot |\Delta\omega^2|^{-1/2})$, with a periodic prefactor. In case (iv) the behavior is $\Delta H \sim \exp(-\mathrm{const} \cdot |\Delta\omega^2|^{-1})$, multiplied by a power and a more complicated amplitude; see (5.29).

In cases (ii) and (iii) we had to restrict ourselves to the limit $p \ll 1$. It would be interesting to extend our results to general values of p. One might wonder whether the prefactor of the leading exponential decay still involves a periodic function of one variable, such as in Eqs. (4.14) and (4.30), or that it becomes more complicated, for instance, as in Eq. (5.29).

Another point of interest is to extend the present method to derive the Lifshitz singularities in the wavenumber-dependent spectral density, starting from the equations of Halperin.[15] We discuss this topic in Ref. 10, starting from a different approach.

APPENDIX. $H(\omega^2)$ IN THE LIMIT $M \to \infty$

When $M = \infty$ the infinite masses break up the chain into independent segments. This was noted first by Domb *et al.*[9] Say that there are infinitely heavy masses at sites 0 and n. Then the eigenmodes have the form $a_k = \mathrm{sn}\, k\beta$, with $\beta = \pi(n-m)/n$, with $1 \leqslant m \leqslant n-1$. The eigenfrequency is $\omega = 2\sin(\frac{1}{2}\beta)$. The probability for this succession to occur is $(1-p)^2 p^{n-1}$. Hence the IDS is

$$H(\omega^2) = (1-p) + \sum_{n=1}^{\infty} \sum_{m=1}^{n-1} (1-p)^2 p^{n-1} \theta(\beta - \pi + \pi m/n) \qquad \text{(A1)}$$

The first term represents the contribution of the $\omega = 0$ mode of the infinitely heavy masses. It can be checked that (A1) is normalized to unity.

First we calculate $H(\omega_s^2)$, where $\omega_s \equiv 2\sin(\frac{1}{2}\beta_s)$, $\beta_s \equiv (l-k)\pi/l$, with k

and l integer and mutual prime. Note that all eigenfrequencies mentioned above occur with finite probability $(1-p)^2 p^{n-1}/(1-p^n)$, where the denominator accounts for the fact that islands $HL^{n-1}H$, $HL^{2n-1}H$, $HL^{3n-1}H$, etc., all give a same frequency. Therefore one has to be more exact in what is meant by $H(\omega_s^2)$. We shall calculate

$$H(\omega_s^2-0)=1-\sum_{n=2}^{\infty}\sum_{m=1}^{n-1}(1-p)^2\ p^{n-1}\,\theta\left(\frac{k}{l}-\frac{m}{n}+0\right) \tag{A2}$$

We define $b(n)$, $1\leqslant b(n)\leqslant l-1$, by

$$nk/l=[nk/l]+b(n)/l \tag{A3}$$

It follows that

$$H(\omega_s^2-0)=1-(1-p)^2\sum_{n=2}^{\infty}[nk/l]\,p^{n-1} \tag{A4}$$

The same result is valid at the special frequency when M is finite but larger than some critical value M_c. Next we set $\beta=\beta_s-\varepsilon$ and calculate

$$H(\omega_s^2-0)-H(\omega^2)=\sum_{n=2}^{\infty}\sum_{m=1}^{n-1}(1-p)^2\,p^{n-1}\,I_{nm} \tag{A5}$$

with $I_{nm}=1$ if $k/l<m/n<k/l+\varepsilon/\pi$ and zero otherwise. Performing the sum over m, we have

$$H(\omega_s^2-0)-H(\omega^2)=\sum_{n=1}^{\infty}(1-p)^2p^{n-1}\left\{\left[\frac{n\varepsilon}{\pi}+\frac{nk}{l}\right]-\left[\frac{nk}{l}\right]\right\} \tag{A6}$$

The term with $n=1$ could be added because it vanishes anyhow. Decomposing

$$n=n_1l+n_2,\qquad 1\leqslant n_2\leqslant l-1;\quad 0\leqslant n_1<\infty \tag{A7}$$

we find, using (A3),

$$\begin{aligned}\left[\frac{n\varepsilon}{\pi}+\frac{nk}{l}\right]-\left[\frac{nk}{l}\right]&=\left[\frac{n\varepsilon}{l}+\frac{n_2k}{l}\right]-\left[\frac{n_2k}{l}\right]\\&=\left[\frac{n\varepsilon}{\pi}+\frac{b(n_2)}{l}\right]-\left[\frac{b(n_2)}{l}\right]\\&=\left[\frac{n\varepsilon}{\pi}+\frac{b(n_2)}{l}\right]\end{aligned} \tag{A8}$$

This does not vanish if $n > \pi\{l-b(n_2)\}/l\varepsilon$. In the leading-order terms the degeneracy factor (A8) equals unity:

$$H(\omega_s^2-0)-H(\omega^2)$$

$$\simeq \sum_{n_2=1}^{l-1} \sum_{n_1=1+[\pi\{l-b(n_2)\}/l^2\varepsilon-n_2/l]}^{\infty} (1-p)^2 p^{n_1 l+n_2-1}$$

$$=\frac{1-p}{1-p^l} p^{n_2+l-1} \sum_{n_2=1}^{l-1} p^{l[\pi\{l-b(n_2)\}/l^2\varepsilon-n_2/l]} \tag{A9}$$

By far the largest contribution comes when $b(n_2)=l-1$, which happens when $n_2=a$, with a defined by $(l-k)a=1 \pmod{l}$:

$$H(\omega_s^2-0)-H(\omega^2)=(1-p^l)^{-1}(1-p)\,p^{l+a-1}p^{l[\pi/l^2\varepsilon-a/l]} \tag{A10}$$

Finally, we recall that H is discontinuous at ω_s^2:

$$H(\omega_s^2+0)-H(\omega_s^2-0)=(1-p)^2p^{l-1}/(1-p^l) \tag{A11}$$

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