Journal of Statistical Physics, Vol. 18, No. 1, 1978

A Generalization of Rayleigh's Theorem for the Infinite Harmonic Crystal

Leo van Hemmen[1]

Received May 31, 1977

We show that if one replaces N masses in an infinite harmonic, perfect ν-dimensional crystal by N_1 lighter and N_2 heavier ones such that $N_1 + N_2 = N$ is finite, then one introduces at most νN_1 (isolated) bound states. This can be considered as an extension of the results of Romerio and Wreszinski.

KEY WORDS: Lattice dynamics; impurities; isolated frequencies.

Consider the equations of motion of an infinite harmonic crystal in ν dimensions, with $\mathbb{Z}^\nu$ labeling the particles. Let M_n be the mass at the site $n \in \mathbb{Z}^\nu$ and let $\alpha = 1,..., \nu$; then[1]

$$M_n \ddot{x}_\alpha(n) = -\sum_{m,\beta} \Phi_{\alpha,\beta}^{n,m}\, x_\beta(m) \tag{1}$$

where m runs through $\mathbb{Z}^\nu$, $\beta = 1,..., \nu$, and $x_\beta(m)$ is the deviation of the mth particle in the Cartesian β-direction of $\mathbb{R}^\nu$. In (1), $\Phi = \{\Phi_{\alpha,\beta} | \alpha, \beta = 1,..., \nu\}$ is called the *interaction matrix*. We assume

$$\Phi_{\alpha,\beta}^{n,m} = \Phi_{\alpha,\beta}^{n-m}; \qquad \Phi_{\alpha,\beta}^{n-m} = 0, \qquad |n-m| > N_0 \tag{2}$$

that is, a translationally invariant, finite-range interaction. For an extensive study of the infinite harmonic crystal we refer to Ref. 2 (cf. also Ref. 3). By a (canonical) transformation we can rewrite (1) in the form

$$\ddot{x}_\alpha(n) = -\sum_{m,\beta} M_n^{-1/2} \Phi_{\alpha,\beta}^{n,m} M_m^{-1/2} x_\beta(m) \tag{3}$$

Supported by the Netherlands Organization for the Advancement of Pure Research (Z.W.O.).

[1] Institut des Hautes Etudes Scientifiques, Bures-sur-Yvette, France.

Upon introducing the diagonal mass matrix $\mathbf{M}$, defined by $(\mathbf{M}x_\alpha)(n) = M_n x_\alpha(n)$, and putting $x = (x_\alpha)$, we find that (3) is nothing but

$$\ddot{x} = -\mathbf{M}^{-1/2}\Phi\mathbf{M}^{-1/2}x \equiv -\Phi_\mu x \tag{4}$$

We are interested in $\sigma(\Phi_\mu)$, the spectrum of $\mathbf{M}^{-1/2}\Phi\mathbf{M}^{-1/2}$ as an operator in $\mathscr{H} = \bigoplus_1^\nu l^2(\mathbb{Z}^\nu)$. We say $x \in \mathscr{H}$ describes a *bound state* if $x \neq 0$ and $\Phi_\mu x = \lambda x$, or, equivalently, if x is an eigenvector with eigenvalue λ. Clearly, x is more or less "localized." In addition, we assume $\Phi x = 0 \Leftrightarrow x = 0$, i.e., $\lambda = 0$ is never an eigenvalue. By stability, $\Phi \geqslant 0$.

If $M_n = M$, $\forall n \in \mathbb{Z}^\nu$, $\mathbf{M} = M\mathbb{1}$ and the spectrum of $M^{-1}\Phi \equiv \Phi_0$ is well known (Ref. 2, p. 131 and Section 3.4): It is absolutely continuous and consists of a closed interval $[0, P]$. Actually, by Fourier transformation, Φ_0 is unitarily equivalent to the *dynamical matrix* $D(k)$ which is defined on the Brillouin zone (BZ); in this case we have ν acoustic modes.[1] Running waves with wave vector $k \in$ BZ are associated with the spectrum of Φ_0; evidently, they are not localized at all! We now perturb this pleasant situation somewhat.

Denote by $|\Lambda|$ the number of points in $\Lambda \subseteq \mathbb{Z}^\nu$. Let $\Lambda = \Lambda_1 \cup \Lambda_2$, and let $\mathbb{Z}^\nu = \Lambda_1 \cup \Lambda_2 \cup (\mathbb{Z}^\nu - \Lambda)$ be a partition of $\mathbb{Z}^\nu$ into three disjoint regions with finite $N = |\Lambda| = |\Lambda_1| + |\Lambda_2| = N_1 + N_2$ and such that

$$M_n < M, \quad n \in \Lambda_1; \qquad M_n > M, \quad n \in \Lambda_2 \tag{5}$$

while $M_n = M$ for $n \notin \Lambda$, i.e., we replace some masses by lighter ones and some by heavier ones. Problem: Describe $\sigma(\Phi_\mu)$ and, more specifically, give the number of eigenvalues—including their multiplicities. This is also of interest for ergodic theory because one can show[2,3] that if Φ_μ does not have any eigenvalue [that is, the point spectrum $\sigma_p(\Phi_\mu)$ is empty], then the system is not only ergodic, but also weakly mixing, or even Bernoulli when the singular continuous spectrum is absent. We now turn to the solution of our problem.

