

Models of a Structural Phase Transition with General Anharmonicity and Disorder

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It is shown how the self-consistent phonon Ansatz leads to a new class of exactly soluble models of a structural phase transition. Both nonpolynomial anharmonicity and disorder are analyzed in detail. In the classical limit, the thermodynamics is obtained and sufficient conditions on the anharmonicity are given to ensure a soft-mode phase transition. Diagonal disorder has been studied numerically. It is found that in three dimensions a pronounced mobility edge, separating localized and delocalized phonon states, may exist.

KEY WORDS: Structural phase transition; anharmonicity; disorder; soft mode; large deviations.

1. INTRODUCTION

A structural phase transition⁽¹⁾ occurs when a material changes its crystallographic structure. At many of these transitions, the atoms in the distorted phase are slightly displaced, away from their equilibrium positions of the high-temperature phase. One therefore has to pay careful attention to the nature of the interaction potentials. Since most explanations have been performed in the context of the *self-consistent phonon approximation* and Landau's theory of phase transitions,⁽²⁾ a microscopic underpinning of these phenomenological considerations (see, e.g., ref. 1) seems highly desirable.

Some years ago Schneider *et al.*⁽³⁾ proposed an interesting model to describe structural phase transitions of the above-mentioned type. This

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model has been extended recently⁽⁴⁾ so as to allow a more realistic but still somewhat special nonpolynomial anharmonicity. It has been solved exactly through the use of the approximating Hamiltonian method.^(5,6) Since the operators involved are all unbounded, the ref. 4 incorporated an extension of the usual theory,^(7,8) which presupposes bounded operators only.

The aim of the present paper is threefold. First, we will demonstrate how the results of ref. 4 can be generalized to a large class of Hamiltonians with *non*polynomial anharmonicity. To this end, a large-deviation method developed by van Hemmen^(9,10) will turn out to be instrumental. We restrict ourselves to the classical mechanical context. The second object of this work is to show that the self-consistent phonon Ansatz [cf. Eq. (1.4) below] leads to a new class of *exactly* soluble models and to prove that the solutions agree with what is usually called the "self-consistent phonon approximation."^(1,2) So we also establish the status of this approximation by showing the conditions under which it gives rise to exact results. In addition, the large-deviation method^(9,10) allows us to handle efficiently "impurities" which correspond to external (quenched) random fields or random distortions and which are linear or quadratic in the displacements. It will be shown that the second possibility ("quadratic disorder") is closely related to the Anderson model.^(11,12)

To describe a structural phase transition, we start with the following Hamiltonian:

$$\tilde{H}_A = H_A^{(0)} + \sum_{l \in A} U(Q_l^2) \quad (1.1)$$

where U is the anharmonicity corresponding, for instance, to a double-well potential, and

$$H_A^{(0)} = \sum_{l \in A, \alpha} \frac{1}{2m} P_{l, \alpha}^2 + \frac{1}{4} \sum_{\substack{l, l' \in A \\ \alpha, \alpha'}} (Q_{l, \alpha} - Q_{l', \alpha}) \Phi_{ll'}^{\alpha\alpha'}(Q_{l, \alpha} - Q_{l', \alpha'}) \quad (1.2)$$

describes the lattice in the harmonic approximation. Moreover, $Q_l = \{Q_{l, \alpha}\}_{\alpha=1}^n$ and $P_l = \{P_{l, \alpha}\}_{\alpha=1}^n$ are the displacement and momentum of a particle with mass m at the site l of, say, the d -dimensional (hyper) cubic lattice \mathbb{Z}^d , while $A \subset \mathbb{Z}^d$ is a finite domain with $N = |A|$ sites. The anharmonicity U has the form

$$U(Q_l^2) = \frac{a}{2} Q_l^2 + W(Q_l^2) \quad (1.3)$$

A typical example is $U(x) = -Ax^2 + Bx^4$, $A, B > 0$; the particular case considered in ref. 4 is $a > 0$, $W(x) = \frac{1}{2}b \exp(-\delta x)$; $b, \delta \geq 0$.

To attain further progress, the Hamiltonian (1.1) has to be simplified. It was noticed in ref. 4 that an exactly soluble mean-field (self-consistent phonon) Hamiltonian may be obtained through the *Ansatz*

$$U(Q_i^2) \rightarrow U\left(N^{-1} \sum_{i \in A} Q_i^2\right) \tag{1.4}$$

To simplify the notation, we restrict ourselves, without loss of generality, to only one degree of freedom and take $n = 1$. Note that the harmonic part of (1.3), corresponding to $\frac{1}{2}aQ_i^2$, is invariant under the transformation (1.4). We therefore incorporate it into $H_A^{(0)}$ and rewrite the Hamiltonian in the form

$$H_A = T_A^{(a)} + NW\left(N^{-1} \sum_{i \in A} Q_i^2\right) \tag{1.5}$$

with

$$T_A^{(a)} = \frac{a}{2} \sum_{i \in A} Q_i^2 + \frac{1}{4} \sum_{i, i' \in A} \Phi_{ii'}(Q_i - Q_{i'})^2 \tag{1.6}$$

Two remarks are in order. First, we have dropped the kinetic energy term since in classical statistical mechanics it is irrelevant. Second, for translationally invariant $\Phi_{ii'} = \Phi_{i-i'}$, the first term in (1.6) stabilizes the lattice.⁽¹³⁾ We will assume this translation invariance throughout what follows. Furthermore, for the sake of simplicity, $\Phi_{i-i'} = 0$ if $|i-i'| > R$, that is, we assume a finite-range interaction.

In Section 2 we derive an explicit expression for the free energy density $f(\beta)$ of the model (1.5) without specifying the function W . This allows quite a bit of freedom to model practical situations. The (exact) solution is obtained through a simple and elegant method (see refs. 9, 10, and 14) based on the philosophy of the theory of large deviations. This approach allows us to generalize those results of refs. 4–6 which were obtained in the classical limit. In Section 3 we indicate how the effect of “impurities” can be incorporated into the Hamiltonian (1.5). The thermodynamic behavior of the system with a “quadratic disorder” in the Einstein phonon approximation is discussed there together with the phonon localization problem. A summary may be found in Section 4.

2. FREE ENERGY DENSITY: ANHARMONICITY AND PHASE TRANSITIONS

In this section we calculate exactly (in the thermodynamic limit) the free-energy density

$$f(\beta) = \lim_{N \rightarrow \infty} (-\beta N)^{-1} \ln Z_N(\beta)$$

for the Hamiltonian (1.5) and describe the class of nonpolynomial anharmonicity for which this is allowed.

