Journal of Statistical Physics, Vol. 17, No. 5, 1977

On the Spectrum of the Dynamical Matrix for a Class of Disordered Harmonic Systems

M. Romerio [1] and W. F. Wreszinski [1]

Received February 1, 1977; revised March 21, 1977

We study some aspects of the effect of mass disorder on the spectrum of the dynamical matrix of an infinite crystal in the harmonic approximation. Under suitable conditions on the masses, it is shown that the spectrum contains an absolutely continuous part and a nonempty set of isolated point eigenvalues of finite multiplicity whose number is smaller than or equal to the number of impurity atoms if the latter is finite. These conditions are satisfied only in the limiting case of zero concentration of each species of impurity. We draw some conjectures and make remarks on the spectrum under less restrictive conditions on the masses and briefly compare them with known results for random harmonic systems.

KEY WORDS: Lattice vibrations; dynamical matrix; disordered system; absolutely continuous and pure point spectrum; localized modes.

1. INTRODUCTION AND SUMMARY

Consider the formal Hamilton function for lattice vibrations in a harmonic crystal in ν dimensions:

$$H_\Lambda = \sum_{\mathbf{n} \in \Lambda \subset \mathbb{Z}^\nu} \frac{p_\mathbf{n}^2}{2M_\mathbf{n}} + \frac{1}{2} \sum_{\mathbf{n},\mathbf{m} \in \Lambda \subset \mathbb{Z}^\nu} u_\mathbf{n} K_{\mathbf{n}-\mathbf{m}} u_\mathbf{m} \tag{1}$$

where K is some function[2] of positive type and finite range, the $u_\mathbf{n}$ are displacement variables about the equilibrium positions, and the $p_\mathbf{n}$ are the

Supported in part by the Swiss National Fund (to M.R.) and the Eidgenössische Stipendienkommission für ausländische Studierende (to W. F. W.).

[1] Institut de Physique, Université de Neuchâtel, Neuchâtel, Switzerland.

[2] In general, the displacements $U_\mathbf{n}$ are vectors and various quantities treated here as scalars, such as K, become matrices. Our methods can be trivially modified to handle this case, but the notation becomes rather involved.

corresponding momenta (we shall leave a precise mathematical formulation to Section 2). We assume for simplicity a Bravais lattice (only one atom per unit cell). Hamiltonian (1) describes a disordered system with a priori arbitrary but fixed masses $M_{\mathbf{n}}$ at sites $\mathbf{n}$. We shall be interested in the case of an infinite lattice (which we identified with $\mathbb{Z}^\nu$) and shall henceforth refer to fixed sets of masses $\{M_{\mathbf{n}}\}_{\mathbf{n}\in\mathbb{Z}^\nu}$ as "mass configurations." In a more realistic system with impurities, the couplings $K(\mathbf{n}-\mathbf{m})$ should also be replaced by general functions $K(\mathbf{n},\mathbf{m})$. However, "pure mass disorder," as described by (1), already exhibits several features distinguishing ordered from disordered systems.[1,3] Since we are primarily interested in qualitative information about the frequency spectrum, we restrict ourselves in this paper to these (simpler) systems.

The lattice-vibrational frequencies $\omega(q)$ satisfy in the limit of an infinite crystal the eigenvalue equation[1,2]

$$\omega(\mathbf{q})^2\eta(\mathbf{q}) = [1/(2\pi)^\nu]\int_B d\mathbf{q}'\,\rho(\mathbf{q}-\mathbf{q}')\tilde{K}(\mathbf{q}')\eta(\mathbf{q}') \qquad \mathbf{q}\in B, \quad \eta\in\mathscr{H}\equiv L^2(B, d^\nu\mathbf{q}) \tag{2}$$

where $B = [-\pi, \pi]^\nu$ is the first Brillouin zone in ν dimensions, and (formally)

$$\tilde{K}(\mathbf{q}) = \sum_{\mathbf{n}\in\mathbb{Z}^\nu}[\exp(i\mathbf{q}\cdot\mathbf{n})]K_{\mathbf{n}}, \qquad \mathbf{q}\in B \tag{3}$$

$$\rho(\mathbf{q}) = \sum_{\mathbf{n}\in\mathbb{Z}^\nu}(1/M_{\mathbf{n}})\exp(i\mathbf{q}\cdot\mathbf{n}), \qquad \mathbf{q}\in B \tag{4}$$