As $(\mathbf{M}^{-1} - M^{-1}\mathbb{1})$ is a finite-rank operator (or equivalently trace class because there is only a finite number of masses in nature), the same holds for $(\mathbf{M}^{-1/2} - M^{-1/2}\mathbb{1})$ and thus also for

$$\mathbf{M}^{-1/2}\Phi\mathbf{M}^{-1/2} - M^{-1/2}\Phi M^{-1/2} = \Phi_\mu - \Phi_0 \tag{6}$$

According to Ref. 4, $\sigma_{ac}(\Phi_\mu) = \sigma_{ac}(\Phi_0)$. But not only does the absolutely continuous spectrum remain the same; the essential spectrum does not change either.[4,5] So we can expect only isolated eigenvalues of finite multiplicity *outside* $[0, P]$, and accordingly we focus our attention on that part of $\sigma_p(\Phi_\mu)$. One easily shows that $\lambda \in \sigma_p(\mathbf{M}^{-1/2}\Phi\mathbf{M}^{-1/2})$ is equivalent to $\lambda \in \sigma_p(\Phi^{1/2}\mathbf{M}^{-1}\Phi^{1/2})$ and that the multiplicity is the same in both cases; the second representation has the advantage of being linear in $\mathbf{M}^{-1}$, and thus in the perturbation.

Au fond, we have to generalize "Rayleigh's theorem" (Ref. 1, Chapter VIII) to the case of an *infinitely* extended system; to do this the use of the *Weinstein–Aronszajn* (WA) *determinant*[4] will be instrumental. Let $S = T + A$, where $A = \sum_{j=1}^{m} |x_j\rangle\langle e_j|$, $m < +\infty$, and define the WA determinant as

$$\omega(\zeta) \equiv \omega(\zeta; T, A) = \det\{\delta_{jk} + (e_j, R(\zeta)x_k)\} \tag{7}$$

where $R(\zeta) = (T - \zeta)^{-1}$. In our case $T = \Phi_0$, or the like; $\omega(\zeta)$ is then a meromorphic function in $\Delta = \mathbb{C}\backslash[0, P]$. Introduce, furthermore, the multiplicity function

$$\nu(\zeta; \omega) = \begin{cases} k & \text{if } \zeta \text{ is a zero of } \omega \text{ of order } k \\ -k & \text{if } \zeta \text{ is a pole of } \omega \text{ of order } k \\ 0 & \text{for other } \zeta \in \Delta \end{cases}$$

and

$$\tilde{\nu}(\zeta; T) = \begin{cases} 0 & \text{if } \zeta \notin \sigma(T) \\ \dim \mathbf{P} & \text{if } \zeta \text{ is an isolated point of } \sigma(T) \\ +\infty & \text{in all other cases} \end{cases}$$

where $\mathbf{P}$ is the projection associated with the isolated point ζ of $\sigma(T)$. Then the (first) WA formula says[4]

$$\tilde{\nu}(\zeta; S) = \tilde{\nu}(\zeta; T) + \nu(\zeta; \omega) \tag{8}$$

So the function $\tilde{\nu}$ gives precise information about the isolated points of the spectrum.

Theorem. The number of bound states (including multiplicity) outside $[0, P]$ does not exceed νN_1.

Proof. By induction. Suppose the theorem holds for $N = N_1 + N_2$. We replace the mass M at x by M_x; either (a) $M_x < M$ or (b) $M_x > M$.

(I) $\nu = 1$. The (first) WA formula (8) says, with

$$T = \Phi^{1/2}\mathbf{M}_N^{-1}\Phi^{1/2}, \qquad A = (M_x^{-1} - M^{-1})P_x \equiv \mu|e\rangle\langle e| \tag{9}$$

and P_x as the projection on the site x, that

$$\omega(\zeta; T, A) = 1 + \mu(\Phi^{1/2}e, [\Phi^{1/2}\mathbf{M}_N^{-1}\Phi^{1/2} - \zeta]^{-1}\Phi^{1/2}e) \tag{10}$$