The method we use is based on the theory of large deviations. To explain it, let us introduce the variable $m_N = N^{-1} \sum_{l \in A} Q_l^2$. To calculate the partition function $Z_N(\beta)$ for the Hamiltonian (1.5), we note that the space of configurations $\{\mathbf{Q}^{(A)}\}$ can be pictured more geometrically as a union of surfaces, or fibers, $m = m_N(\mathbf{Q}^{(A)})$ with $0 \leq m < \infty$, so that

$$\begin{aligned} Z_N(\beta) &= \int_0^\infty dm \int_{\{\mathbf{Q}^{(A)}: m_N = m\}} \prod_{l \in A} dQ_l \exp(-\beta H_A) \\ &= \int_0^\infty dm e^{-\beta N W(m)} Z_N(\beta, m) \end{aligned}$$

Here $Z_N(\beta, m)$ is the partition function of the system with the Hamiltonian $T_A^{(a)}$ of (1.6) in the microcanonical ensemble $m_N(\mathbf{Q}^{(A)}) = m$. Now we define the probability distribution

$$\begin{aligned} P_N(dm) &= [Z_{N,a}(\beta)]^{-1} Z_N(\beta, m) dm \\ Z_{N,a}(\beta) &= \int \prod_{l \in A} dQ_l \exp(-\beta T_A^{(a)}) \end{aligned} \tag{2.1}$$

Consequently, the free energy density $f(\beta)$ has the form

$$f(\beta) = f_a(\beta) - \lim_{N \rightarrow \infty} \frac{1}{\beta N} \ln \int_0^\infty P_N(dm) \exp[-\beta N W(m)] \tag{2.2}$$

where $f_a(\beta)$ is the free energy density for the harmonic system (1.6) in the grand canonical ensemble:

$$f_a(\beta) = \lim_{N \rightarrow \infty} \left(-\frac{1}{\beta N} \right) \ln Z_{N,a}(\beta) \tag{2.3}$$

Now we consider the c -function^(9,10)

$$c_N(t) = \frac{1}{N} \ln \left\langle \exp t \sum_{l \in A} Q_l^2 \right\rangle_{T_A^{(a)}} = \frac{1}{N} \ln \int_0^\infty P_N(dm) e^{tNm} \tag{2.4}$$

Here $\langle - \rangle_{T_A^{(a)}}$ is the finite-volume Gibbs state for the Hamiltonian $T_A^{(a)}$. The sequence $\{c_N(t)\}_N$ obviously has the following properties:

- (i) Functions $\{c_N(t)\}_N$ are finite and convex for $t < \beta\alpha/2$.
- (ii) For $t < \beta\alpha/2$ the pointwise limit $c(t) = \lim_{N \rightarrow \infty} c_N(t)$ exists and has the form

$$c(t) = \beta[f_\alpha(\beta) - f_{\alpha-2t/\beta}(\beta)] \tag{2.5}$$

- (iii) $c(t)$ is differentiable for $t < \beta\alpha/2$.

This means that the sequence of probability distributions $\{P_N(dm)\}_N$ has a large-deviation property with the entropy function $c^*(m)$,^(9,10,14) where

$$c^*(m) = \sup_{t < \beta a/2} [tm - c(t)] \tag{2.6}$$

is the Legendre transformation of $c(t)$. In other words,

$$P_N(dm) \sim dm \exp[-Nc^*(m)] \tag{2.7}$$

as $N \rightarrow \infty$.

To apply (2.7) to the evaluation of (2.2), one has to formulate some conditions on the function $W(m)$. We assume that there is $m_c \geq 0$ such that for $m \geq m_c$ one has (see Fig. 1)

$$a + 2W'(m) \geq 0 \tag{2.8}$$

and the integral in (2.2) converges for an arbitrary N . Then, using a Laplace argument and Eqs. (2.2) and (2.7), we get

$$f(\beta) = f_a(\beta) - \inf_m [W(m) + \beta^{-1}c^*(m)] \tag{2.9}$$

If we assume in addition that $W(m)$ is continuously differentiable on $(0, \infty)$ and is such that $W(m) + \beta^{-1}c^*(m)$ reaches its infimum at a single point $\bar{m} = \bar{m}(\beta)$, then by exploiting the identities

$$c^*(m) = m\tilde{t}(m) - c(\tilde{t}(m)), \quad \partial_m c^*(m) = \tilde{t}(m), \quad \partial_t c(\tilde{t}(m)) = m$$

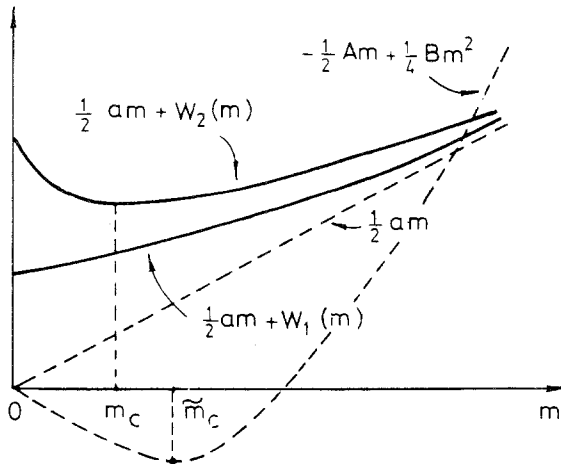


Fig. 1. Anharmonic potentials W_1 and W_2 corresponding to two different regimes considered in the text. For the first case, $a + 2W'_1(m) \geq 0$; for the second, $a + 2W'_2(m_c) = 0$, $m_c > 0$.

one can rewrite Eq. (2.9) as

$$f(\beta) = f_{a+2W'(\bar{m})}(\beta) + [W(\bar{m}) - \bar{m}W'(\bar{m})] \tag{2.10}$$

Here $\bar{m}(\beta)$ satisfies the fixed-point equation

$$m = \partial_c [-\beta \partial_m W(m)] \tag{2.11}$$

Therefore, our model (1.5) is thermodynamically equivalent to a harmonic system (1.6) with renormalized constant a : $a \rightarrow a + 2W'(\bar{m})$.

In passing, we note that the particular case considered by ref. 4 corresponds to $W(m) = \frac{1}{2}b \exp(-\delta m)$, $b > 0$, $\delta > 0$. It describes a structural phase transition in the mean-field (self-consistent phonon) model which mimics a double-well potential with Gaussian anharmonicity.

