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Determination of the inelastic neutron scattering cross section by the spectral moments method: application to incommensurate crystals and quasi-crystals

C Benoit
Groupe de Dynamique des Phases Condensées (Unité Associée au CNRS 233), Université de Montpellier, USTL 34060, Montpellier Cédex, France

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Abstract. If we work directly with the dynamic matrix, the spectral moments method allows the direct determination of the response of harmonic materials without any calculation of eigenvalues or eigenvectors. The method selects directly in the frequency spectrum the active modes with the right magnitude. We present here a new development of this method and we apply it to the determination of the inelastic neutron scattering cross section of systems. We illustrate these results via applications to several models: a perfectly dimerised chain, chains with incommensurate distortions and quasi-crystals.

1. Introduction

Many physical properties of a many-body system are closely related to the spectrum of the Schrödinger equation. Of particular interest for physical applications are the density of states and the behaviour of the wavefunction (localised, extended, chaotic or non-chaotic). Examples include harmonic solids, band theory and the Ising model. Recently, many physical systems have been made which have a quasi-crystal or fractal structure (Family and Landau 1984). The vibrational properties and mechanical behaviour of these systems are very different from those of ordinary objects, and calculations of the physical properties of these non-crystalline systems require special techniques that do not make use of the translational invariance. The problem of determining the vibrational properties of a disordered system was first solved by Dyson (1953) for a linear chain and these systems have been widely studied since the work of Dean (1960). Ingenious methods were also developed to study some other properties of one-dimensional systems (Mattis and Lieb 1966). Unfortunately, neither the methods nor the results can in general be extended to the three-dimensional case. Also several different approaches have been developed; the most important are the recursion method (see Haydock *et al* 1972) and for a review see Haydock (1980)) and the moments method (Cyrot-Lackmann 1967, Gaspard and Cyrot-Lackmann 1973).

The recursion method is an adaptation of the Lanczos (1950) algorithms to solid state physics. In this method, we first choose a particular vector and then set up new orthogonal bases (Krylov space) (Saad 1981). In this new base the Hamiltonian takes a tridiagonal form. The eigenvalues of this matrix are easily obtained by iteration. This method is

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numerically very stable and fast, needs to store only two vectors and is unique in obtaining the local and global properties of local orbital interactions *en masse* (Kelly 1980, Ishii and Fujiwara 1980). However, the continued-fraction coefficients cannot be averaged as these are strongly non-linear on the density of state, and knowledge of the total density of state involves the sum of the local densities of states (Heine 1980). A second method makes use of the moments of the density of state. Since the work of Montroll (1942), various computational methods have been devised: the modified moments method (Blumstein and Wheeler 1973, Wheeler *et al* 1974), the generalised moments method (Cyrot-Lackmann 1967, Gaspard and Cyrot-Lackmann 1973, Lambin and Gaspard 1982) which has the advantage of both moments method (linearity of the moments) and the recursion method (stability). Recently, Jurczek (1985) proposed an improved moments method that permits one to determine exactly the coefficients of the continued-fraction representation of the electronic density of states. He showed, also, that both methods are equivalent.

However, it is well known that the density of states often exhibits many gaps and sharp features. For such systems the representations of density of states from moments suffer from the inability to reproduce accurately the singularities. We are faced, in practice, with the asymptotic behaviour of the continued-fraction coefficients (Turchi *et al* 1982). Furthermore, any of these methods permits us to compute easily and with accuracy the eigenstates of the systems. It is well known that, in particular for large systems, if the eigenvalues can, in principle, be easily found, the determination of the eigenvectors with acceptable accuracy is a non-trivial problem (Isaacson and Keller 1966, Dean 1972). However, the determination of many physical properties requires good knowledge of the eigenstates of the Schrödinger equation or eigenvectors of the dynamic matrix. For instance, it is well known that, for harmonic solids, it is necessary to compute the eigenvectors to calculate the infrared absorption or the Raman scattering spectra of the system.

