# **Special Frequencies and Lifshitz Singularities** in Binary Random Harmonic Chains

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We consider a one-dimensional chain of coupled harmonic oscillators; the mass of each atom is a random variable taking only two values (M or 1). We investigate the integrated density of states  $H(\omega^2)$  near special frequencies: a given frequency  $\omega_s$  with rational wavelength becomes "special" if the mass ratio M exceeds a certain critical value  $M_c$ . We show that H has essential singularities of the types  $H_{sg} \sim \exp(-C_1 |\omega^2 - \omega_s^2|^{-1/2})$  or  $\exp(-C_2 |\omega^2 - \omega_s^2|^{-1})$ , according to the value of M and the sign of  $(\omega^2 - \omega_s^2)$ . The Lifshitz singularity at the band edge is analyzed in the same way. In each case, the constant  $C_1$  or  $C_2$  is evaluated explicitly and compared with a vast amount of numerical work. All these exponential singularities are modulated by periodic amplitudes. The properties of the eigenfunctions with frequencies close to the special values are also discussed, and are illustrated by numerical data.

**KEY WORDS:** Density of states; random harmonic chains; one-dimensional systems; special frequencies; Lifshitz singularities.

# 1. INTRODUCTION

The behavior of random one-dimensional harmonic chains has been studied intensively since the work of Dyson<sup>(14)</sup> (see the review by Lieb and Mattis<sup>(15)</sup>). An important contribution was also made by Dean,<sup>(16)</sup> who

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performed a numerical calculation of the spectral density of binary harmonic chains. He found two outstanding features: the spectral density has "high values" at frequencies connected to islands of light particles embedded in a sea of heavy ones, whereas it "vanishes" at certain "special frequencies."

The first feature was recently studied by Nieuwenhuizen and Luck,<sup>(11)</sup> extending an argument of Halperin.<sup>(17)</sup> The outcome is that the "high values" are actually infinitely high, since the integrated spectral density is only Hölder-continuous, with an exponent  $2\alpha$  less than unity. The values of frequency where this happens form a dense set in a high-frequency interval when the mass ratio M and the fraction of light masses p obey a certain inequality. The power-law behavior of the integrated spectral density  $H(\omega^2)$  is multiplied by a periodic amplitude. Starting from the Dyson–Schmidt<sup>(2,14)</sup> integral equation for the invariant function  $Z(u; \omega^2)$  and from an identity relating  $H(\omega_1^2) - H(\omega_2^2)$  to the Z functions at  $\omega_1^2$  and  $\omega_2^2$ , both the power law of  $H(\omega^2)$  and the periodic function were related to a similar behavior of the function  $Z(u, \omega^2)$ . In the present paper, we study analogous behavior in  $H(\omega^2)$  near the band edge and special frequencies.

The occurrence of periodic functions, multiplying power-law or exponential singularities, is quite general in one-dimensional disordered systems with discrete distributions of the random variables. Examples are diffusion in a random medium<sup>(23)</sup> and the random field Ising model.<sup>(24)</sup> An even simpler was discussed by de Calan *et al.*,<sup>(25)</sup> namely the study of the random variable,  $z = 1 + x_1 + x_1 x_2 + x_1 x_2 x_3 + \cdots$ , given the identically independently distributed  $x_i$ . Also, the essential singularities of  $H(\omega^2)$  at special frequencies, including the well-known Lifshitz singularity at the band edge, have periodic amplitudes.

Periodic functions also occur in approximate real-space renormalization group treatments of higher dimensional models, or, equivalently, on hierarchical lattices (see, for instance, Derrida *et al.*<sup>(27)</sup>). The study of these periodic functions is known to be a difficult mathematical problem.<sup>(28)</sup>

The existence of *special frequencies*, where the integrated spectral density has an exponential singularity, was explained by Matsuda<sup>(5)</sup> and Hori<sup>(6)</sup>: a given frequency with rational wavelength becomes "special" if the mass ratio M of heavy and light particles exceeds a critical value  $M_c$ , depending on the value of the frequency. This happens for the first time for M = 2. Then an infinity of special frequencies exist, which accumulate at the high-frequency band edge. For M = 3 a new set of special frequencies arises. If the mass ratio becomes infinite, all frequencies with rational wavelength are special. The integrated spectral density at those frequencies was derived by Domb *et al.*<sup>(18)</sup>

The nature of special frequencies is such that in no chain of the ensem-

ble can an eigenfrequency cross the special frequency if one varies, for instance, the value of M. Hence, the value of  $H(\omega^2)$  at the special frequency  $\omega_s$  calculated for  $M = \infty$  holds for all  $M \ge M_c$ . The subject of the present paper, namely the behavior of the integrated spectral density  $H(\omega^2)$  in the neighborhood of  $\omega_s^2$ , has been a challenging problem for quite a while.

In passing, we note that the band edge  $\omega_{\text{max}}$  is also a special frequency. Lifshitz<sup>(10)</sup> gave a simple physical explanation for the existence of an exponential singularity in  $H(\omega_{\text{max}}^2) - H(\omega^2) = 1 - H(\omega^2)$ . Van Hemmen<sup>(26)</sup> analyzed this behavior in the  $M = \infty$  case. He also noted a similar behavior around  $\omega = 0$ ; in fact, for  $M = \infty$  all "rational" frequencies exhibit a singular behavior. We recall the argument of Lifshitz in Section 4.1 (it is the simplest case of a special frequency). For a recent review of this and related points, see Simon.<sup>(19)</sup>

The authors of Ref. 11 also reported on the Lifshitz singularity. For  $\omega_s^2 = \omega_{\max}^2$  they found the behavior

$$1 - H(\omega^2) \approx \exp(-cx |\ln p|) P(x/\mu) \qquad (x \to \infty)$$
(1.1)

where c is a constant depending on the mass ratio, p is the probability for the occurrence of light masses,

$$x = |\omega_s^2 - \omega^2|^{-1/2} \tag{1.2}$$

P is a periodic function with unit period, and the scale  $\mu$  satisfies  $c\mu = 1$ .