Suppose, for instance, that $N_1 = 2$; $\Phi^{1/2}\mathbf{M}_N^{-1}\Phi^{1/2}$ is self-adjoint, so $\omega(\zeta)$ may be rewritten in the form (putting $\Phi^{1/2}e = f$)

$$\omega(\zeta) = 1 + \mu\int_0^P (\lambda - \zeta)^{-1}\, d\|E_\lambda f\|^2 + \sum_{i=1}^{N_1} \mu(\lambda_i - \zeta)^{-1}|(e_i, f)|^2 \tag{11}$$

and we now expect two poles, say in λ_1 and λ_2. We find the new bound

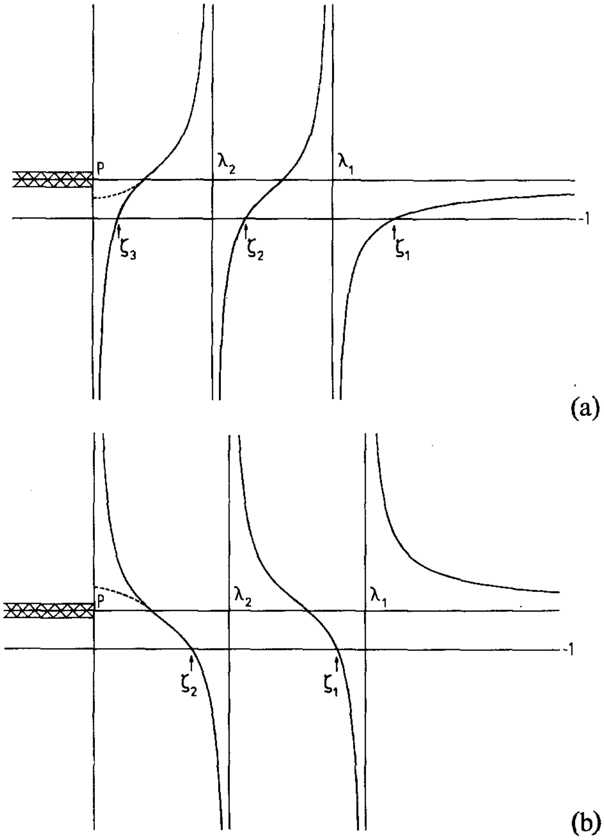

Fig. 1. (a) $\omega(\zeta) - 1$ when $\mu > 0$ ($M_{N+1} < M$); (b) $\omega(\zeta) - 1$ when $\mu < 0$ ($M_{N+1} > M$).

states where $\omega(\zeta) = 0$ and $\zeta > P$; see Fig. 1. The zeros of $\omega(\zeta)$ are the points ζ_i where the plotted $[\omega(\zeta) - 1]$ crosses the horizontal line -1. The dotted lines, though characteristic for the infinite system, will not enter the picture before (III) and (IV).

Clearly, $\omega(\zeta)$ has three zeros when $\mu > 0$ and only two when $\mu < 0$. Moreover, the order of the zeros is *one*; to see this, it suffices to prove $\omega'(\zeta_i) \neq 0$. When $\zeta \notin \sigma(T)$, $\omega(\zeta)$ is analytic in a neighborhood of ζ and

$$\omega'(\zeta) = \mu(\Phi^{1/2}e, [\Phi^{1/2}\mathbf{M}_N^{-1}\Phi^{1/2} - \zeta]^{-2}\Phi^{1/2}e) \tag{12}$$

being zero implies

$$|\Phi^{1/2}\mathbf{M}_N^{-1}\Phi^{1/2} - \zeta|^{-1}\Phi^{1/2}e = 0 \Rightarrow \Phi^{1/2}e = 0 \tag{13}$$

so $e = 0$ and we have a contradiction. Ergo, $\omega'(\zeta_i) \neq 0$. Notice that the slopes of the curves in Fig. 1 are in agreement with (12). Finally, if there is not a pole in λ_2 (e.g.), ζ_2 moves to the left in Fig. 1a but ζ_3 is missing. There is no problem, however, for in this case $\tilde{\nu}(T, \lambda_2) = +1$, while $+1$ would be compensated by $\nu(\omega, \lambda_2) = -1$ if there were a pole in λ_2. An analogous argument applies to Fig. 1b.

(II) $\nu = 2$. Nothing changes essentially. Only

$$A = \mu|e_1\rangle\langle e_1| + \mu|e_2\rangle\langle e_2| \tag{14}$$

as the interaction matrix is now 2×2, and we add these two projection operators one after the other. Also here $|\omega(\zeta)|$ is supposed to blow up when ζ approaches P from above. Intuitively, the reason is the following. Take $N_1 = 1$ and $N_2 = 0$. P is the *maximum* of a certain eigenvalue $\omega_i(k)^2$ of the dynamical matrix $D(k)$, say $P = \omega_i(k_0)^2$. A Taylor expansion then gives

$$\omega_i(k)^2 - \omega_i(k_0)^2 = \tfrac{1}{2}(k - k_0)^2(\omega_i^2)''(k_0) + \cdots \tag{15}$$

in a neighborhood of k_0 when $\nu = 1$, while an analogous relation holds when $\nu = 2$; cf. also Ref. 2, Figs. VII.7–VII.11. Combining (10) and (15) gives the desired result. In (IV) we shall point out what can be said in general.