For harmonic solids, these difficulties are partially removed if we calculate directly the response function of the system (Galtier and Benoit 1981). While for electronic systems the calculus of the response function involves transitions between different states, for harmonic systems, from Bose statistics and properties of the harmonic oscillator, the calculation of the response function corresponds to the determination of the one-phonon density of states weighted by the optical activity of the modes. Using these properties, we have shown (Benoit 1987, hereafter referred to as I) that the moments method could be applied to direct determination with the exact magnitude of the infrared absorption or ($T = 0$ K) Raman scattering spectra. The method that we shall call the spectral moments method is fast, stable and linear and requires usually the determination of a few coefficients of the continued fraction.

In I, this method was applied only to the determination of the activity of optical processes. For these processes the momentum transfer is equal to zero. We show here that the spectral moments method can also be applied to the determination of the inelastic neutron scattering cross section of solids. In such a process, it is necessary to determine the spectrum of scattered particles for many different momentum transfers. So, in the following, we show how the spectral moments method can be applied to the determination of the inelastic neutron scattering cross section and how it is possible to obtain easily a great number of spectral generalised moments for a given direction of the momentum transfers. In § 3, to test the method, we determine the inelastic neutron scattering cross section of a perfectly dimerised chain and a chain with incommensurate distortions. Finally, we determine the response function of a quasi-crystal; the properties of the eigenstates of the quasi-periodic structure have been known to be difficult to determine.

2. General theory

For a harmonic crystal, it can be shown (Peretti and Jouanin 1965) that the inelastic neutron scattering cross section is given by

$$\sigma(\boldsymbol{q}, \omega) = \frac{k}{k^0} \sum_j \sum_{\alpha\beta} \frac{f_{j\alpha}(\boldsymbol{q}) q_\alpha f^*_{j\beta}(\boldsymbol{q}) q_\beta (\delta(\omega - \omega_j) - \delta(\omega + \omega_j))}{2\omega_j} \tag{1}$$

with

$$f_{j\alpha}(\boldsymbol{q}) = \sum_n c_n \exp(-w_n) \exp(-\mathrm{i}\boldsymbol{q} \cdot \boldsymbol{r}^0_n) e_{\alpha n}(j) m_n^{-1/2} \tag{2}$$

where $n(\omega) = 1/[\exp(h\omega/kT) - 1]$, $\hbar\boldsymbol{q}$ and $\hbar\omega$ are the momentum and energy transferred by the neutron to the scattering system, $\boldsymbol{k}^0$ and $\boldsymbol{k}$ are the initial and final wavevectors of the neutron, c_n the scattering length factors of the nth nucleus, $\exp(-w_n)$ the Debye–Waller factor, $\boldsymbol{r}^0_n$ the position of the nth atom, ω_j the frequency and $\boldsymbol{e}_j$ the eigenvector of the normal mode j. $\sigma(\boldsymbol{q}, \omega)$ is anti-symmetric in ω. As the eigenvalues of the dynamic matrix $\mathbf{D}$ are the squares of the frequencies, it follows that it is not possible to use equation (1) directly in a moments method. However, to check a dynamic model, it is only necessary to evaluate, for instance, the low-temperature spectra at low frequencies. So we now evaluate a function $\sigma'(\boldsymbol{q}, \omega)$ which is identical with $\sigma(\boldsymbol{q}, \omega)$ for $T \rightarrow 0$ and $\omega \leqslant 0$ and is symmetric. Let $\sigma'(\boldsymbol{q}, \omega)$ be defined by

$$\sigma'(\boldsymbol{q}, \omega) = \frac{k}{k^0} \sum_j \frac{|\boldsymbol{f}_j(\boldsymbol{q}) \cdot \boldsymbol{q}|^2 (\delta(\omega - \omega_j) + \delta(\omega + \omega_j))}{2\omega_j}. \tag{3}$$