The η are related to displacement variables $u_{\mathbf{n}}\in l^2(\mathbb{Z}^\nu)$ by Fourier transformation:

$$u_{\mathbf{n}} = [1/(2\pi)^\nu]\int d^\nu p\,[\exp(i\mathbf{p}\cdot\mathbf{n})]\,\eta(\mathbf{p}) \tag{5}$$

The operator (formally) defined by the rhs of (2) is called a "dynamical matrix."[1,2] In this paper, we study some aspects of its spectrum.

The study of a number of models (for instance, the model of a single impurity at the origin imbedded on an otherwise perfect harmonic crystal[1,2]) suggests that for some infinite systems the spectrum of the dynamical matrix should consist of the union of an absolutely continuous part (corresponding to the perfect crystal) and a number of isolated point eigenvalues, which represent localized modes (with $|u_{\mathbf{n}}|$ of rapid decrease in $|\mathbf{n}|$). The number of the latter should be smaller or equal to the number of impurity atoms. In the case, for instance, of two-component systems consisting of a species of

[3] For a large class of harmonic systems, it can be shown that pure "mass disorder" is equivalent to pure "coupling disorder" (J. Hammerberg, private communication). The results of this paper are therefore applicable to some systems of the latter type.

"heavy" atoms and a species of "light" atoms, these localized modes may be interpreted as normal modes of vibration of groups of "light" atoms surrounded by "heavy" atoms (chains consisting of a number of "light" atoms lying between two "heavy" atoms in one dimension[1]).

In Section 2, precise conditions on the mass configurations are given under which the above-mentioned features of the spectrum may be proven rigorously. We believe that the framework given there is the appropriate one for the formulation and proof of various results in the literature (in particular, for those connected to Rayleigh's theorems[1]).

The assumptions in Section 2 hold only in the limiting case of zero concentration of each species of impurity atom. In Section 3, we make some remarks and conjectures about the spectrum under less restrictive assumptions on the masses, and briefly compare them with known results[3,4] for the random harmonic chain.

2. MATHEMATICAL FORMULATION AND RESULTS

To formulate the problem in a mathematically precise manner, we split out from ρ—for the moment still formally—a delta measure, corresponding to a perfect crystal where all the atoms have the greatest mass, by writing

$$1/M_{\mathbf{n}} = \lambda_{\mathbf{n}} + 1/M \tag{6}$$

where

$$0 < a \leqslant \inf_{\mathbf{n}\in\mathbb{Z}^\nu} M_{\mathbf{n}} \leqslant \sup_{\mathbf{n}\in\mathbb{Z}^\nu} M_{\mathbf{n}} \equiv M < \infty \tag{7}$$

It follows that $\lambda_{\mathbf{n}} \geqslant 0$, $\forall \mathbf{n} \in \mathbb{Z}^\nu$. On $\tilde{K}$ we assume: $\tilde{K}$ is bounded and continuously differentiable on B and

$$\nabla\tilde{K} \neq \mathbf{0} \quad \text{almost everywhere on } B \tag{8a}$$

and

$$\tilde{K}(\mathbf{q}) \geqslant 0 \qquad \forall \mathbf{q} \in B \tag{8b}$$

Letting now

$$\boldsymbol{\varphi}(\mathbf{q}) = \tilde{K}^{1/2}(\mathbf{q})\eta(\mathbf{q}) \tag{9}$$