To analyze possible phase transitions in the system (1.5), one has to take into account the explicit formula for the free energy density $f_a(\beta)$. Using (2.5), one gets for (2.11)

$$m = \lim_{N \rightarrow \infty} \beta^{-1} I_d^{(N)}(m) = \lim_{N \rightarrow \infty} \frac{1}{\beta N} \frac{1}{\Omega_{q=0}^2(m)} + \lim_{N \rightarrow \infty} \frac{1}{\beta N} \sum_{\substack{q \in A^* \\ (q \neq 0)}} \frac{1}{\Omega_q^2(m)} \tag{2.12}$$

where

$$\Omega_q^2(m) = [a + 2W'(m)] + [\tilde{\Phi}(0) - \tilde{\Phi}(q)]$$

Here $\{\Omega_q\}_{q \in A^*}$ are the frequencies of the harmonic system corresponding to (2.10) with periodic boundary conditions, the wavevectors q belong to the Brillouin zone A^* of A , and $\tilde{\Phi}(q)$ is the (discrete) Fourier transform of $\Phi_{l-l'}$, $l, l' \in A$.

As follows from (2.12), there are (at least) two different regimes for the behavior of the “order parameter” $\bar{m}(\beta)$.

First, let $a + 2W'(m) \geq \varepsilon > 0$ for $m > 0$ and $a + 2W'(0) \geq 0$ (see Figs. 1 and 2); then the contribution of the term corresponding to $\Omega_{q=0}^2$ [see Eq. (2.12)] tends to zero. Thus, Eq. (2.11) assumes the form

$$m = \frac{\beta^{-1}}{(2\pi)^d} \int_{\mathcal{B}} d^d q \Omega_q^{-2}(m) \equiv \beta^{-1} I_d(m) \tag{2.13}$$

where $\mathcal{B} = \{q: |q^\alpha| \leq \pi, \alpha = 1, 2, \dots, d\}$. Accordingly, there is no structural phase transition of the soft-mode type.⁽¹⁾

The second possibility corresponds to the case when $a + 2W'(m)$ reaches zero for an $m_c > 0$; see Fig. 1. For finite N , Eq. (2.12) then has the solution \bar{m}_N approaching m_c (when $N \rightarrow \infty$) for $\theta \leq \theta_c$; for $\theta > \theta_c$ one has

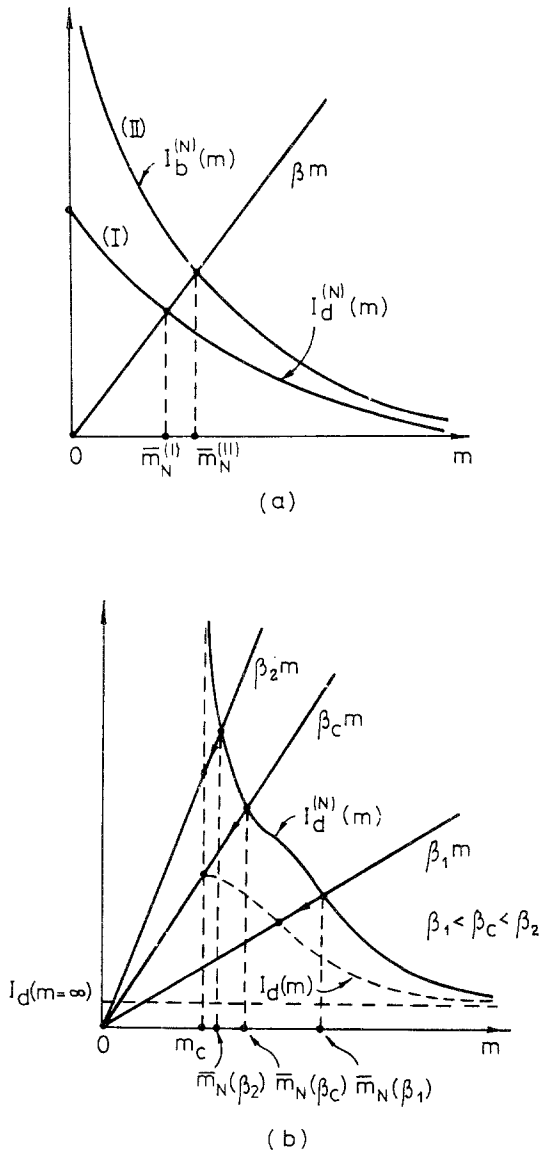


Fig. 2. (a) Graphical solution of Eq. (2.12) for the cases (I) $a + 2W'(m) > 0$ and (II) $a + 2W'(m) = 0$ at $m = 0$. (b) Situation when $a + 2W'(m)$ vanishes at $m = m_c > 0$. Arrows indicate how \bar{m}_N converges to m_c or $\bar{m}(\beta)$, respectively, for $\beta > \beta_c$ or $\beta \leq \beta_c$.

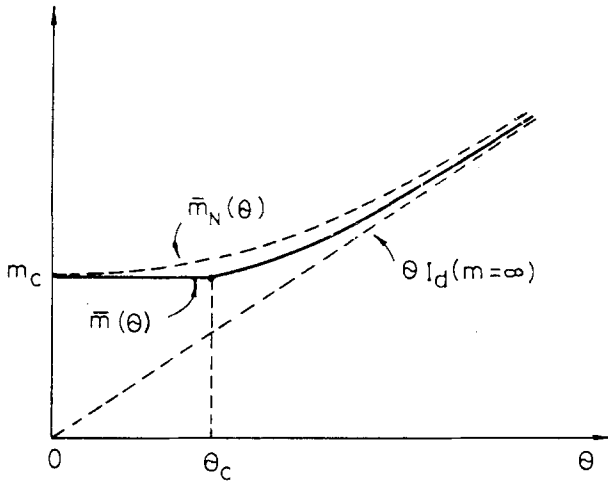


Fig. 3. Temperature dependence of the "order parameter" $\bar{m}(\theta)$. Here m_c and θ_c are defined by Eq. (2.14).