We see that $\sigma'(\boldsymbol{q}, \omega)$ is a function of the square of the frequency. We obtain with

$$u = \omega^2 \qquad \lambda_j = \omega_j^2 \tag{4}$$

$$g^n(\boldsymbol{q}, u) = \sigma'(\boldsymbol{q}, \omega) = \frac{k}{k^0} \sum_j |\boldsymbol{f}_j(\boldsymbol{q}) \cdot \boldsymbol{q}|^2 \delta(u - \lambda_j). \tag{5}$$

Defining a structure factor vector $|F(\boldsymbol{q})\rangle$ by

$$|F(\boldsymbol{q})\rangle = \left(\frac{k}{k^0}\right)^{1/2} \sum_{\alpha n} c_n^* \exp(-w_n)(m_n)^{-1/2} \exp(\mathrm{i}\boldsymbol{q} \cdot \boldsymbol{r}^0_n) q_\alpha |\alpha n\rangle \tag{6}$$

equation (3) can now be expressed as

$$g^n(\boldsymbol{q}, u) = \sum_j |\langle F(\boldsymbol{q})|j\rangle|^2 \delta(u - \lambda_j). \tag{7}$$

It is easy to show (see I) that

$$g^n(\boldsymbol{q}, u) = (-1/\pi) \lim_{\varepsilon \rightarrow 0_+} [\mathrm{Im}\{R^n(\boldsymbol{q}, z)\}] \tag{8}$$

with $z = u + \mathrm{i}\varepsilon$ ($\varepsilon \rightarrow 0_+$) and

$$R^n(\boldsymbol{q}, z) = \langle F(\boldsymbol{q})|(z\mathbf{I} - \mathbf{D})^{-1}|F(\boldsymbol{q})\rangle. \tag{9}$$

To calculate $g^n(\boldsymbol{q}, u)$, we need to determine $R^n(\boldsymbol{q}, z)$. This can be achieved by expanding $R^n(\boldsymbol{q}, z)$ in a continued-fraction expansion:

$$R^n(\boldsymbol{q}, z) = a_0/[\![z - a_1 - b_1/\{z - a_2 - b_2/[z - a_3 - b_3/(\ldots)]\}]\!]. \qquad (10)$$

The coefficients b_s are positive; a_s and b_s are real and are correlated to the moments of $g^n(\boldsymbol{q}, u)$. It is possible to show that the coefficients a_s and b_s are given by the following relations (Jurczek 1985):

$$a_{s+1} = \bar{\nu}_{s,s}/\nu_{s,s} \qquad b_s = \nu_{s,s}/\nu_{s-1,s-1} \qquad (11)$$

with $a_0 = \nu_{0,0}$.

The generalised moment $\nu_{s,s}$ and $\bar{\nu}_{s,s}$ are given in I by

$$\nu_{s,s} = \langle F(\boldsymbol{q})|P_s(\mathbf{D})P_s(\mathbf{D})|F(\boldsymbol{q})\rangle \qquad (12a)$$

$$\bar{\nu}_{s,s} = \langle F(\boldsymbol{q})|P_s(\mathbf{D})\mathbf{D}P_s(\mathbf{D})|F(\boldsymbol{q})\rangle \qquad (12b)$$

where

$$P_{s+1}(u) = uP_s(u) - a_{s+1}P_s(u) - b_sP_{s-1}(u). \qquad (13)$$

Now, with the help of equations (11)–(13), it is possible to determine exactly the successive coefficients a_s and b_s. However, in practice, the use of equations (12) involves a great number of products and the method is not very convenient for very large systems. Let us show that it is possible to simplify the computation of the moments. Equations (12) can be written

$$\nu_{s,s} = \mathrm{Tr}[\mathbf{Q}(q)P_s(\mathbf{D})P_s(\mathbf{D})] \qquad (14)$$

$$\bar{\nu}_{s,s} = \mathrm{Tr}[\mathbf{Q}(q)P_s(\mathbf{D})\mathbf{D}P_s(\mathbf{D})] \qquad (15)$$

with the operator $\mathbf{Q}(q)$ given by

$$\mathbf{Q}(q) = |F(\boldsymbol{q})\rangle\langle F(\boldsymbol{q})|. \qquad (16)$$