We shall show that a very analogous behavior to (1.1) is present to the right and the left of special frequencies inside the spectrum. The main difference is that the probability p has to be replaced by the probability of occurrence of the relevant successions of one heavy and a certain number of light masses. A first attempt to do so was made by Ventevogel<sup>(13)</sup> in the case  $\omega^2 < \omega_z^2$ .

The case  $\omega^2 < \omega_s^2$ ,  $M > M_c$  turns out to be most interesting. Equation (1.1) remains valid (see Section 4.4), but now p has to be replaced by p', and

$$x = (\omega_s^2 - \omega^2)^{-1}$$
(1.3)

The factor c is again evaluated (Section 4.4). Also here a periodic amplitude is observed numerically. The same holds for the critical case  $(M = M_c; \omega^2 < \omega_s^2)$  (Section 4.3). There the exponent of x is again equal to -1/2, as in Eq. (1.2).

The exponents -1/2 and -1 in Eqs. (1.2) and (1.3) were already reported in a note by Englisch,<sup>(22)</sup> but no values for the constants c were

given. For a related model, a numerical calculation was performed by Gubernatis and Taylor.<sup>(12)</sup> These authors, however, fitted both sides of the special frequency by a behavior of the form (1.1)–(1.2). Our claim is that this is only correct at one side.

Binary mass distributions therefore generate a quite complicated behavior of  $H(\omega^2)$ . For smoother distributions, such singularities do not occur, apart from the Lifshitz singularity at the band edge.<sup>(29)</sup> This was indeed found to be the case for the exactly soluble models with exponential and gamma distributions.<sup>(20)</sup>

Regardless of whether or not the integrated density of states has a great deal of structure, thermodynamic quantities, such as the specific heat, are smooth functions of temperature.<sup>(26)</sup> A computation of the derivative of this quantity with respect to temperature was reported in Ref. 21, using a finite number of terms of the low-frequency expansion for the integrated density of states and the inverse localization length. For all models considered in Ref. 21, dC/dT is a smooth function; only its global shape depends on the mass distribution.

The setup of the paper is as follows. In Section 2, we give some general definitions and sketch the derivation of the Dyson-Schmidt integral equation. In Section 3, we discuss the phenomenon of special frequencies and investigate properties of the function  $Z(u; \omega^2)$ , which is a Cantor function at these frequencies. In Section 4, we present arguments that yield the exponents of Eq. (1.1) in the different cases  $\omega^2 \uparrow 4$  (Section 4.1),  $\omega^2 \downarrow \omega_s^2$  (Section 4.2),  $\omega^2 \uparrow \omega_s^2$ ,  $M = M_c$  (Section 4.3), and  $\omega^2 \uparrow \omega_s^2$ ,  $M > M_c$  (Section 4.4). The predictions are compared with a vast amount of numerical data, and the properties of eigenfunctions are analyzed in detail.

# 2. BASIC DEFINITIONS. THE SCHMIDT FUNCTION

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

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

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

$$\mathbf{A}_{n} = \begin{pmatrix} 2 - m_{n}\omega^{2} & -1\\ 1 & 0 \end{pmatrix} \mathbf{A}_{n-1} \equiv T_{m_{n}}\mathbf{A}_{n-1}$$
(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 transfer matrix. 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  $\beta$  (wave number) through

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

Then the matrices

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

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

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

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

where  $Q_{\beta}$  is given by

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

The angle  $\gamma$  is defined by

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

One easily verifies the relation

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

The basic variables in Eqs. (2.5)–(2.6) are  $\beta$  and  $\gamma$ , rather than M and  $\omega^2$ . Various other models, such as tight-binding models,<sup>(1)</sup> random alloy models,<sup>(2,3)</sup> and systems equivalent to harmonic chains with negative random masses,<sup>(4)</sup> can be mapped onto the same set of transfer matrices. In all these models, special frequencies may appear for binary distributions of the appropriate random variables.

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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  $\varphi_n$  by

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

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

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

$$= R_{\beta}(\varphi_n) \pmod{2\pi} \qquad \text{if} \quad m_n = M \tag{2.9b}$$

where

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

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, such as in (2.5c). Although this notation is not fully correct, we denote the Möbius transform attached to  $Q^N$  by  $R^N$ . We also note that prefactors in Q matrices, such as  $(\cos \gamma)^{-1}$  in Eq. (2.5c), drop out from the definition of the Möbius transform R. In particular, matrices (+Q) and (-Q) correspond to the same Möbius transform. In the following, we shall tacitly forget about the sign of Q matrices, and often write  $\pm Q$  instead of Q.