$a + 2W'(\bar{m}_N) > 0$ and $\bar{m}_N \rightarrow \bar{m}(\beta < \beta_c)$ as $N \rightarrow \infty$; see Figs. 2 and 3. Here the critical temperature $\theta_c = \beta_c^{-1}$ is determined by the condition (see Fig. 2)

$$m_c = \theta_c I_d(m_c), \quad a + 2W'(m_c) = 0 \tag{2.14}$$

This situation corresponds to the well-known structural phase transition with a soft-mode^(1,2)

$$\bar{m}(\beta) = \begin{cases} \bar{m}(\beta), & \beta \leq \beta_c \\ m_c, & \beta > \beta_c \end{cases} \quad \Omega_{q=0} = \begin{cases} > 0, & \theta > \theta_c \\ 0, & \theta \leq \theta_c \end{cases} \tag{2.15}$$

Here, as above, $\bar{m}(\beta)$ is the solution of Eq. (2.13).

In the particular case $W(m) = \frac{1}{2}b \exp(-\delta m)$ the phase transition occurs only if $\kappa = \delta^{-1} \ln(\delta b/a) > 0$, while $m_c(\kappa) = \kappa > 0$ [$m_c(\kappa) = 0$ for $\kappa < 0$].⁽⁴⁾ Then one gets (see Fig. 3)

$$\begin{aligned} \bar{m}_N(\beta > \beta_c) &= m_c + \frac{\exp(\delta m_c)}{\delta^2 b(\beta - \beta_c) N} + O(N^{-1}) \\ \bar{m}_N(\beta \leq \beta_c) &= \theta I_d(\bar{m}(\beta)) + O(N^{-1}) \end{aligned} \tag{2.16}$$

Summarizing: Eqs. (2.10) and (2.11) contain all the relevant information about the system. Under suitable conditions, to be specified elsewhere, they may give rise to either a smooth thermodynamic behavior or a soft-mode structural phase transition.

3. FREE ENERGY DENSITY: ANHARMONICITY AND DISORDER

The impurities in the anharmonic lattice (1.1) create randomness in the parameters on which the Hamiltonian depends. Here we consider the case where the single-particle potential is random (“quadratic disorder”):

$$V_{\xi_l}(Q_l^2) = V(\xi_l Q_l^2) \tag{3.1}$$

The $\{\xi_l\}_{l \in \mathbb{Z}^d}$ are, e.g., independent, identically distributed (i.i.d.) random variables (random field on the lattice \mathbb{Z}^d). As compared to (1.3), we add the random potential $V_{\xi_l}(Q_l^2)$ to the deterministic $W(Q_l^2)$.

In the particular case of ref. 4, one has

$$V_{\xi_l}(Q_l^2) = \frac{1}{2}b \exp(-\delta \xi_l Q_l^2) \tag{3.2}$$

which corresponds to a Gaussian perturbation with random width.

To construct an exactly soluble anharmonic lattice with “impurities,” we use the *Ansatz* (1.4) (self-consistent phonon model), which in this case says

$$V_{\xi_l}(Q_l^2) \rightarrow V\left(N^{-1} \sum_{l \in A} \xi_l Q_l^2\right) \tag{3.3}$$

Now we are again in the position known from refs. 9, 10, and 14. So we can use the scheme based on the theory of large deviations adapted to the case (3.3). Namely, we introduce for a fixed configuration $\xi = \{\xi_l\}_{l \in \mathbb{Z}^d}$ two variables

$$m_N = \frac{1}{N} \sum_{l \in A} Q_l^2; \quad q_N = \frac{1}{N} \sum_{l \in A} \xi_l Q_l^2 \tag{3.4}$$

Then, as a first step toward the calculation of the free energy density for the anharmonic model with (anharmonic) impurities

$$H_A = T_A^{(a)} + NW(m_N) + NV(q_N) \tag{3.5}$$

one has to calculate the *c*-function (cf. Section 2)

$$c(\mathbf{t}) = \lim_{N \rightarrow \infty} \frac{1}{N} \ln \langle \exp(\mathbf{t} \cdot \mathbf{w}_N) \rangle_{T_A^{(a)}} \tag{3.6}$$

Here $\mathbf{t} = (t_1, t_2)$ and $\mathbf{w}_N = (Nm_N, Nq_N)$ are vectors in \mathbb{R}^2 .

The right-hand side of (3.6) can be represented as a difference of two free energy densities

$$c(\mathbf{t}) = \beta f_a(\beta) - \lim_{N \rightarrow \infty} \beta f_{a-2t_1/\beta - 2t_2/\beta}^{(N)}(\beta | \xi) \tag{3.7}$$

Here $f_{a-2(t_1+t_2)/\beta}^{(N)}$ corresponds to a harmonic system with a random single-particle harmonic potential

$$H_A^{(t)}(\xi) = T_A^{(a)} - \frac{t_1}{\beta} \sum_{l \in A} Q_l^2 - \frac{t_2}{\beta} \sum_{l \in A} \xi_l Q_l^2 \tag{3.8}$$

But now we can refer to the conventional wisdom about random systems^(15,16) and state that, for t_1, t_2 , and ξ such that $\text{Prob}(\{t_1 + t_2 \xi_l < a\}_{l \in \mathbb{Z}^d}) = 1$ the limit in (3.7) exists and is independent of ξ for almost all configurations ξ . Therefore, with probability one the c -function (3.7) exists, is independent of ξ , and is a convex function of the vector argument \mathbf{t} . The same is valid for its Legendre transform

$$\begin{aligned} c^*(\mathbf{w}) &= \sup_{\mathbf{t}} [t_1 m + t_2 q - c(\mathbf{t})] \\ &= \bar{t}_1(\mathbf{w}) m + \bar{t}_2(\mathbf{w}) q - c(\bar{\mathbf{t}}(\mathbf{w})) \end{aligned} \tag{3.9}$$

Using the Laplace argument, one gets for the free energy density of the model (3.5) the following expression (cf. Section 2):

$$\begin{aligned} f(\beta) &= \lim_{N \rightarrow \infty} \left(-\frac{1}{\beta N} \right) \ln \left[\int dm \int dq \exp\{-\beta N[W(m) + V(q)]\} \right. \\ &\quad \times \int \prod_{\substack{l \in A \\ \{\mathbf{Q}^{(A)}: m_N = m, q_N = q\}}} dQ_l \exp(-\beta T_A^{(a)}) \left. \right] \\ &= f_a(\beta) + \inf_{\mathbf{w}} \left[W(m) + V(q) - \frac{c^*(\mathbf{w})}{\beta} \right] \end{aligned} \tag{3.10}$$

Here we assume that the functions W and V are differentiable and satisfy the inequality

$$a + 2W'(m) + 2V'(q) \geq 0 \tag{3.11}$$

This inequality guarantees the stability of the system (3.5); see below.