we obtain formally from (2) the integral equation for $\boldsymbol{\varphi}$:

$$\omega(\mathbf{q})^2\boldsymbol{\varphi}(\mathbf{q}) = \frac{1}{M}\tilde{K}(\mathbf{q})\boldsymbol{\varphi}(\mathbf{q}) + \frac{1}{(2\pi)^\nu}\int_B d\mathbf{q}'\, \tilde{K}^{1/2}(\mathbf{q})\rho_1(\mathbf{q}-\mathbf{q}')\tilde{K}^{1/2}(\mathbf{q}')\boldsymbol{\varphi}(\mathbf{q}') \tag{10}$$

where $\rho_1 = \rho - (1/M)\delta$. We are therefore led to investigate the spectrum of the operator

$$H = H_0 + V \tag{11}$$

[4] See also the review by Lebowitz, and Ref. 15.[4]

where H_0 is the bounded symmetric operator defined on all $\varphi \in \mathscr{H}$ by

$$(H_0\varphi)(\mathbf{q}) = (1/M)\tilde{K}(\mathbf{q})\varphi(\mathbf{q}) \tag{12}$$

and V is defined by

$$V = \tilde{K}^{1/2} P \tilde{K}^{1/2} \tag{13}$$

where P is defined by

$$(P\varphi)(\mathbf{q}) \equiv \sum_{\mathbf{n}\in\mathbb{Z}^\nu} \lambda_{\mathbf{n}}(e_{\mathbf{n}}, \varphi) e_{\mathbf{n}}(\mathbf{q}) \tag{14}$$

where

$$e_{\mathbf{n}}(\mathbf{q}) \equiv [1/(2\pi)^{\nu/2}] \exp(i\mathbf{q}\cdot\mathbf{n}) \tag{15}$$

Let $\|\tilde{K}\|_0 = \inf_{\mathbf{p}\in B} \tilde{K}(\mathbf{p}) \geqslant 0$ [by (8b)] and $\|\tilde{K}\|_\infty \equiv \sup_{\mathbf{p}\in B} \tilde{K}(\mathbf{p}) < \infty$ [by (8a)]. By (7) and (13), V is a bounded operator on $\mathscr{H}$, with

$$\|V\| \leqslant \|\tilde{K}\|_\infty \left(\sup_{\mathbf{n}\in\mathbb{Z}^\nu} \lambda_{\mathbf{n}} \right) \tag{16}$$

It is also symmetric and positive, whence the spectrum of H is a subset of $\mathbb{R}_+$. From (8a) it follows that the spectrum Σ_{H_0} of H_0 is absolutely continuous (see, e.g., Ref. 5, p. 518, Example 19)[5]:

$$\Sigma_{H_0} = \Sigma_{H_0}^{\mathrm{ac}} = (1/M)[\|\tilde{K}\|_0, \|\tilde{K}\|_\infty]$$

Throughout this section, we shall require the $|\lambda_{\mathbf{n}}|_{\mathbf{n}\in\mathbb{Z}^\nu}$ to satisfy the condition

$$0 < \sum_{\mathbf{n}\in\mathbb{Z}^\nu} \lambda_{\mathbf{n}} < \infty \tag{17}$$

P is then a trace-class operator (see Refs. 5–7).

Proposition 2.1. Under condition (17),

$$\Sigma_H^{\mathrm{ac}} = \Sigma_{H_0} \tag{18}$$

and the part of Σ_H in the complement of Σ_{H_0} consists of isolated eigenvalues with finite multiplicity.