In representation $|\alpha n\rangle$ the elements $\langle\alpha n|\mathbf{Q}(q)|\beta n'\rangle$ are given by

$$\begin{aligned}\langle\alpha n|\mathbf{Q}(\boldsymbol{q})|\beta n\rangle &= \langle\alpha n|F(\boldsymbol{q})\rangle\langle F(\boldsymbol{q})|\beta n'\rangle \\ &= (k/k^0)|\boldsymbol{q}|^2 N\langle\alpha n|\mathbf{Q}'(q)|\beta n'\rangle \exp[\mathrm{i}\boldsymbol{q}\cdot(r_n^0 - r_{n'}^0)]\end{aligned} \qquad (17)$$

with

$$\mathbf{Q}'(q) = |F'(\boldsymbol{q})\rangle\langle F'(\boldsymbol{q})| \qquad (18)$$

and

$$|F'(\boldsymbol{q})\rangle = N^{-1/2}\sum_{\alpha n} c_n^* \exp(-w_n)\,(m_n)^{-1/2}\,\frac{q_\alpha}{\boldsymbol{q}}|\alpha n\rangle \qquad (19)$$

where N is a norm and we have, without loss of generality, that

$$\langle F'(\boldsymbol{q})|F'(\boldsymbol{q})\rangle = 1. \qquad (20)$$

It follows from (18) and (20) that

$$\mathrm{Tr}[\mathbf{Q}'(q)] = \mathrm{Tr}[\mathbf{Q}'(q)^n] = 1 \qquad \forall n. \qquad (21)$$

Equation (21) shows that all eigenvalues are equal to zero except one which is equal to unity. Let λ_1 be this value. We obtain

$$\lambda_1 = 1 \qquad \lambda_i = 0 \qquad \text{for } i \neq 1. \tag{22}$$

From (18) and (20), it is clear that the eigenvectors $|\lambda_1\rangle$, corresponding to the eigenvalue λ_1, are given by

$$|\lambda_1\rangle = |F'(\boldsymbol{q})\rangle \tag{23}$$

since

$$\mathbf{Q}'(\boldsymbol{q})|\lambda_1\rangle = |F'(\boldsymbol{q})\rangle\langle F'(\boldsymbol{q})|\lambda_1\rangle = |F'(\boldsymbol{q})\rangle = \lambda_1|\lambda_1\rangle. \tag{24}$$

As $|\lambda_1\rangle$ is known, it is possible by Schmidt's orthogonalisation method (Isaacson and Keller 1966) to generate a set of linear independent vectors which are the eigenvectors of operator $\mathbf{Q}'(\boldsymbol{q})$. The matrix $\mathbf{U}$ which diagonalises $\mathbf{Q}'(\boldsymbol{q})$ may be found by compounding the eigenvectors of $\mathbf{Q}'(\boldsymbol{q})$ into a matrix. If $\mathbf{Q}_d$ is the diagonal form of $\mathbf{Q}'(\boldsymbol{q})$, we have

$$\mathbf{Q}_d = \mathbf{U}^+\mathbf{Q}'(\boldsymbol{q})\mathbf{U} \tag{25}$$

with

$$\left.\begin{aligned}(\mathbf{Q}_d)_{11} &= 1\\ (\mathbf{Q}_d)_{ij} &= 0 \qquad \text{otherwise.}\end{aligned}\right. \tag{26}$$

Now we substitute equation (25) into (14) and, taking into account (17), one obtains

$$\begin{aligned}\nu_{s,s} &= (k/k^0)|\boldsymbol{q}|^2 N\,\mathrm{Tr}[\mathbf{Q}'(\boldsymbol{q})P_s(\mathbf{D}'(\boldsymbol{q}))P_s(\mathbf{D}'(\boldsymbol{q}))]\\ &= (k/k^0)|\boldsymbol{q}|^2 N\,\mathrm{Tr}[\mathbf{U}\mathbf{Q}_d\mathbf{U}^+P_s(\mathbf{D}'(\boldsymbol{q}))P_s(\mathbf{D}'(\boldsymbol{q}))].\end{aligned} \tag{27}$$