One can derive an explicit expression for the infimum in (3.10) without evaluating $c^*(\mathbf{w})$ explicitly. To this end, we note that a minimizing \mathbf{w} in (3.10) satisfies

$$\nabla c^*(\mathbf{w}) = -\beta \{W'(m), V'(q)\} \tag{3.12}$$

To obtain ∇c^* , we return to (3.9) and differentiate the last term, realizing that we need not take into account the *implicit* dependence upon m and q , since $\bar{\mathbf{t}}(\mathbf{w})$ maximizes the expression in the middle. This gives

$$\nabla c^*(\mathbf{w}) = \bar{\mathbf{t}} = \{\bar{t}_1(\mathbf{w}), \bar{t}_2(\mathbf{w})\} \tag{3.13}$$

Comparing (3.12) and (3.13), we obtain $\bar{\mathbf{t}}$ itself. Since $\bar{\mathbf{t}}$ also satisfies $\mathbf{w} = (m, q) = \nabla c(\bar{\mathbf{t}})$, we are left with a fixed-point equation for m and q ,

$$\begin{aligned} m &= \partial_{t_1} c(-\beta W'(m), -\beta V'(q)) \\ q &= \partial_{t_2} c(-\beta W'(m), -\beta V'(q)) \end{aligned} \tag{3.14}$$

Let us denote the solutions to (3.14) by $\bar{\mathbf{w}}$. We then get from (3.10)

$$f(\beta) = f_{\mathbf{a}(\bar{\mathbf{w}})}(\beta) + W(\bar{m}) - \bar{m}W'(\bar{m}) + V(\bar{q}) - \bar{q}V'(\bar{q}) \tag{3.15}$$

We have to minimize (3.15) with respect to all $\bar{\mathbf{w}}$ which satisfy (3.14). Here $\mathbf{a}(\bar{\mathbf{w}}) = (a + 2W'(\bar{m}), 2V'(\bar{q}))$. Consequently, $f_{\mathbf{a}(\bar{\mathbf{w}})}(\beta)$ is the free energy density for the system with the Hamiltonian (3.8), where $t_1 = -2\beta W'(\bar{m})$, $t_2 = -2\beta V'(\bar{q})$, i.e., the Eqs. (3.14) are equivalent to

$$\begin{aligned} m &= \lim_{N \rightarrow \infty} \left\langle \frac{1}{N} \sum_{l \in \mathcal{A}} Q_l^2 \right\rangle_{H_A^{\mathbf{a}(\bar{\mathbf{w}})}(\xi)} \\ q &= \lim_{N \rightarrow \infty} \left\langle \frac{1}{N} \sum_{l \in \mathcal{A}} \xi_l Q_l^2 \right\rangle_{H_A^{\mathbf{a}(\bar{\mathbf{w}})}(\xi)} \end{aligned} \tag{3.16}$$

Summarizing: The anharmonic system with ‘‘impurities’’ described by the Hamiltonian (3.5) has an exact solution represented in a (very) implicit form by Eqs. (3.14)–(3.16). Therefore, to analyze the effect of anharmonic disorder in the framework of the Hamiltonian (3.5), one should either simplify the model or use numerical calculations.

3.1. Einstein Phonons

In the case of Einstein phonons, $\Phi_{l-l'}$ vanishes for $l \neq l'$ and the phonons are completely localized.⁽¹⁾ For the sake of simplicity, we take into consideration only anharmonic disorder, i.e., $W = 0$. Then the effective (approximating) Hamiltonian (3.8) takes the form

$$H_A^{\mathbf{a}(\bar{\mathbf{w}})}(\xi) = \frac{a}{2} \sum_{l \in \mathcal{A}} Q_l^2 + V'(\bar{q}) \sum_{l \in \mathcal{A}} \xi_l Q_l^2 \tag{3.17}$$

For the free energy density (3.15) one gets

$$\begin{aligned} f(\beta) &= V(\bar{q}) - \bar{q}V'(\bar{q}) - \lim_{N \rightarrow \infty} \frac{1}{\beta N} \sum_{l \in \mathcal{A}} \ln \left[\frac{\pi}{\beta[a/2 + V'(\bar{q})\xi_l]} \right]^{1/2} \\ \bar{q} &= \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{l \in \mathcal{A}} \xi_l \frac{\theta}{2[a/2 + V'(\bar{q})\xi_l]} \end{aligned} \tag{3.18}$$

At this stage one should specify the random field $\{\xi_l\}_{l \in \mathbb{Z}^d}$. Here we consider i.i.d. binary random variables $\{\xi_l = \pm 1\}$; $\text{Prob}\{\xi_l = +1\} = p$, $\text{Prob}\{\xi_l = -1\} = q = 1 - p$. Then one can calculate limits (3.18) in the explicit form

$$\begin{aligned}
 f(\beta) &= V(\bar{q}) - \bar{q}V'(\bar{q}) + \frac{1}{2\beta} \left\{ p \ln \left[\beta \left(\frac{a}{2} + V'(\bar{q}) \right) \right] \right. \\
 &\quad \left. + (1-p) \ln \left[\beta \left(\frac{a}{2} - V'(\bar{q}) \right) \right] \right\} - \frac{\pi}{2\beta} \tag{3.19} \\
 \bar{q} &= \left[a \left(p - \frac{1}{2} \right) - V'(\bar{q}) \right] \left(2\beta \left\{ \left(\frac{a}{2} \right)^2 - [V'(\bar{q})]^2 \right\} \right)^{-1}
 \end{aligned}$$

For a particular case of the potential (3.2) one has $V'(q) = -\frac{1}{2}b \delta e^{-\delta q}$ and $\delta b < a$ [stability condition (3.11)], while $f(\beta)$ and $\bar{q}(\beta)$ are smooth functions of β . The critical value $p = p_c$ corresponds to the condition

$$a(p - \frac{1}{2}) + \frac{1}{2}\delta b = 0$$

For $p = p_c$ the parameter \bar{q} vanishes for all temperatures, while for $p > p_c$ one has $\bar{q} > 0$ and for $p < p_c$, $\bar{q} < 0$; $\bar{q} = 0$ only for $\theta = 0$.