Proof. The trace-class operators form a two-sided ideal of the algebra of bounded operators on a Hilbert space (see, e.g., Ref. 6, p. 207). Hence V defined by (13) is also trace-class. It is also symmetric, whence (18) follows by a theorem of Kato (Ref. 5, Theorem 4.4, p. 540). The second part follows from the stability of the essential spectrum of a bounded symmetric operator by compact perturbations (Ref. 7, p. 362). ■

Remark 2.1. Condition (17) includes the case of a finite number of impurity atoms of various species imbedded in a crystal containing in addition

[5] We denote by Σ_A^{ac} the absolutely continuous part of the spectrum Σ_A of an operator A on $\mathscr{H}$.

an infinite number of atoms of the same species and mass M; results of the same type are given in Refs. 13 and 14. It is sufficient to take

$$M_{\mathbf{n}} = M \qquad \forall \mathbf{n} \notin \Lambda, \qquad \Lambda \text{ a finite subset of } \mathbb{Z}^{\nu} \tag{19}$$

In this case, V is degenerate, of rank not exceeding the number of points in Λ. The masses $M_{\mathbf{n}}$ of the impurity atoms are all smaller than M, and, depending on how much smaller, one may have the situation described in Section 1, where the set of isolated eigenvalues is not empty:

Proposition 2.2. Assume that

$$\|\tilde{K}^{-1}\|_1 \equiv [1/(2\pi)^{\nu}] \int_B d\mathbf{p}\, \tilde{K}^{-1}(\mathbf{p}) < \infty \tag{20}$$

Then there exists $\alpha < 1$ such that if

$$M_{\mathbf{n}} < \alpha M \qquad \text{for some } \mathbf{n} \in \mathbb{Z}^{\nu} \tag{21}$$

the isolated point spectrum of H is not empty.

Proof. Let $\varphi_{\mathbf{n}}$ be defined by

$$\boldsymbol{\varphi}_{\mathbf{n}}(\mathbf{p}) \equiv \tilde{K}^{-1/2}(\mathbf{p}) e_{\mathbf{n}}(\mathbf{p})$$

Then $\boldsymbol{\varphi}_{\mathbf{n}} \in \mathscr{H}$ and $\|\varphi_{\mathbf{n}}\|^2 = \|\tilde{K}^{-1}\|_1$. By (11)–(13),

$$(\boldsymbol{\varphi}_{\mathbf{n}}, H\boldsymbol{\varphi}_{\mathbf{n}})/\|\boldsymbol{\varphi}_{\mathbf{n}}\|^2 = 1/(M_{\mathbf{n}}\|\boldsymbol{\varphi}_{\mathbf{n}}\|^2) = 1/(M_{\mathbf{n}}\|\tilde{K}^{-1}\|_1) \tag{22}$$

We recall that $(\|\tilde{K}\|_{\infty}/M)$ is the upper bound of $\Sigma_{H_0}^{\mathrm{ac}}$ and that by Proposition 2.1 the part of the spectrum Σ_H in the complement of $\Sigma_{H_0}^{\mathrm{ac}}$ is an isolated point spectrum Σ_I. Hence it follows from (22) that Σ_I is not empty if

$$1/(M_{\mathbf{n}}\|\tilde{K}^{-1}\|_1) > (1/M)\|\tilde{K}\|_{\infty} \tag{23}$$

Inequality (23) is equivalent to (21), with

$$\alpha \equiv 1/(\|\tilde{K}^{-1}\|_1 \|\tilde{K}\|_{\infty})$$

We have

$$1 = [1/(2\pi)^{\nu}] \int_B d\mathbf{p}\, \tilde{K}^{-1}(\mathbf{p})\tilde{K}(\mathbf{p}) \leqslant \|\tilde{K}^{-1}\|_1 \|\tilde{K}\|_{\infty} \tag{24}$$

Equality in (24) is equivalent to

$$[1/(2\pi)^{\nu}] \int_B d\mathbf{p}\, \tilde{K}^{-1}(\mathbf{p})[\|\tilde{K}\|_{\infty} - \tilde{K}(\mathbf{p})] = 0$$