Next, taking into account the cyclic properties of the trace, one obtains

$$\nu_{s,s} = (k/k^0)|\boldsymbol{q}|^2 N\,\mathrm{Tr}[\mathbf{Q}_d P_s(\mathbf{D}_t(\boldsymbol{q}))P_s(\mathbf{D}_t(\boldsymbol{q}))] \tag{28}$$

with $\mathbf{D}'(\boldsymbol{q})$ such that

$$\langle\alpha n|\mathbf{D}'(\boldsymbol{q})|\beta n'\rangle = \langle\alpha n|\mathbf{D}|\beta n'\rangle \exp[\mathrm{i}\boldsymbol{q}\cdot(\boldsymbol{r}_n^0 - \boldsymbol{r}_{n'}^0)] \tag{29}$$

and

$$\mathbf{D}_t(\boldsymbol{q}) = \mathbf{U}^+\mathbf{D}'(\boldsymbol{q})\mathbf{U}. \tag{30}$$

We obtain in the same way for equation (15)

$$\bar{\nu}_{s,s} = (k/k^0)|\boldsymbol{q}|^2 N\,\mathrm{Tr}[\mathbf{Q}_d P_s(\mathbf{D}_t(\boldsymbol{q}))\mathbf{D}_t(\boldsymbol{q})P_s(\mathbf{D}_t(\boldsymbol{q}))] \tag{31}$$

and, now taking into account equation (26), one obtains for (28) and (31)

$$\nu_{s,s} = (k/k^0)|\boldsymbol{q}|^2 N[P_s(\mathbf{D}_t(\boldsymbol{q}))P_s(\mathbf{D}_t(\boldsymbol{q}))]_{11}. \tag{32}$$

$$\bar{\nu}_{s,s} = (k/k^0)|\boldsymbol{q}|^2 N[P_s(\mathbf{D}_t(\boldsymbol{q}))\mathbf{D}_t(\boldsymbol{q})P_s(\mathbf{D}_t(\boldsymbol{q}))]_{11}. \tag{33}$$

Finally, the one-phonon differential cross section (3), can easily be obtained from (8), (11), (32) and (33). We consider only the case of the coherent scattering by materials and assume that the experimental procedure is the 'constant-$\boldsymbol{q}$' method (Brockhouse 1966). Now, if we neglect the dependence of the Debye–Waller factor on $\boldsymbol{q}$, we have the following.

(i) The determination of the moments requires the determination of only one term of the matrix products.

(ii) The matrix $\mathbf{U}$ is independent of the magnitude of the scattering vector q. The matrix $\mathbf{U}$ depends only on the direction of q and the physical coefficients of the system. So it is necessary to compute $\mathbf{U}$ only once for every direction of q and not for every magnitude of the scattering vector.

(iii) From equations (32) and (33), we observe that it is necessary to compute only one line of the matrix $P_s(\mathbf{D}_t(q))$.

(iv) $\mathbf{D}_t(q)$ is not the Fourier transform of the dynamic matrix but corresponds to the representation of the operator $\mathbf{D}$ in the base of eigenvectors $|\lambda_i)$, every term being multiplied by the phase factor $\exp[\mathrm{i}q \cdot (r_n^0 - r_{n'}^0)]$.

In practice, one calculates a finite number of coefficients a_s and b_s and we are then faced with the problem of the termination of the continued fraction. However, with the method developed here, it is easy to calculate the spectrum for every step of the iteration. After several tests, we employ here the same type of termination that was used for a dimerised chain and chains with topological defects in I. In the following, we illustrate this method by determining the inelastic neutron scattering cross section for several models.