(III) $\nu = 3$. When $\nu = 3$, however, the reasoning around (15) breaks down and we may get the dotted line near P and thus no bound states. If $\mu > 0$ is large enough, the dotted line will cross -1 in $\zeta_1 > P$ and we are done again. A rough estimate for such a μ is

$$\mu(e_1, \Phi e_1) > P \tag{16}$$

(IV) $\nu = 1, 2$, or 3. As soon as the dotted line appears above -1, the number of bound states does not increase any more. At the left-hand side of zero we never get a bound state: In case of $\mu < 0$ the function $[\omega(\zeta) - 1]$ is monotonically *decreasing* from zero to $M/M_n - 1$ when ζ goes from $-\infty$ to 0; the case $\mu > 0$ is trivial. Of course this last result also follows from general considerations (positivity). ∎

Let us add some remarks. First, notice that the order of the zeros of $\omega(\zeta)$ corresponds with the multiplicity of the eigenvalues. Second, we recovered the result that any mass $< M$ ($> M$) does (does not) give a bound state when being placed in a perfect one-dimensional lattice.[6,7] Third, there is a quite natural argument (not a proof) that there are no bound states inside $[0, P]$ when $\nu = 1$ or 2. Suppose on the contrary that they were there. We then would have, after a Fourier transformation of $\Phi^{1/2}\mathbf{M}^{-1}\Phi^{1/2}x = \lambda x$ with $\lambda \in [0, P]$, that $\lambda = \omega_i(k_0)^2$ while at the same time

$$\hat{x}(k) = [\lambda - D(k)]^{-1} \sum_{n=1}^{\nu N} \mu_n \hat{f}_n(k)(f_n, x) \qquad \text{[a.e.]} \tag{17}$$

But

$$[\lambda - D(k)]^{-1} = \sum_{i=1}^{\nu} [\omega_i(k_0)^2 - \omega_i(k)^2]^{-1}|d_i\rangle\langle d_i| \tag{18}$$

and the functions $[\omega_i(k_0)^2 - \omega_i(k)^2]^{-1}$ are *not* in $L^2(\mathrm{BZ})$ when $\nu = 1$ or 2, so we do not expect that $\hat{x}$ will be there either. Thus $x \in \mathscr{H}$ cannot be realized, prohibiting λ to be an eigenvalue.

Finally we remark that these techniques can be applied equally well to nonprimitive lattices. They enable us to strengthen considerably the results of Romerio and Wreszinski,[8] who used completely different (and more global) methods. Let us add that the assertions of Ref. 8 on the spatial decay properties of the eigenvectors x satisfying $\mathbf{M}^{-1/2}\Phi\mathbf{M}^{-1/2}x = \lambda x$ with $\lambda \notin [0, P]$ are actually much better than is stated. When the interaction is finite range, the components of x tend to zero *exponentially*, as follows from a relation like (17) (study $\Phi\mathbf{M}^{-1}y = \lambda y$ with $y = \mathbf{M}^{1/2}x$ and $M_n = M$ when $|n|$ is sufficiently large) combined with an analyticity argument; cf. Ref. 2, Section 3.4, and Ref. 7.

ACKNOWLEDGMENTS

I express my gratitude to Stig Andersson and George Hagedorn for some stimulating discussions, and to Prof. D. Ruelle and Prof. N. H. Kuiper for the hospitality extended to me at the IHES.

REFERENCES

1. A. A. Maradudin *et al.*, *Theory of Lattice Dynamics in the Harmonic Approximation*, 2nd ed. (Academic Press, New York, 1971).
2. J. L. van Hemmen, Dynamics and ergodicity of the infinite harmonic crystal, thesis, Univ. of Groningen (1976); available from University Microfilms, number 77-70,001.
3. O. E. Lanford III and J. L. Lebowitz, *Springer Lecture Notes in Physics*, No. 38 (1975), p. 144.
4. T. Kato, *Perturbation Theory for Linear Operators* (Springer-Verlag, New York, 1966), esp. pp. 540, 244.
5. M. Schechter, *Spectra of Partial Differential Operators* (North-Holland, Amsterdam, 1971), Ch. 1.
6. R. I. Cukier and P. Mazur, *Physica* **53**:157 (1971).
7. O. Madelung, *Festkörpertheorie III* (Springer-Verlag, 1973), pp. 70–74.
8. M. Romerio and W. F. Wreszinski, On the spectrum of the dynamical matrix for a class of disordered harmonic systems, Preprint, Univ. de Neuchâtel (1977).