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

$$\varphi_0 = 2\beta; \qquad \varphi_{N+1} = 0 \tag{2.11}$$

In order to study the integrated spectral density, we now briefly derive the integral equation of Dyson<sup>(14)</sup> and Schmidt.<sup>(2)</sup> 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

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

satisfies

$$Z_n(u) = pZ_{n-1}(2 - \omega^2 - 1/u) + qZ_{n-1}(2 - M\omega^2 - 1/u) - \theta(-u) + Z_n(0)$$
(2.14)

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where  $\theta$  is the Heaviside step function, defined by  $\theta(x) = 1$  for x > 0 and 0 for  $x \le 0$ . The integrated density of states  $H(\omega^2)$  can be related to Z(u) at given  $\omega^2$ : for a large but finite chain,  $H(\omega^2)$  is approximately equal to the number of changes of sign in the sequence  $a_n$   $(1 \le n \le N)$ , divided by N. 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)

$$H(\omega^2) = \operatorname{Prob}\{Y < 0\} = Z(0)$$
(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  $n \to \infty$ 

$$Z(u) = pZ(2 - \omega^2 - 1/u) + qZ(2 - M\omega^2 - 1/u) - \theta(-u) + H(\omega^2)$$
(2.16)

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

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

$$V(\phi) = pV(\phi - 2\beta) + qV(R_{\beta}(\phi)) - I(0 < \phi < 2\beta) + H(\omega^{2})$$
 (2.19)

Here *I* is the characteristic function of an interval:

$$I(\varphi_0 < \varphi < \varphi_1) = 1, \qquad \varphi_0 < \varphi \pmod{2\pi} < \varphi_1$$
$$= 0, \qquad \text{elsewhere} \qquad (2.20)$$

# 3. AT A SPECIAL FREQUENCY

In this section, we briefly review the argument of Matsuda<sup>(5)</sup> and Hori<sup>(6)</sup> explaining the existence of special frequencies. We also consider some aspects of the function Z(u), which is the distribution function of a Cantor set for these frequencies.

Let us recall an old conjecture of Saxon and Hutner,<sup>(7)</sup> which was proven by Luttinger.<sup>(8)</sup> Suppose that one has pure crystals of A-type atoms, B-type atoms,.... Then the forbidden frequencies that are common to pure A, B,... crystals are also forbidden in an arbitrary substitutional alloy consisting of A, B,..., and if there is a gap near a frequency forbidden to A, B,..., then also the composite lattice has a gap near that frequency. This argument also holds for ordered lattices formed by infinite repetitions of constituent parts of a (not necessarily disordered) composite lattice. This theorem was applied to special frequencies in the random mass chain by Hori<sup>(5)</sup> and Matsuda<sup>(6)</sup>; we now follow their argument; see Eq. (8.9).

In our random lattice, the constituent parts may be chosen to be the subsequences of one heavy and an arbitrary number of light masses, to be denoted by  $HL^{a-1}$  ( $a=1, 2,..., \infty$ ). For a given value of a, the periodic chain  $(HL^{a-1})^{\infty}$  has a finite number of gaps, corresponding to values of  $\omega$  such that the Möbius transform  $R_{a\beta}$  is hyperbolic. This follows from (2.7) and our convention that  $R_{a\beta}$  is the Möbius transform associated with  $Q_{a\beta}$ . The reason is that, if n is lowered, the phase  $\varphi_n$  starts from  $\varphi_{N+1} = 0$  [see (2.11)] and moves toward the attracting fixed point of  $R_{a\beta}$ . Then it cannot satisfy the second boundary condition  $\varphi_0 = 2\beta$ , implying that the present frequency is not an eigenfrequency of the chain.

This already implies that any inhomogeneous chain that would not have more than L successive light masses would have gaps near special frequencies. The width of these gaps vanishes as  $L \to \infty$ , and hence the random chain under consideration has no (finite) gap in its spectrum. The essential singularities of  $H(\omega^2)$  at special frequencies can therefore be viewed, in a heuristic way, as infinitesimal versions of Saxon and Hutner's gaps.

Throughout the following, a Möbius transformation with real coefficients is called hyperbolic if it has two distinct real fixed points, parabolic if it has one single real fixed point (with a derivative  $\pm 1$ ), and elliptic if its two fixed points are complex conjugate. It turns out that the matrices  $R_{\alpha\beta}$ (a = 1, 2,...) can only be hyperbolic or parabolic if  $\beta/\pi$  is rational:

$$\beta = \pi (l - k)/l \tag{3.1}$$

with *l* and *k* integer  $(1 \le k \le l-1)$ , and mutual prime. In this situation, a sequence of *l* light particles leaves the phase invariant (mod  $2\pi$ ) and  $R_{(a+l)\beta} = R_{a\beta}$ . Thus, we only need to satisfy the condition

$$\left|\frac{\cos(\gamma + a\beta)}{\cos\gamma}\right| \ge 1, \qquad a = 1, ..., l \tag{3.2}$$

Let us define for future use the integers a(n) by

$$n = a(n)(l-k) \pmod{l}, \qquad 1 \le n \le l; \quad 1 \le a(n) \le l \tag{3.3}$$

which exist in virtue of Bezout's identity for mutual primes, and also

$$\lambda = \pi/l \tag{3.4}$$

One has a(l) = l, a(l-k) = 1, and for k = 1, a(n) = l - n. Equation (3.2) is always satisfied for a = l. For a = 1, ..., l - 1 it is satisfied provided it is satisfied for a(1). This requires in the present situation

$$\cos(\gamma + \lambda) \leqslant -\cos\gamma \tag{3.5}$$

or

$$\gamma \geqslant \gamma_c \equiv \frac{1}{2}\pi (1 - 1/l) \tag{3.6}$$

From (2.6) follows the equivalent condition that, at given k and l, the mass ratio exceeds the critical value  $M_c$ :

$$M \ge M_e = 1 + \tan(k\pi/2l) \operatorname{cotan}(\pi/2l) \tag{3.7}$$

A frequency  $\omega$  is called a *special frequency*  $\omega_s$  if both (3.1) and (3.6)–(3.7) are satisfied. In order to show that for no chain in the ensemble can this frequency be an eigenfrequency, Matsuda<sup>(5)</sup> and Hori<sup>(6)</sup> considered the location of the fixed points of the transformations  $R_{n\lambda}$  (n = 1,..., l). They are given by

$$\psi^{\pm}(\delta) = \delta \pm v(\delta), \qquad \delta = \lambda, ..., n\lambda$$
 (3.8)

where  $v(\delta)$  is defined by

$$\cos v(\delta) = \sin(\gamma + \delta) / \sin \gamma, \qquad 0 \le v(\delta) \le \pi \tag{3.9}$$