3. Illustrations of the method

Let us consider a chain of N masses, each coupled to its nearest neighbours. We study the longitudinal vibrations of this chain. Firstly, as for the study of the dielectric properties of the system in I, we consider a perfectly dimerised chain. The elastic

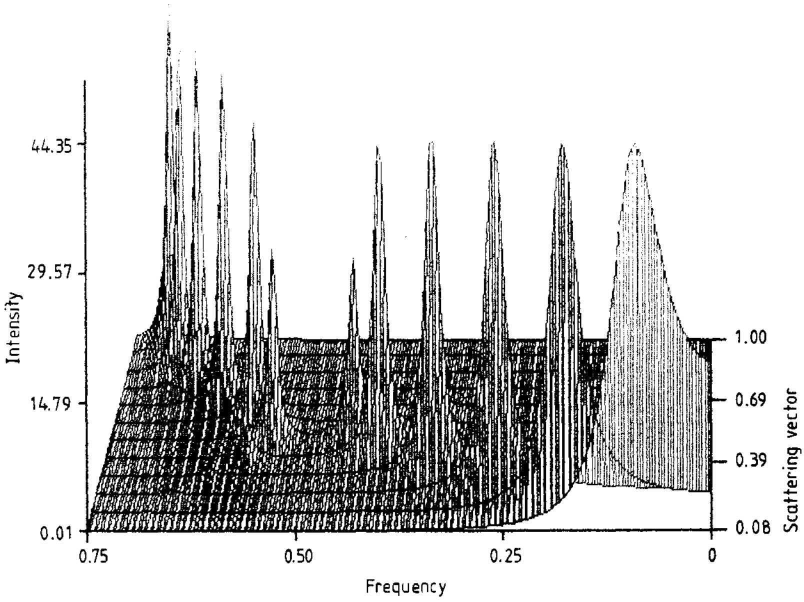

Figure 1. The inelastic neutron scattering cross section for 12 values of the scattering vector for a perfect chain with $m = 1$, $k_1 = 0.100$, $k_2 = 0.025$ and with 32 spectral moments.

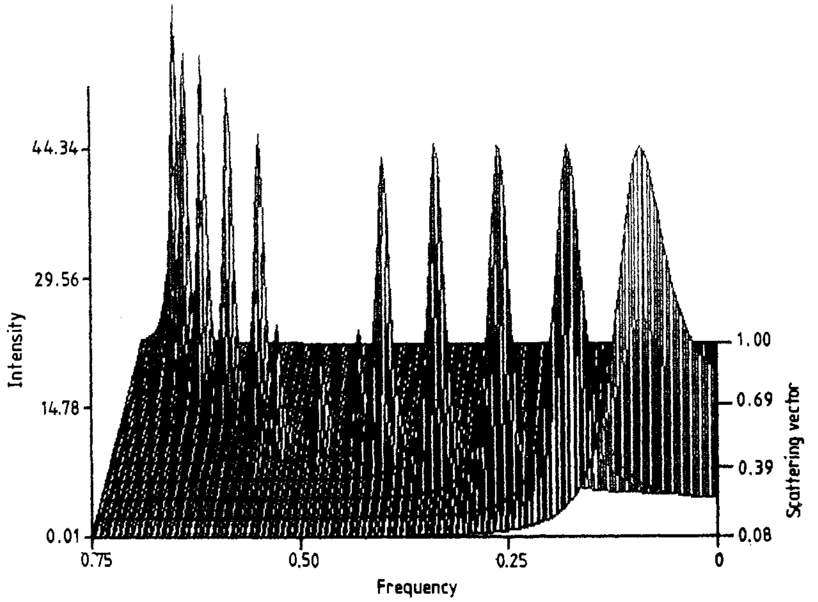

Figure 2. The inelastic neutron scattering cross section for 12 values of the scattering vector for a chain with incommensurate soliton lattice with $m = 1$, $k_1 = 0.100$, $k_2 = 0.025$, $\alpha = \sqrt{2}a$, $z = 1.5$ and with 32 spectral moments.