Since $\tilde{K}^{-1}(\mathbf{p}) \geqslant 0$ and $\tilde{K}$ is bounded, this last condition can hold only if $\tilde{K}(\mathbf{p}) = \|\tilde{K}\|_{\infty}$ almost everywhere on B. This is excluded by the gradient condition in (8a). Hence $\alpha < 1$. ■

Remark 2.2. As an example, take the case of nearest neighbor (nn) interactions, corresponding to the formal interaction Hamiltonian

$$\tfrac{1}{2}J \sum_{\substack{\mathbf{n}\in\mathbb{Z}^\nu \\ \mathbf{m}\ \text{nn of}\ \mathbf{n}}} (u_{\mathbf{n}} - u_{\mathbf{m}})^2$$

This leads [by (3)] to

$$\tilde{K}(\mathbf{p}) = J\left(\nu - \sum_{i=1}^{\nu} \cos p_i\right), \qquad \mathbf{p} \equiv (p_i)_{i=1}^{\nu} \tag{25}$$

Conditions (8) are clearly satisfied, but assumption (20) requires $\nu \geqslant 3$. In particular, if $\nu = 3$, $\|\tilde{K}\|_\infty = 6J$, and

$$\|\tilde{K}^{-1}\|_1 = 0.5054620197J^{-1}$$

(this is the Watson integral[8]), whence

$$\alpha = 1/3.0327721182 \simeq 1/3 \tag{26}$$

More generally, suppose that $\nu \geqslant 3$ and

$$\tilde{K}(\mathbf{q}) = J_0 + \sum_{l=1}^{N} J_l \sum_{\boldsymbol{\delta}_l} \cos(\mathbf{q}\cdot\boldsymbol{\delta}_l) \tag{27}$$

where, for each $l \geqslant 1$, $\boldsymbol{\delta}_l$ runs over the set of lth nearest neighbors of the origin, and conditions are imposed on the $\{J_l\}_{l\geqslant 0}$ in order to guarantee the validity of (8). Condition (20) is then, for $\nu = 3$, easily seen to be equivalent to the following constraint:

$$\left(\frac{\partial^2 \tilde{K}(\mathbf{p})}{\partial p_i^{\,2}}\right)_{\mathbf{p}=0} = -\sum_{l=1}^{N} J_l \sum_{n_i^l} (n_i^l)^2 \neq 0, \qquad i = 1, 2, 3 \tag{28}$$

where $\sum_{n_i^l}$ is a sum over the ith coordinates of the lth nearest neighbors. This assumption is equivalent to the existence of the continuum (elastic) limit where the frequencies $\omega(\mathbf{p}) \sim_{|\mathbf{p}|\to 0} |\mathbf{p}|$. ■

By methods of Ghirardi and Rimini[9] (see also Ref. 10), one may prove the following bound on the number N_E of eigenvalues of H in the interval (E, ∞), where $E > \|\tilde{K}\|_\infty/M$:

Proposition 2.3.

$$N_E < A(E) \equiv \int_{B\times B} d\mathbf{p}\, d\mathbf{p}'\, |V(\mathbf{p}, \mathbf{p}')|^2 [E - \tilde{K}(\mathbf{p})/M]^{-1} [E - \tilde{K}(\mathbf{p}')/M]^{-1} \tag{29}$$

where

$$V(\mathbf{p}, \mathbf{p}') \equiv \frac{1}{(2\pi)^\nu} \tilde{K}^{1/2}(\mathbf{p}) \sum_{\mathbf{n}\in\mathbb{Z}^\nu} \lambda_{\mathbf{n}} \{\exp[i(\mathbf{p} - \mathbf{p}')\cdot\mathbf{n}]\} \tilde{K}^{1/2}(\mathbf{p}') \quad ■ \tag{30}$$