It satisfies  $0 \le v(\delta) \le \delta$  when  $\pi - 2\gamma \le \delta \le \pi$ . Note that for n = l there is only one fixed point  $\psi^{\pm}(\pi) = 0$ , because  $R_{l\lambda}$  is parabolic. Since  $d\psi^{-}(\delta)/d\delta < 0$ , the *attracting* fixed points  $\psi^{-}(n\lambda)$  lie in the segment  $S = [0; \psi^{-}(\lambda)]$ . We call S the *sink interval*. It has no overlap with the region  $[\psi^{+}(\lambda); 2\pi]$ , where the *repelling* fixed points  $\psi^{+}(n\lambda)$  are located. Figure 1 illustrates the discussion.

The transformation  $R_{l\lambda} = R_0$  always attracts the phase in the clockwise direction; also, the other  $R_{n\lambda}$  keep the phase in S if it was there initially. Hence, the phase, starting from  $\varphi_{N+1} = 0$ , will remain trapped in the sink interval S. Therefore, the boundary condition on the left end of the chain,  $\varphi_0 = 2\beta$ , cannot be satisfied for any sequences  $\{R_{\lambda n_1}, ..., R_{\lambda n_N}\}$ . Hence, for no chain in the ensemble (having a heavy mass at one of the ends) is the frequency under consideration an eigenfrequency. This is the theorem of Hori and Matsuda.



Fig. 1. Schematic picture of the fixed points of the transformations  $HL^{a-1}$  at a special frequency. (•) Attracting fixed points:  $\psi^{-}(n\pi/l)$  for n = 1, ..., l. ( $\bigcirc$ ) Repelling fixed points:  $\psi^{+}(n\pi/l)$  for n = 1, ..., l. For n = l, the points coincide  $[\psi^{\pm}(\pi) = 0]$ .

All these aspects are closely connected to the behavior of the Schmidt function at the special frequency. Iterating Eq. (2.19) l-1 times and using  $2l\beta = 0 \pmod{2\pi}$ , we find

$$V_{s}(\varphi) = \sum_{a=1}^{l} r_{a} V_{s}(R_{a\beta}(\varphi)) + q^{-1} H(\omega_{s}^{2})$$
$$- q^{-1} \sum_{a=1}^{l} r_{a} I(-2\beta < \varphi - 2a\beta < 0)$$
(3.10)

where

$$r_a = qp^{a-1}/(1-p^l), \qquad a = 1,...,l$$
 (3.11)

and the subscript s reminds us that we are at a special frequency.

The solution of this equation is a devil's staircase: assuming  $V_s(\varphi) = V_s(0^+)$  for  $0 < \varphi < \psi^+(\lambda)$ , one finds that this assumption is consistent with (3.10). Using this knowledge, one finds that  $V_s(\varphi)$  is constant at the preimage  $R_{2\lambda}^{-1}\{[0, \psi^+(\lambda)]\}$ , and so on. For a typical situation, a plot of  $V_s(\varphi)$  at a special frequency is presented in Fig. 2.

We can calculate  $H(\omega_s^2)$  from (3.10); choosing, for instance,  $\varphi = 0^+$ ,

$$H(\omega_s^2) = \sum_{n=1}^{l-k} r_{a(n)}$$
(3.12)

For k = 1, this becomes simpler:

$$H(\omega_s^2) = (1 - p^{l-1})/(1 - p^l)$$
(3.13)



Fig. 2. Schmidt function  $V_s(\phi)$  versus against  $\phi/2\pi \in [0; 1]$  at the special frequency  $\omega_s^2 = 3$ . Here l = 3, k = 1; p = 0.4, M = 2.5.

This result was first derived by Borland.<sup>(9)</sup> An expression equivalent to (3.12) is

$$H(\omega_s^2) = 1 - q^2 \sum_{j=1}^{\infty} p^{j-1} [jk/l]$$
(3.14)

where [x] denotes the integer part of x.

In the following, we shall need the behavior of  $V_s$  for  $\varphi$  close to  $\varphi = 2\pi$ and  $\varphi = \psi^+(\lambda)$ . For  $R_{(l-1)\lambda}^{-1}(0) < \varphi < 2\pi$ , Eq. (3.10) reduces to

$$1 - V_s(\varphi) = r_l \{ 1 - V_s(R_0(\varphi)) \}$$
(3.15)

where the parabolic transformation R acts as a translation on the variable  $\cot(\frac{1}{2}\varphi)$ :

$$\operatorname{cotan}\left[\frac{1}{2}R_0(\varphi)\right] = \operatorname{cotan}\left(\frac{1}{2}\varphi\right) - 2 \tan\gamma \tag{3.16}$$

implying that the solution of Eq. (3.15) reads

$$1 - V_s(2\pi - \varphi) = \exp(\frac{1}{2} \ln r_t \cot \alpha \gamma \cot \alpha \frac{1}{2}\varphi)$$
$$\times P_0(\frac{1}{2} \cot \alpha \gamma \cot \alpha \frac{1}{2}\varphi)$$
(3.17)

where  $P_0$  is a periodic function with unit period, which the present analysis cannot predict. For small  $\varphi$ , we have asymptotically

$$1 - V_s(2\pi - \varphi) \approx \exp(\ln r_t \operatorname{cotan} \gamma \varphi^{-1}) P_0(\operatorname{cotan} \varphi^{-1}) \qquad (3.18)$$