constants are given by

$$\Phi(n, n+1) = (k_1 + k_2)/2 + (k_1 - k_2)/4[\rho(n+1) - \rho(n)] \tag{34}$$

with $\rho(n) = (-1)^n$ for the dimerised chain. It is well known that for this system the frequencies are given for the acoustic ($j = 1$) and optic ($j = 2$) modes by (Seitz 1940)

$$[\omega_j(q)]^2 = \llbracket (k_1 + k_2) + (-1)^j\{(k_1 + k_2)^2 - 4k_1k_2[\sin(qa)]^2\}^{1/2} \rrbracket / m \tag{35}$$

with $q = 2\pi p/Na$ and $-N/2 < p \leq N/2$. a is the lattice parameter. Now we apply the spectral moments method. We choose m and c_n equal to unity and we neglect the dependence on q in the front term in (32) and (33). In order to check the accuracy of the method, we compare the frequencies of the peaks of the inelastic cross section for several scattering vectors q between 0 and $2\pi/a$, with the exact values given by (35).

The results are shown in figure 1. We observe that the acoustic modes are principally active in the first Brillouin zone while the optic modes are principally active in the second Brillouin zone. However, we observe some weak peaks corresponding to optical modes in the first Brillouin zone and acoustic modes in the second Brillouin zone (not visible on the figure). We recall that for the undimerised chain the acoustic and optic modes are respectively strictly active in the first and second Brillouin zones. The values of the frequencies calculated by the spectral moment method agree very well with the values obtained with (35).

We now consider a dimerised chain with solitons. We choose a soliton lattice incommensurate with the crystal lattice. The elastic constants are obtained with the help of (34) with the order parameter $\rho(n)$ given by:

$$\rho(n) = (-1)^n \prod_i \tanh\left(\frac{n - l_i}{z}\right) \tag{36}$$

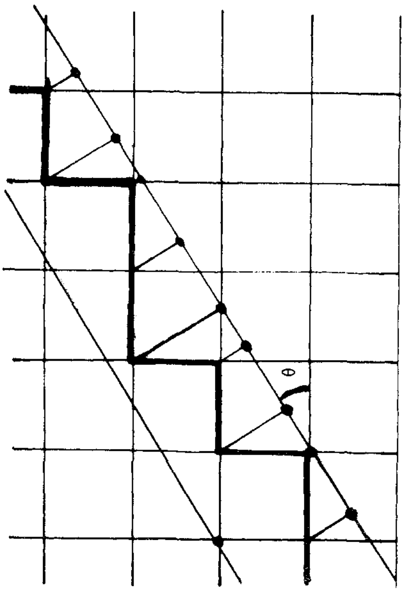

Figure 3. Construction of a one-dimensional quasi-crystal by the projection method.

with $l_i = i\alpha$, where α/a is an incommensurate number.

The inelastic scattering cross section for different values of q are given in figure 2. It can be seen that the system presents a new scattering peak in the phonon gap. This result agrees with the frequency distribution calculated in I by the moments method for a chain with solitons as defects. However, we now find that the new mode is active in inelastic neutron scattering experiments for $|q| = \pi/a$, i.e. for the boundary of the first Brillouin zone of the unperturbed chain. This result is in agreement with the conclusion of Su *et al* (1980) that the defect state arises from combinations of the zone boundary states.

Finally we consider a quasi-crystal; the properties of the eigenstates of the quasi-periodic structure have been known to be difficult to determine (Luck 1986, Kohmoto *et al* 1987). We choose the well known projection method to generate an almost periodic tiling of the chain with short and long segments of respective lengths $s = \sin\theta$ and $c = \cos\theta$ where θ is the angle between the x axis and the strip used to construct the tiling (figure 3). We choose $\tan\theta = \frac{1}{2}(\sqrt{5} - 1)$. In order to generalise the results obtained by Luck (1986), we use a nearest-neighbour potential (short-range forces) and a screened Coulombic potential (long-range forces). The nearest-neighbour force constants for short and long bounds, respectively, are taken as equal to $\frac{1}{2}$ and 1, which correspond to the values used in the work of Luck (1986) for the short-range part. The long-range potential is given by

$$\Phi = \frac{A}{2} \sum_{nn'}{}' \frac{1}{|r_n - r'_n|} \exp(-\alpha|r_n - r'_n|) \qquad (37)$$

where r_n represents the position of the nth atom, and A and α are constants of the potential. It is not possible with such a potential to use for instance the transfer matrix method. Furthermore the properties of the eigenstates of the quasi-periodic structure are known to be difficult to determine. We have shown in figure 4(a) the integrated