It is easy to prove that, if $\nu = 1, 2$,

$$A(E) \xrightarrow[E\downarrow(\|\tilde{K}\|_\infty/M)]{} +\infty \tag{31}$$

while $A(E)$ remains finite as $E \downarrow (\|\tilde{K}\|_\infty/M)$ if $\nu = 3$ for a large class of functions $\tilde{K}$, which includes (25). This *may* be an indication that there might (for $\nu = 1, 2$) be accumulation of the eigenvalues at the boundary point $E = \|\tilde{K}\|_\infty/M$. We do not expect this to happen, however, if there is a finite number of impurity atoms:

Proposition 2.4. Let (19) hold and $N(\Lambda)$ be the number of points in Λ. If N is the number of discrete eigenvalues of H, then

$$N \leqslant N(\Lambda) \tag{32}$$

Proof. P is of finite rank $N(\Lambda)$ (see Remark 2.1), and V is also of finite rank r such that (see, e.g., Ref. 5, p. 160)

$$r \leqslant N(\Lambda) \tag{33}$$

Since V is a positive self-adjoint operator of rank r, there exists an orthonormal system $\{\Phi_i\}_{i=1}^r$ such that

$$V = \sum_{i=1}^{r} \mu_i(\Phi_i, \cdot)\Phi_i, \qquad \mu_i > 0$$

Let ν_i ($i \geqslant 1$) be defined by

$$\nu_1 = \max_{\|\Phi\|=1} (\Phi, H\Phi)$$

$$\nu_i = \min_{\Psi_1,\ldots,\Psi_{i-1}} \max_{\Phi\in(\Psi_1,\ldots,\Psi_{i-1})^\perp, \|\Phi\|=1} (\Phi, H\Phi), \qquad i \geqslant 2$$

It follows that $\nu_i \geqslant \nu_{i+1}$ and that

$$\begin{aligned}
\nu_i &= \min_{\Psi_1,\ldots,\Psi_{i-1}} \max_{\Phi\in(\Psi_1,\ldots,\Psi_{i-1})^\perp, \|\Phi\|=1} \left[(\Phi, H_0\Phi)\right. \\
&\qquad \left. + \sum_{k=1}^{r} \mu_k |(\Phi_k, \Phi)|^2\right] \\
&\leqslant \max_{\Phi\in(\Phi_1,\ldots,\Phi_{i-1})^\perp \|\Phi\|=1} (\Phi, H_0\Phi) \\
&\leqslant \max_{\|\Phi\|=1} (\Phi, H_0\Phi) \equiv \nu_0 \qquad \text{if} \quad i \geqslant r+1
\end{aligned} \tag{34}$$

On the other hand, it follows from the fact that V is positive that, for all $i \geqslant 2$,

$$\nu_i \geqslant \min_{\Psi_1,\ldots,\Psi_{i-1}} \max_{\Phi\in(\Psi_1,\ldots,\Psi_{i-1})^\perp, \|\Phi\|=1} (\Phi, H_0\Phi) \tag{35}$$

By a version of Weyl's min-max principle (Proposition A.1 of the appendix) applied to H_0, it follows that the right-hand side of (35) is independent of i and is the upper end of the essential spectrum of H_0, namely ν_0. Hence from (35) we get

$$\nu_i \geqslant \nu_0 \qquad \text{for all } i \tag{36}$$

From (34) and (36) it follows that $\nu_i = \nu_0$ for all $i \geqslant r + 1$. Hence, by the

same Proposition A.1, ν_{r+1} is the upper end of the essential spectrum of H and there are at most r (discrete) eigenvalues of H. The final assertion follows from (33). ■

Remark 2.3. (1) A similar argument was used by Perez[11] to prove that the number of two-magnon bound states in the Heisenberg ferromagnet in ν dimensions is less than or equal to ν.

(2) The above proposition also provides a general variational principle which might be useful for the numerical calculation of the energies of all localized modes.

(3) Result (32) is optimal because we expect the discrete eigenvalues of H to dissolve in the continuum where the mass ratios $M_{\mathbf{n}}/M$ get sufficiently close to one.