For  $\psi^+(\lambda) < \varphi < R_{2\lambda}^{-1}(\psi^+(\lambda))$ , Eq. (3.10) has the form

$$V_s(\varphi) = r_{a(1)} V_s(R_\lambda(\varphi)) \tag{3.19}$$

When  $M > M_c (\gamma > \gamma_c)$ ,  $R_{\lambda}$  has a derivative larger than unity at  $\psi^+(\lambda)$ :

$$\alpha \equiv \frac{d}{d\varphi} R_{\lambda}(\varphi) \bigg|_{\psi^{+}(\lambda)} = \frac{\sin \gamma \sin \nu(\lambda) + \cos(\pi - \gamma - \lambda)}{-\sin \gamma \sin \nu(\lambda) + \cos(\pi - \gamma - \lambda)}$$
(3.20)

and the solution of (3.19) is asymptotically

$$V_{s}(\varphi + \psi^{+}(\lambda)) \approx \varphi^{\zeta} P_{1}\left(\frac{\ln \varphi}{\ln \alpha}\right), \qquad \varphi \downarrow 0$$
(3.21)

where the exponent  $\zeta$  reads

$$\zeta = -\frac{\ln r_{a(1)}}{\ln \alpha} \tag{3.22}$$

In the critical case  $(M = M_c; \gamma = \gamma_c)$  one has  $\psi^{\pm}(\lambda) = \lambda$ , and, in analogy with (3.18), one derives easily

$$V_{s}(\varphi + \lambda) - V_{s}(\lambda)$$
  

$$\approx \exp(\varphi^{-1} \operatorname{cotan} \gamma_{c} \ln r_{a(1)}) P_{2}(\varphi^{-1} \operatorname{cotan} \gamma_{c}), \qquad \varphi \downarrow 0 \quad (3.23)$$

Again,  $P_1$  and  $P_2$  are periodic functions with unit period.

Finally, a similar behavior is present at the band edge ( $\omega^2 = 4$ ). For  $v > 1 + \frac{1}{4}(M-1)^{-1}$ , Eq. (2.16) becomes

$$Z_{s}(-1+1/v) = pZ_{s}[-1+1/(v-1)]$$
(3.24)

The solution is, for  $v \ge \frac{1}{4}(M-1)^{-1}$ ,

$$Z_s(-1+1/v) = p^v P_3(v)$$
(3.25)

where  $P_3$  also has unit period. This is indeed an exact relation. Related properties of  $H(\omega^2)$ , to be derived later, are only asymptotic expressions.

# 4. INTEGRATED SPECTRAL DENSITY NEAR SPECIAL FREQUENCIES

#### 4.1. Lifshitz Singularity at the Band Edge

The behavior of the integrated density of states  $H(\omega^2)$  near special frequencies is very similar to its behavior at the band edge. Another way of

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expressing this is to say that  $\omega^2 = 4$  is also a special frequency, namely with k = 0 and l = 1, so that  $\beta = \pi$  [see Eqs. (2.3), (3.1)]. We therefore briefly discuss the argument of Lifshitz<sup>(10)</sup> for the behavior of  $1 - H(\omega^2)$  as  $\omega^2 \uparrow 4$ .

Lifshitz makes the following observation: an eigenfunction with frequency close to  $\omega^2 = 4$  can only be supported by a large succession of light masses. Let

$$\omega^2 = 2 + 2\cos[\pi/(N+1)]$$
(4.1)

with N integer and  $N \ge 1$ . Such a frequency corresponds to an eigenmode  $a_n = \sin[(n - n_0) \pi/(N + 1)]$  of a succession of N light particles if they were enclosed between infinitely heavy particles (fixed walls) at  $n_0$  and  $n_0 + N + 1$ . The fact that the heavy particles are not infinitely heavy is not important, since they damp such a mode anyway. The probability of occurrence of such a succession of particles is  $q^2 p^N$ , and by definition the probability of occurrence of eigenvalues between  $\omega^2$  and  $\omega^2 = 4$  equals  $H(4) - H(\omega^2) = 1 - H(\omega^2)$ , so we have

$$1 - H(\omega^2) \sim p^N q^2 \tag{4.2}$$

Eliminating N from (4.1) and (4.2), one finds the Lifshitz singularity

$$1 - H(\omega^2) \sim p^{\pi(4-\omega^2)^{-1/2}} = \exp[-\pi |\ln p| (4-\omega^2)^{-1/2}]$$
(4.3)

Considering N as a wavelength, the square root arises because the dispersion curve  $\omega = \sin(\frac{1}{2}\beta)$  is flat at the band edge.

In Fig. 3, we present the interesting part of the eigenfunction with  $\omega^2$  closest to 4 in a random chain of 1024 particles. The mass ratio is M = 4



Fig. 3. Eigenfunction of a random chain with 1024 particles with p = 1/2, M = 4. The eigenfrequency  $\omega^2 = 3.9033$  is the one closest to the band edge  $\omega^2_{Max} = 4$ . ( $\bullet$ ,  $\bigcirc$ ) Light and heavy atoms, respectively.

and p = q = 1/2. The eigenfunction is evaluated by exactly diagonalizing the  $1024 \times 1024$  matrix, using the stable QR algorithm. One observes that the eigenmode indeed is localized on light masses. Their number N = 9 should be compared with the theoretical prediction N = 9.06 from Eq. (4.1) and the value of  $\omega^2$ .