3.2. Localization of Phonons. Numerical Results

Localization of phonons is one of the most intriguing phenomena in a harmonic lattice with disorder. In a recent paper⁽¹⁷⁾ (see also ref. 18) this phenomenon was observed in a lattice with random masses. In our model (3.5) (for simplicity we put $W = 0$ and $\Phi_{ll'} = \Phi \delta_{l,l'+\rho}$, $\|\rho\| = 1$) anharmonic disorder leads to the effective Hamiltonian

$$H_A^{(a)} = \frac{a}{2} \sum_{l \in A} Q_l^2 + \frac{1}{4} \Phi \sum_{l, \rho} (Q_l - Q_{l+\rho})^2 + V'(\bar{q}) \sum_{l \in A} \xi_l Q_l^2 \tag{3.20}$$

Therefore, the eigenvalue problem for phonon frequencies $\{\omega\}$ is given by

$$(m\omega^2 - a)Q_l = \varepsilon_l Q_l + (-\Delta Q)_l, \quad \varepsilon_l = \xi_l V'(\bar{q}) \tag{3.21}$$

where $(\Delta Q)_l = \sum_{\rho} Q_{l+\rho} - 2dQ_l$ is the discretized Laplacian. As above, we consider this problem for an i.i.d. random field $\{\xi_l\}_{l \in \mathbb{Z}^d}$: $\text{Prob}\{\xi_l = 1\} = p$, $\text{Prob}\{\xi_l = -1\} = 1 - p$. Then Eq. (3.21) is equivalent to an Anderson model with a binary distribution (see, e.g., ref. 19),

$$\begin{aligned}
 EQ_l &= \varepsilon_l Q_l - \sum_{\rho} Q_{l+\rho} \tag{3.22} \\
 E &= m\omega^2 - a - 2d, \quad \varepsilon_l = \pm \varepsilon, \quad \varepsilon = V'(\bar{q})
 \end{aligned}$$

Our procedure to exhibit localization of phonons and to find a mobility edge follows that developed in recent papers.^(17,19) Through an exact numerical diagonalization we find all the eigenvalues and eigenvectors of the problem (3.24) for $A \subset \mathbb{Z}^d$ ($d=3$) and a fixed realization ε of the random field $\{\varepsilon_l\}_{l \in \mathbb{Z}^d}$. Then we examine the inverse participation ratio (IPR)

$$\text{IPR}(Q_E) = \sum_{l \in A} Q_{l,E}^4 / \left(\sum_{l \in A} Q_{l,E}^2 \right)^2 \quad (3.23)$$

for each eigenvector $Q_E = \{Q_{l,E}\}_{l \in A}$. Delocalized phonons are expected to have small IPR of order $|A|^{-1}$, while localized ones show larger values of IPR; e.g., the IPR equals one if Q_E is localized at one site as for Einstein phonons. For a given random field $\{\varepsilon_l\}_{l \in \mathbb{Z}^d}$ we need not average over many samples (or configurations ε), since localization/delocalization phenomena should occur with probability one, i.e., for almost all realizations ε of the random field. This means that for large $N = |A|$ (say, $N \simeq 1000$) all samples show essentially the same behavior; see refs. 15 and 16.

To display the results, we arrange the eigenvalues $\{E_k\}$ in an ascending sequence $E_1 < E_2 < \dots < E_N$ and plot the IPR *against the label k* .

Insofar as the amplitude ε of the random field $\{\varepsilon_l\}_{l \in A}$ is a function of the "order parameter" $\bar{q}(\beta)$ [see Eqs. (3.16), (3.22)], the interesting problem is whether localization/delocalization of phonons depends on ε . The importance of percolation effects as the site energies $\{\varepsilon_l\}_{l \in A}$ increase in absolute value was observed in refs. 17–19.

A numerical simulation has been performed for three-dimensional $10 \times 10 \times 10$ systems with periodic boundary conditions for $p=0.25$ and $p=0.50$ and $\varepsilon=1, 2$, and 4.

If $p=0.25$, then $\varepsilon_l = -\varepsilon$ percolates (for $d=3$, site percolation threshold $p_c=0.312$), but $\varepsilon_l = +\varepsilon$ does not. Since $2d$ is equal to the norm of the kinetic energy (hopping) operator K , $(KQ)_l = -\sum_{\rho} Q_{l+\rho}$, for $\varepsilon \geq 2d$ the positive-energy eigenstates of the problem (3.24) are expected to be localized on finite clusters with $\varepsilon_l = +\varepsilon$, whereas the eigenstates corresponding to negative energies may be spread out on the percolating (infinite) cluster of sites with $\varepsilon_l = -\varepsilon$. Figures 4–6 confirm this observation. It turns out, however, that there is something like a critical $\varepsilon_c < 2d$ such that for $\varepsilon \leq \varepsilon_c$ there is no localization whatsoever, whereas for $\varepsilon > \varepsilon_c$ the states with $E > 0$ do localize. Note that the upper row gives the labels $k=100, 200, \dots$, explicitly and the lower row gives the corresponding eigenvalues E_k , $100 \leq k \leq 1000$.

For $\varepsilon=1$, the IPR criterion shows (see Fig. 4) the complete absence of

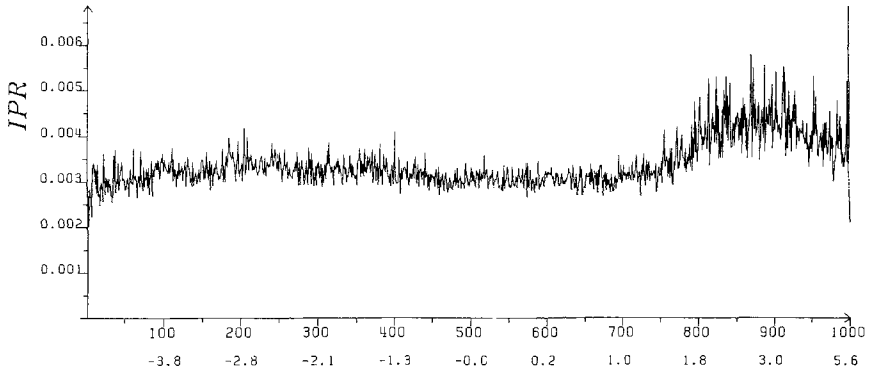


Fig. 4. The inverse participation ratio (IPR) of a $10 \times 10 \times 10$ system with $p=0.25$ and $\varepsilon=1$ plotted against the label k . Below the labels $k=100, 200, \dots, 1000$, one can find the eigenvalues E_k . The sites l with $\varepsilon_l = -1$ percolate ($p_c=0.312$ for site percolation when $d=3$) but their counterparts do not. Note the extremely small values of the IPR and the complete absence of localized states.

localized states. For $\varepsilon=2$, the IPR gives a similar picture: only for $E \gtrsim 1$ does the IPR increase appreciably, suggesting a tendency to localization, but these states are still delocalized. Finally, for $\varepsilon=4$ the positive-energy eigenstates do localize with clear mobility edge at $E=0$.