We finally consider the space-decay properties of the $U_{\mathbf{n}}$ for the discrete spectrum, recalling transformation (9). Let $\tilde{K}$ be given by (37) (with suitable $\{J_l\}_{l=0}^{N}$; see Remark 2.2).

Proposition 2.5. Under the assumptions of Proposition 2.4, let $\eta \in \mathscr{H}$ satisfy the eigenvalue equation

$$(H_0 + P\tilde{K})\eta = E\eta, \qquad E > (\|\tilde{K}\|_\infty/M) \tag{37}$$

and $U_{\mathbf{n}}$ be related to η bu (5). Then

$$\sum_{N\in\mathbb{Z}^\nu} (1 + |\mathbf{n}|)^k |u_{\mathbf{n}}| < \infty \qquad \forall k \in \mathbb{Z}_+ \tag{38}$$

Proof. By (37)

$$\eta(\mathbf{p}) = [E - \tilde{K}(\mathbf{p})/M]^{-1} \times \int_B d\mathbf{p}' \left\{ \sum_{\mathbf{n}\in\Lambda} \lambda_{\mathbf{n}} \exp[i(\mathbf{p} - \mathbf{p}')\cdot\mathbf{n}] \right\} \tilde{K}(\mathbf{p}')\eta(\mathbf{p}'), \qquad \mathbf{p} \in B \tag{39}$$

$\mathbf{p} \to \tilde{K}(\mathbf{p})$ given by (27) is a periodic function of each component p_i of $\mathbf{p}$ with period 2π. From this, (39), and the fact that $\eta \in \mathscr{H}$, it follows that η is infinitely differentiable, and any partial derivative of η is a periodic function of each component of its argument with period 2π. Hence (38) follows by a standard result (e.g., Ref. 12, Theorem 513, p. 528).[6] ■

3. REMARKS ON THE CASE OF NONZERO CONCENTRATION AND COMPARISON WITH RANDOM HARMONIC SYSTEMS

Both condition (17) and the condition

$$\sum_{\mathbf{n}\in\mathbb{Z}^\nu} \lambda_{\mathbf{n}}^2 < \infty \tag{40}$$

[6] The falloff may actually be proven to be exponential; see Ref. 15.

(which implies that V is a Hilbert–Schmidt operator) can hold only if the number of impurity atoms of each species is finite—that is, in the limiting case of zero concentration of each species of impurity. If condition (17) is relaxed, however, and only (40) is required, there no longer exists a general proof that $\Sigma_H^{ac} = \Sigma_{H_0}$: there exist Hilbert–Schmidt operators V such that $H = H_0 + V$ has a pure point spectrum (everywhere dense in Σ_{H_0}) (Theorem of Weyl–von Neumann; Ref. 5, p. 523). Mathematically, the whole problem consists in finding a proof of asymptotic completeness for a class of bounded but nonlocal potentials, and where the "kinetic energy" is a function satisfying (8). On the other hand, it seems to us possible that Weyl–von Neumann phenomena occur for certain mass configurations, yielding a pure point spectrum for the dynamical matrix. We discuss below some reasons why (and conditions under which) this might be expected.

In Ref. 3, Casher and Lebowitz considered the flux density J in the steady state in a harmonic crystal whose ends, separated by a distance L, were kept in contact with heat reservoirs at different temperatures. They proved that J does not tend to zero as $L \to \infty$ (and therefore the thermal conductivity[3] is infinite) if the spectrum of the dynamical matrix contains an absolutely continuous part. For zero impurity concentration one expects infinite thermal conductivity just as for the perfect harmonic crystal. If it is nonzero, however, one might expect that collisions between lattice waves and impurities would be sufficient in number to provide a finite thermal conductivity (and hence no ac spectrum) for *certain* distributions of impurities. This cannot be expected for a harmonic crystal with an arbitrary distribution of impurities (with nonzero concentration) because periodic configurations (corresponding to a unit cell containing two or more different atoms) give rise to infinite thermal conductivity and an ac spectrum.