# 4.2. To the Right of a Special Frequency

For frequencies to the right of  $\omega_s$ , we define  $\omega = 2 \sin \frac{1}{2}\beta$  by

$$\beta = \pi (l-k)/l + \varepsilon \equiv \beta_s + \varepsilon \tag{4.4}$$

Now the transformation  $R_{l\beta}$  associated with one heavy and l-1 light masses becomes elliptic, since we are inside the spectrum of an ordered chain with unit cell HL<sup>*l*-1</sup>. Also, the transformation connected to a sequence of *l* light masses ( $\varphi \rightarrow \varphi - 2l\varepsilon$ ) is elliptic, but we shall soon show that this is irrelevant. The matrix  $Q_{l\beta}$  is advantageously written as

$$\pm Q_{I\beta} = \cos \mu + i \sin \mu A \tag{4.5}$$

where  $0 < \mu < \pi$  is defined by

$$\cos \mu = \frac{\cos(\gamma + l\varepsilon)}{\cos \gamma} \tag{4.6a}$$

and

$$A = \frac{1}{\sin \mu \cos \gamma} \begin{pmatrix} -\sin(\gamma + l\varepsilon) & -\sin \gamma \ e^{+il\varepsilon} \\ \sin \gamma \ e^{-il\varepsilon} & \sin(\gamma + l\varepsilon) \end{pmatrix}$$
(4.6b)

The sign in (4.5) is chosen such that  $\cos \mu = +1$  if  $\varepsilon = 0$ . Because  $A^2 = 1$ , the Nth power of  $Q_{l\beta}$  has the form (4.5) with  $\mu \to N\mu$ . An eigenfunction can be found if the phase  $\varphi$ , starting from  $\varphi_{N+1} = 0$ , and then being attracted by several of the  $Q_{a\beta}$  (a = 1,..., l-1), is able to pass zero and reach  $\psi^+(\pi - \lambda)$ . From that point, it can be repelled further in the clockwise direction if the next succession of masses is  $HL^{a(l-1)-1}$ . From Eq. (4.5) it follows that about  $N \simeq \pi/\mu$  transformations  $R_{l\beta}$  are able to do the job:  $\pi/2\mu$ are needed to reach zero, and the other  $\pi/2\mu$  to get away from zero over any fixed angle. From (4.5) it follows that  $N \approx \pi/\mu \sim \varepsilon^{-1/2}$  for small  $\varepsilon$ . Repeated transformations related to *l* light masses can also move the phase away from zero. But about  $1/\varepsilon$  such successions are needed, which is much more. Hence, the  $\varepsilon$  dependence of these transformations may be neglected. Consequently, near the special frequency the integrated density of states

will be determined to leading order by  $\pi/\mu$  successions of one heavy and l-1 light masses:

$$H(\omega^{2}) - H(\omega_{s}^{2}) \sim r_{l}^{N} \sim \exp\{-C_{+} |\ln r_{l}| (\omega^{2} - \omega_{s}^{2})^{-1/2}\}$$
(4.7)

where  $r_l = qp^{l-1}/(1-p^l)$  and

$$C_{+} = \pi \cos(\frac{1}{2}\beta_{s}) \left[\frac{1}{2}l(M-1)\right]^{-1/2}$$
(4.8)

The occurrence of the probability factor  $qp^{l-1}$  is obvious. The factor  $(1-p^l)^{-1}$  comes from the fact that, after each subsequence  $HL^{l-1}$ , a subsequence  $L^l$  or  $L^{2l}$  or  $L^{3l}$ , etc., may be present because they hardly influence the phase. The probability for occurrence of such situations is  $1 + p^l + p^{2l} + \cdots = (1 - p^l)^{-1}$ . Note that a square root of frequency has entered (4.7), because the dispersion (4.5) of an ordered chain  $(HL^{l-1})^{\infty}$  is quadratic for  $\omega^2 \downarrow \omega_s^2$ .

We have made a numerical test of Eq. (4.7). The function  $Z(u; \omega^2)$  and the integrated density of states  $H(\omega^2)$  have been computed by a method, already used in Refs. 11 and 25, which consists in enumerating the  $2^n$ possible values of the displacement  $a_n$  (assuming the boundary conditions  $a_0 = 0$  and  $a_1 = 1$ ). The data presented in the following correspond to n = 18 ( $2^n = 262, 144$ ).

For different values of p, k, l, and M, we have plotted the numerical and analytical values of  $C_+$ . The result is given in Fig. 4; very good agreement with (4.8) is found. Also, the behavior (4.7) is found to be



Fig. 4. Numerical versus analytical values of  $C_+$  for various values of k, l, M, and p.



Fig. 5. Plot of  $\ln[H(\omega^2) - H(\omega_s^2)]$  against  $(\omega^2 - \omega_s^2)^{-1/2}$ . The parameters are k = 1, l = 3, M = 5, p = 0.1. The straight line has a slope  $C_+ \ln r_l = -3.0201$ , predicted by Eqs. (4.7), (4.8).

modulated by a periodic function of  $(\omega^2 - \omega_s^2)^{-1/2}$ , as was already announced in Eq. (1.1). We found that the product of  $C_+$  and the period equals unity (within a few percent). Figure 5 shows a plot which illustrates the oscillatory behavior of  $H(\omega^2)$  in a typical case. In Fig. 6, we present the interesting part of an eigenfunction for  $\omega^2 = 2.0279 > \omega_s^2 = 2$  for our chain with 1024 particles and M=4. One sees that the eigenfunction is appreciably different from zero almost only for successions of one heavy and one, three, or five light masses. This agrees with the argument given above, since l=2, and hence  $l-1 \pmod{2} = 1$ , 3, 5,.... In total, five of these successions are present, to be compared to  $(\pi/\mu) - 1 = 6.55$  from Eq. (4.6).



Fig. 6. Eigenfunction of the same chain as in Fig. 3, with  $\omega^2 = 2.0279$ , closest to the special frequency  $\omega_s^2 = 2$  from the right. ( $\bullet$ ,  $\bigcirc$ ) Light and heavy atoms, respectively.