On the other hand, if $p=0.50$, then both $\varepsilon_l = +\varepsilon$ and $\varepsilon_l = -\varepsilon$ percolate in $d=3$. For $\varepsilon=1$ we again observe a complete absence of localized states; see Fig. 7. One gets a similar picture for $\varepsilon=2$ (Fig. 8). But for $\varepsilon=4$ the picture is more complicated (Fig. 9). First, we observe resonances: delocalized

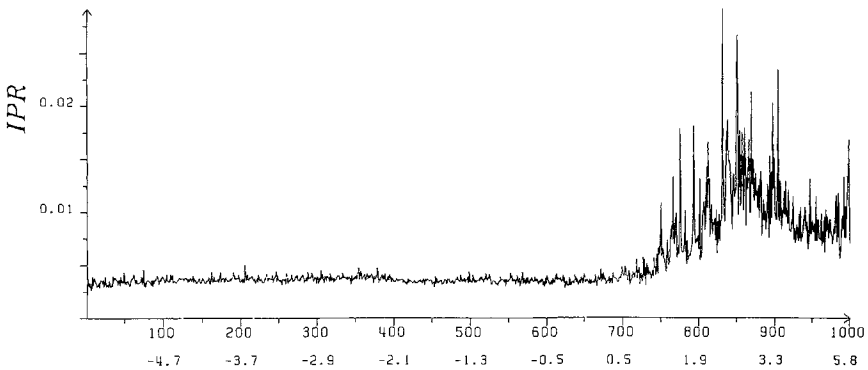


Fig. 5. As Fig. 4, for $\varepsilon=2$. There is a well-pronounced increasing of the IPR for $k \gtrsim 750$, which anticipates localization. However, all the states are still delocalized. Note the difference in scale between the cases $\varepsilon=1$ and $\varepsilon=2$.

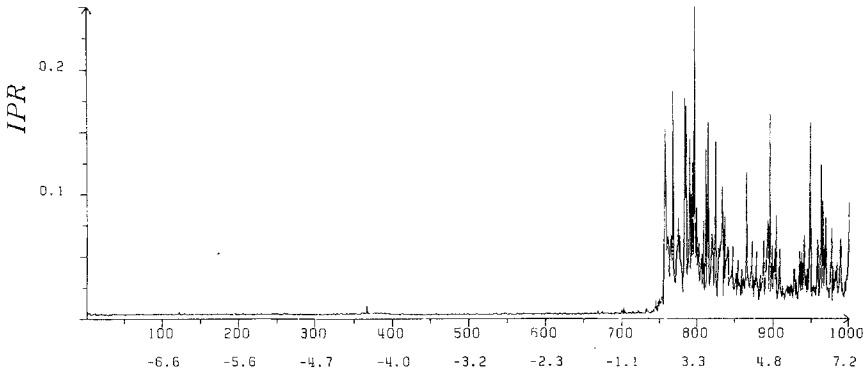


Fig. 6. As Fig. 4, for $\varepsilon = 4$. A clear mobility edge appears at $E = 0$; the states for $E > 0$ are localized. So $\varepsilon = 4$ is already beyond a critical ε_c . Note the difference in scale between $\varepsilon = 1$ and $\varepsilon = 4$.

eigenstates which are strongly peaked at one or very few sites. Let us consider a small cluster of $\varepsilon_l = -4$ sites surrounded by $\varepsilon_l = +4$ sites such that one of the $\varepsilon_l = +4$ sites is coupled to an infinite cluster of $\varepsilon_l = -4$ sites: this is nothing but cluster screening. Then, the screened particle can “tunnel” through a $\varepsilon_l = +4$ barrier. Therefore, there exists an eigenstate with an appreciable amplitude on the small cluster $\varepsilon_l = -4$ and a small amplitude on the infinite $\varepsilon_l = -4$ cluster. This phenomenon is called a resonance.⁽¹⁷⁾ Figure 9 shows evident resonances at $k \simeq 230, 360, 770, 800, 840,$ and 990 and a bump near $k = 500$. We do not know whether the bump in the middle has any physical relevance, but it is hard to imagine a mobility edge there.

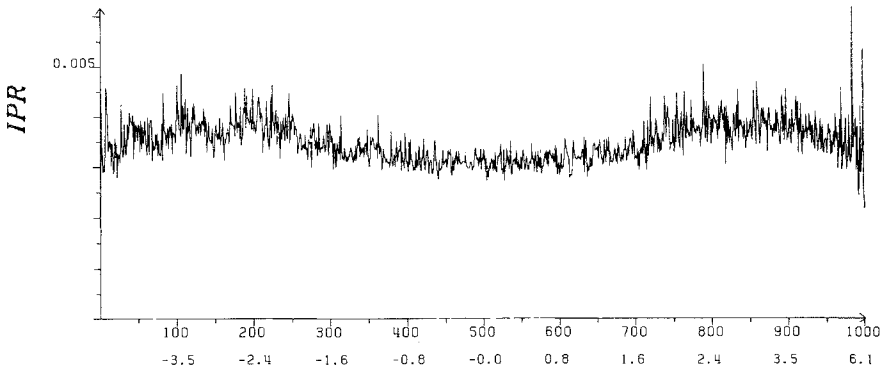


Fig. 7. As Fig. 4, except for the fact that $p = 0.5$. Both $\varepsilon_l = +1$ and $\varepsilon_l = -1$ percolate, since $p_c = 0.312$ for site percolation. Note the extremely small values of the IPR and the complete absence of localized states.