The latter difficulties do not occur for random harmonic chains (corresponding to the mass at each site being an independent random variable). For such systems it was proved in Ref. 3 that the spectrum of the dynamical matrix has, with probability one, no absolutely continuous part. It seems to us to be an interesting open problem to find precise conditions on the masses implying results of comparable generality for the nonrandom case, with nonzero concentration of each species of impurity.

APPENDIX

The following proposition is essentially Proposition II.32 of Ref. 10:

Proposition A.1. Let H be a positive, bounded, self-adjoint operator on a Hilbert space $\mathscr{H}$, and $\{\Psi_i\}_{i=1}^{\infty}$ (varying) orthonormal bases of $\mathscr{H}$. Let

$$\nu_n(H) \equiv \min_{\Psi_1,\ldots,\Psi_{n-1}} \left[\max_{\Phi \in (\Psi_1,\ldots,\Psi_{n-1})^{\perp}, \|\Phi\|=1} (\Phi, H\Phi) \right]$$

Then, either (a) $\nu_n(H)$ is the nth eigenvalue for H, counting multiplicity (and counted from the greatest eigenvalue); or (b) $\nu_n(H)$ is the upper end of the essential spectrum, in which case $\nu_n = \nu_{n+1} = \cdots$ and there are at most $n - 1$ eigenvalues. ■

ACKNOWLEDGMENTS

We are greatly indebted to Prof. J. L. Lebowitz for his critical comments on the manuscript and for his interest. We should also like to thank Dr. J. Hammerberg for fruitful discussions, and the referee for helpful remarks and corrections.

NOTE ADDED IN PROOF

After the completion of this paper, we received van Hemmen's preprint[15] where many of our results are generalized, in particular to include nonprimitive lattices.

REFERENCES

1. A. A. Maradudin, E. W. Montroll, and G. H. Weiss, Theory of Lattice Dynamics in the Harmonic Approximation, in *Solid State Physics, Suppl. 3* (Academic Press, New York, 1963).
2. R. J. Elliott, Impurity and Anharmonic Effects in Lattice Dynamics, in *Proc. Int. School Phys. E. Fermi, Course LV*, S. Califano, ed. (Academic Press, New York, 1975).
3. A. Casher and J. L. Lebowitz, *J. Math. Phys.* **12**:1701 (1971).
4. J. L. Lebowitz, Nonequilibrium Statistical Mechanics, *Cours de Troisième Cycle en Suisse Romande, Summer 1976*, and references therein.
5. T. Kato, *Perturbation Theory for Linear Operators* (Springer Verlag, Berlin, 1966).
6. M. Reed and B. Simon, *Methods of Modern Mathematical Physics*, Vol. 1, *Functional Analysis* (Academic Press, New York, 1972).
7. F. Riesz and B. Sz-Nagy, *Leçons d'Analyse Fonctionnelle*, 4th ed. (Gauthier-Villars, Paris, 1965).
8. G. N. Watson, *Quart. J. Math.* **10**:266 (1939).
9. G. C. Ghirardi and A. Rimini, *J. Math. Phys.* **6**:40 (1965).
10. B. Simon, *Hamiltonians Defined as Quadratic Forms* (Princeton Univ. Press, 1971).
11. J. F. Perez, Thesis, ETH Zürich (1973), (unpublished).
12. F. Trèves, *Topological Vector Spaces, Distributions and Kernels* (Academic Press, New York, 1967).
13. A. O'Connor and J. L. Lebowitz, *J. Math. Phys.* **15**:692 (1974).
14. O. E. Lanford and J. L. Lebowitz, in *Dynamical Systems*, J. Moser, ed. (Lecture Notes in Physics, Vol. 38, Springer Verlag, 1976).
15. L. van Hemmen, A Generalization of Rayleigh's Theorem to the Infinite Harmonic Crystal, Preprint I.H.E.S. (1977).