Also observe that the nontrivial part of the eigenfunction is enclosed by one heavy mass on the left and one heavy and two light masses on the right. Since l=2, the transformation  $L^2$  is close to unity, and the situation is almost the same as in the case where there is a heavy mass on both sides. According to the argument given below Eq. (4.6), the predicted sequence should be  $HL^{a(1)-1}$ . Since l=2, k=1, one finds from Eq. (3.3) that a(1)=1. Thus, the predicted form of the borders of the central part of the eigenfunction indeed is present in the case of Fig. 6.

We finally comment on the exponential behavior of the integrated density of states reported by Gubernatis and Taylor.<sup>(12)</sup> These authors fit their data to a relation of the form (4.7), and find the value 1.482 for the constant in the exponent. When we employ Eq. (4.8) we find the value 2.739 for the same quantity. The reason for this discrepancy may lie in the fact that they have only about ten data points and ignore the periodic structure.

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

The situation to the left of a special frequency in the critical case  $(M = M_c)$  is very similar to the one on the right. We now have

$$\beta = \beta_s - \varepsilon = \pi (l - k)/l - \varepsilon \tag{4.9}$$

and the transformation  $R_{a(1)\beta}$  changes from parabolic to elliptic, just as  $R_{l\beta}$  did in the previous case. A decomposition for  $Q_{a(1)\beta}$  of the form (4.5) introduces  $\mu$  defined by

$$\cos \mu = \pm \cos(\gamma + \bar{a}\beta)/\cos\gamma \qquad (4.10)$$

where  $\bar{a} \equiv a(1)$  satisfies  $\bar{a}\beta = \pi/l - \bar{a}\varepsilon$  [see (3.3)], and the sign is such that  $\mu = 0$  for  $\varepsilon = 0$ . In solving for  $\mu$ , one also has to keep in mind that  $\gamma$  depends on  $\varepsilon$  [see Eqs. (2.6) and (4.9)]. For small  $\varepsilon$  the result is

$$\mu = \left[2 \tan \gamma_s(\bar{a} + b) \varepsilon\right]^{1/2} \left[1 + O(\varepsilon)\right] \tag{4.11a}$$

where

$$b = 2 \frac{d\gamma}{d\beta}\Big|_{\beta_s} = \frac{\sin(\pi/l)}{\sin(k\pi/l)}$$
(4.11b)

Following exactly the same reasoning as in Section 4.2, we conclude that the eigenfunction must be localized on sequences of one heavy and  $(\bar{a}-1) \pmod{l}$  light masses. It must be enclosed between sequences of the form  $HL^{a(2)-1}$ . As a result, we find

$$H(\omega_s^2) - H(\omega^2) \sim \exp\{-C_{-}^{\text{crit}} |\ln r_{\bar{a}}| (\omega_s^2 - \omega^2)^{-1/2}\}$$
(4.12)

where

$$C_{-}^{\text{crit}} = \pi \left[ \sin(\pi k/l) \tan(\pi/2l) / (\bar{a} + b) \right]^{1/2}$$
(4.13)

and

$$r_{\bar{a}} = q p^{\bar{a}-1} (1-p^l)^{-1}$$

In Fig. 7, we present data comparing numerical results for  $C_{-}^{\text{crit}}$ , determined by analyzing  $H(\omega^2)$  using Eq. (4.12), with the prediction (4.13). We have considered situations with various values of k, l, and a(1). The agreement is again very good. Also here the behavior (4.12) is found to be modulated by a periodic function of  $(\omega_s^2 - \omega^2)^{-1/2}$ . The product of  $C_{-}^{\text{crit}}$  and the period is equal to unity (within 2%) in all cases. Figure 8 illustrates the oscillatory behavior of  $H(\omega^2)$ .

In Fig. 9, we present the eigenfunction in a chain with 1024 particles and a mass ratio M = 4 for  $\omega^2 = 0.9895$ . The value  $\omega_s^2 = 1$  corresponds to k = 2, l = 3. This implies  $\bar{a} = 1$ , and our argument predicts that the eigenfunction can only be nonvanishing for subsequences of the form H, HL<sup>3</sup>, HL<sup>6</sup>, etc. One observes that only the first one is present. In counting the number of successions, one has to keep in mind that, since a(2) = 2, the succession HL ends the eigenfunction. Hence we find N = 14, to be compared with  $N = \pi/\mu - 1 = 14.30$  from (4.10). It is rather unexpected to find an eigenfunction located almost only on heavy (but not lazy) masses!



Fig. 7. Numerical versus analytical values of  $C_{-}^{crit}$  for various values of k, l, and p.



Fig. 8. Plot of  $\ln[H(\omega_s^2) - H(\omega^2)]$  against  $(\omega_s^2 - \omega^2)^{-1/2}$ . The parameters are k = 2, l = 7, p = 0.1  $(M = M_c)$ . The straight line has a slope  $C_{\perp}^{\text{crit}} \ln r_{\tilde{a}} = -3.3156$ , predicted by Eqs. (4.12), (4.13).

# 4.4. To the Left of a Special Frequency: General Case

This case turns out to be the most complicated one. We take again  $\beta$  as in Eq. (4.9). The only elliptic transformation present is  $L': \varphi \to \varphi - 2l\epsilon$ . A naive version of the argument for the related situation near the band edge suggests that we should find out for which  $N_1$  the transformation connected to  $\mathrm{HL}^{N_1}$  becomes elliptic. But a short calculation shows that  $\mathrm{HL}^{a-1}\mathrm{HL}^{N_1}$  (a = 1, ..., l-1) still remains hyperbolic: much more than  $N_1$ 



Fig. 9. Eigenfunction of the same chain as in Fig. 3, with  $\omega^2 = 0.9895$ , closest to the special frequency  $\omega_s^2 = 1$  from the left. ( $\bullet$ ,  $\bigcirc$ ) Light and heavy atoms, respectively. Note that for this case M = 4 is equal to the critical mass ratio.