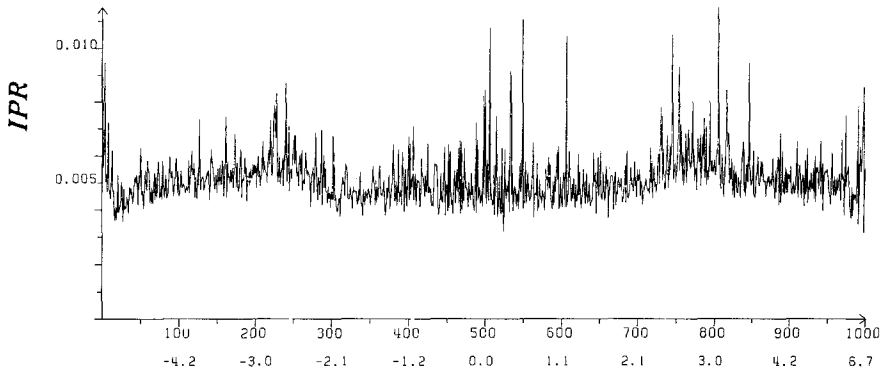


Fig. 8. As Fig. 7, for $\varepsilon=2$. Note the IPR scale and the absence of localized states.

4. SUMMARY

We have obtained a class of exactly soluble models of a structural phase transition. To get an explicit solution, we used a method developed in refs. 9, 10, and 14. In addition, this method allows us to develop results obtained in ref. 4 for a general case of anharmonic (classical) lattices so as to incorporate anharmonic disorder also. Consequently, this method is more efficient than the approximating Hamiltonian method,⁽⁴⁻⁸⁾ though the latter works for quantum lattices as well.

Our main results are as follows.

1. A large class of exactly soluble classical Hamiltonians with non-polynomial anharmonicity is found and an explicit *Ansatz* for constructing

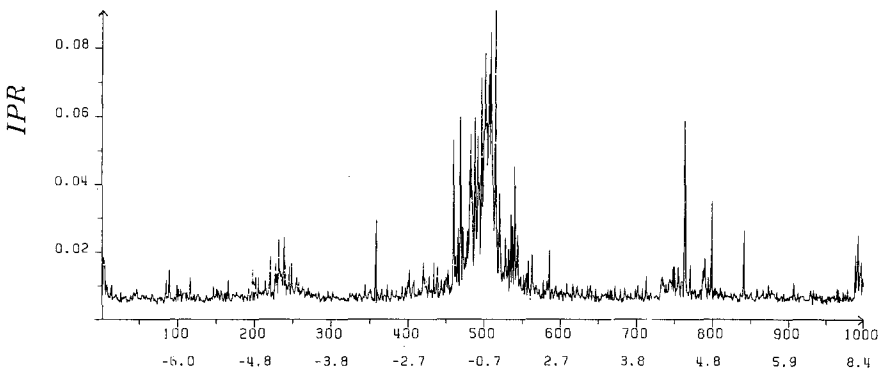


Fig. 9. As Fig. 7, but for $\varepsilon=4$. Note the IPR scale, the well-pronounced resonances at $k \simeq 230, 360, 770, 800, 840,$ and 990 , and the plain bump in the middle at $k \simeq 500$.

such Hamiltonians is presented. The result coincides with that corresponding to the well-known self-consistent phonon approximation.⁽²⁾

2. Two important examples of thermodynamic behavior are considered and sufficient conditions ensuring a soft-mode phase transition are isolated; cf. Figs. 1 and 2.

3. It is shown that the same *Ansatz* gives exactly soluble models of a classical lattice with a general (anharmonic) disorder. In this case the exact solution is less explicit and one needs additional approximations or computer simulations.

4. As a first example, we consider the case of Einstein (completely localized) phonons. Then, one gets explicit formulas for the free energy density and the "order parameter."

5. In the second example the similarity of a "quadratic disorder" to the Anderson model is stressed. Numerical results for a three-dimensional $10 \times 10 \times 10$ system based on the inverse participation ratio criterion predict localization of phonons and a pronounced mobility edge. This occurs if the probability distribution for a random field (corresponding to disorder) is chosen suitably and its amplitude ε exceeds a critical value ε_c . The first condition means that for a binary random field the sites with, e.g., $+\varepsilon$ percolate but their counterparts with $-\varepsilon$ do not.

A possibility of localization and nonergodic behavior in a structural transition model without disorder has been discussed in ref. 20.

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REFERENCES

1. A. D. Bruce and R. A. Cowley, *Structural Phase Transitions* (Taylor & Francis, London, 1981).
2. V. L. Aksenov, N. M. Plakida, and S. Stamenković, *Neutron Scattering by Ferroelectrics* (World Scientific, Singapore, 1987).
3. T. Schneider, E. Stoll, and H. Beck, *Physica* **79A**:201 (1975).
4. S. Stamenković, N. S. Tonchev, and V. A. Zagrebnov, *Physica A* **145**:262 (1987).
5. N. M. Plakida and N. S. Tonchev, *Theor. Math. Phys.* **63**:270 (1985).
6. N. M. Plakida and N. S. Tonchev, *Physica* **136A**:176 (1986).

7. J. G. Brankov, N. S. Tonchev, and V. A. Zagrebnov, *Ann. Phys. (N.Y.)* **107**:82 (1977).
8. J. G. Brankov, N. S. Tonchev, and V. A. Zagrebnov, *J. Stat. Phys.* **20**:317 (1979).
9. J. L. van Hemmen, *Phys. Rev. Lett.* **49**:409 (1982).
10. J. L. van Hemmen, A. C. D. van Enter, and J. Canisius, *Z. Phys. B Condensed Matter* **50**:311 (1983).
11. B. Kramer, G. Bergmann, and V. Bruynseraede, eds. *Localisation, Interaction and Transport Phenomena* (Springer, Berlin, 1985).
12. Y. Nagaoka and H. Fukuyama, eds., *Anderson Localisation* (Springer, Berlin, 1982).
13. J. L. van Hemmen, *Phys. Rep.* **65C**:43 (1980).
14. J. L. van Hemmen, *Phys. Rev. A* **34**:3435 (1986), in: *Mark Kac Seminar on Probability and Physics, Syllabus 1985–1987*, H. Maassen and F. den Hollander, eds. CWI Syllabus Series No. 17 (CWI, Amsterdam, 1988) 41–48, and work in preparation.
15. J. L. van Hemmen, *J. Phys. A* **15**:3891 (1982).
16. L. A. Pastur, *Commun. Math. Phys.* **75**:179 (1980).
17. J. Canisius and J. L. van Hemmen, *J. Phys. C* **18**:4873 (1985).
18. J. Canisius and J. L. van Hemmen, *Phys. Rev. Lett.* **46**:1487 (1981).
19. J. Canisius, J. L. van Hemmen, and T. M. Nieuwenhuizen, *Physica* **131A**:131 (1985).
20. V. L. Aksenov, M. Bobeth, N. M. Plakida, and J. Schreiber, *J. Phys. C* **20**:375 (1987).