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light masses are needed. To find the correct number, let us look at Fig. 1. Suppose that the phase is in the sink interval, close to  $\psi^{-}(\lambda)$ . Only if it is moved in the counterclockwise direction and has passed  $\psi^{+}(\lambda)$  and if the next transformation is  $R_{\bar{a}\beta}$  will it not be attracted back toward the sink interval  $[0; \psi^{-}(\lambda)]$ . Then it is possible to have an eigenfunction. The angle  $\psi^{+}(\lambda) - \psi^{-}(\lambda)$  equals  $2\nu(\lambda)$  [see (3.8)]. Hence, a succession of  $N \simeq 2\nu(\lambda)/2l\varepsilon$  segments of *l* light particles is needed. We thus have

$$H(\omega_s^2) - H(\omega^2) \sim (p^l)^N \tag{4.14a}$$

$$= \exp\{-C_{-}^{\text{gen}} |\ln p| (\omega_s^2 - \omega^2)^{-1}\}$$
(4.14b)

where

$$C_{-}^{\text{gen}} = 2\nu(\lambda)\sin\beta_s \tag{4.15}$$

The factor  $v(\lambda)$  is defined by Eq. (3.9):

$$\cos v(\lambda) = \sin(\gamma + \pi/l) / \sin \gamma, \qquad 0 < v < \pi \tag{4.16}$$

Note that the exponent of  $(\omega_s^2 - \omega^2)$  in (4.14) is -1, to be compared with -1/2 in the critical case. This is not a contradiction, because the factor  $v(\lambda)$  vanishes when the mass ratio approaches its critical value. The reason why the exponent equals -1 is that here the relevant dispersion relation is just that of a chain with only light particles [Eq. (2.3)], and it is not taken at its band edge, so that  $\omega^2$  is *linear* in  $\varepsilon$ .

In Fig. 10, we present data comparing the numerical values of  $C_{-}^{\text{gen}}$  with Eq. (4.15). We have taken various values of k, l, and M. Again the



Fig. 10. Numerical versus analytical values of  $C_{\underline{e}^{n}}$  for various values of k, l, M, and p. The point GT denotes the result for a related model studied by Gubernatis and Taylor.<sup>(12)</sup>



Fig. 11. Plot of  $\ln[H(\omega_s^2) - H(\omega^2)]$  against  $(\omega_s^2 - \omega^2)^{-1}$ . The parameters are k = 1, l = 3, M = 3, p = 0.1. The straight line has a slope  $C_{-}^{\text{gen}} \ln p = -2.8824$ , predicted by Eqs. (4.14), (4.15).

agreement is good. The point GT marks the outcome of a similar calculation performed for the electronic model studied by Gubernatis and Taylor.<sup>(12)</sup> These authors fitted their results to a behavior of the form (4.12). We have redone their calculation, and find that it can be perfectly described by the equivalent of Eq. (4.14), adapted to their model.

Also here we found an amplitude periodic in  $(\omega_s^2 - \omega^2)^{-1}$ . Its period  $\tau$  satisfies  $\tau C_{-}^{\text{gen}} = l$ , within small errors. The occurrence of the factor l here is expected from (4.14a), where, instead of p,  $p^l$  is the relevant factor. Figure 11 illustrates this behavior in a typical case.



Fig. 12. Eigenfunction of the same chain as in Fig. 3 with  $\omega^2 = 1.6779$ , closest to the special frequency  $\omega_s^2 = 2$  from the left. In this situation, the mass ratio M = 4 exceeds the critical value  $M_c = 2$ . ( $\Phi$ ,  $\bigcirc$ ) Light and heavy atoms, respectively.

Nevertheless, we expect that, in front of the behavior (4.14), there should also be a power  $(\omega_s^2 - \omega^2)^{2\zeta}$ , where  $\zeta$  is given by Eq. (3.22). Since the argument is not complete, we will not elaborate on it here. We only note that numerical results seem to confirm the value of  $\zeta$  given in (3.22), within large error bars.

In Fig. 12, we present a plot of an eigenfunction of the same chain as in previous sections, with mass ratio M = 4 and 1024 particles. The frequency  $\omega^2 = 1.6779$  is closest to  $\omega_s^2 = 2$ . Thus, k = 1, l = 2 in this situation. One clearly observes that the eigenfunction is mainly centered at clusters of l = 2 and 3l = 6 light particles. The latter number should be compared with  $v(\lambda)/\varepsilon - 1 = 6.22$ .

# 5. SUMMARY

In this paper, we have discussed several aspects of special frequencies. We have given physical arguments explaining exponential singularities in the integrated density of states  $H(\omega^2)$  near special frequencies (Section 4). These predictions are confirmed by extensive numerical calculations and by the properties of eigenfunctions.

In the numerical calculations, it was always found that the exponential singularities are modulated by periodic functions, with a period simply related to the exponent of the singularity.

We aim to publish in a future paper an analytical derivation of the results of Section 4. The main idea will be to relate the behavior of the integrated density of states  $H(\omega^2)$  near a special frequency  $\omega_s$  to scaling properties of the Schmidt function  $V_s(\varphi)$  at the special frequency.

Nevertheless, several related questions will remain as difficult open problems, e.g., a deeper understanding of the structure of the periodic amplitudes.

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# NOTE ADDED

While completing this work, we received a preprint "Special energies and special frequencies" by M. Endrullis and H. Englisch. Although they use a slightly different approach and have a different interest, they derive essentially the same results for the exponents as we do in Section 4 with our "physical arguments." In particular, in the case studied by Gubernatis and Taylor,<sup>(12)</sup> their results concerning the exponents coincide with ours.

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