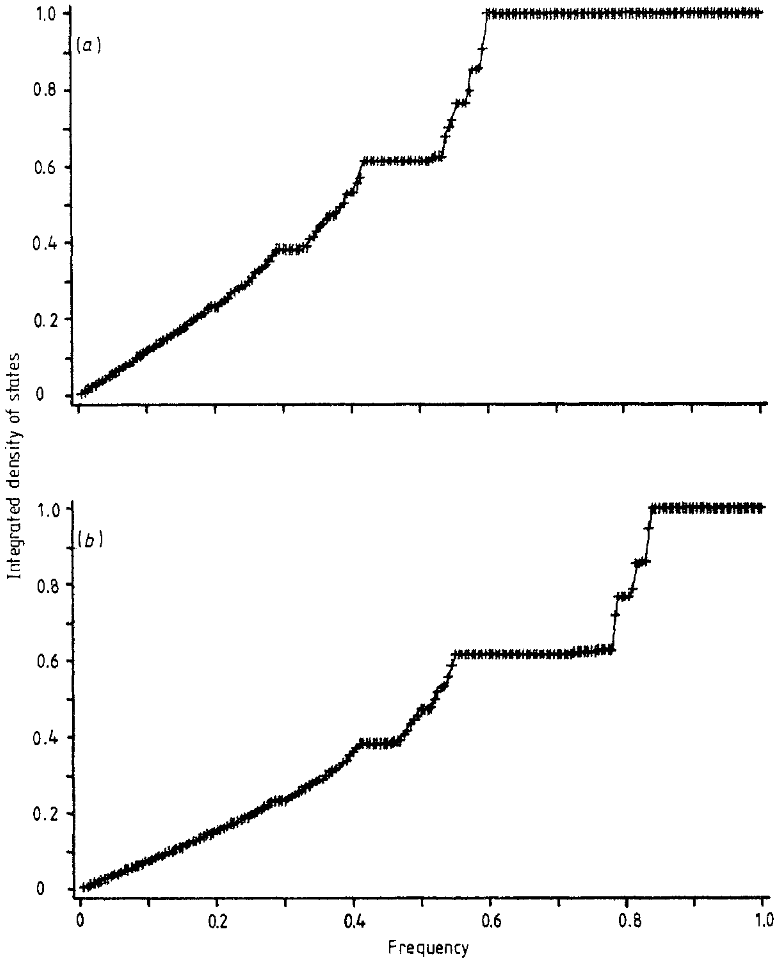

Figure 4. The integrated density of states for a quasi-crystal (*a*) with short-range forces and (*b*) with short- and long-range forces. The short-range force constants for short and long bounds, respectively, are taken equal to $\frac{1}{2}$ and 1 ($A = 0.01$; $\alpha = 0.1$).

density of states for the model with short-range forces and in figure 4(*b*) the integrated density of states for the model with short- and long-range forces (equation (37)) up to third-neighbour forces. We see that with the long-range forces the same structure for the density spectrum is obtained as with short-range forces. The Cantor structure is quite apparent. This structure is certainly intimately related to the quasi-periodicity and not to the range of the forces. In I, we illustrated the spectral moments method by calculating the optical properties of materials. However, it is now possible to take into account, in the determination of the optical properties, the improvements developed in the present paper. So we have given in figure 5 the infrared absorption of a quasi-crystal with 800 atoms. We observe that many modes are now infrared active and that the spectrum is quite different from the spectrum of a disordered system (see I). We now study the scattering properties of a quasi-crystal with 400 atoms. The general results for different scattering vectors are shown in figure 6. We observe that, for small q, only low-frequency

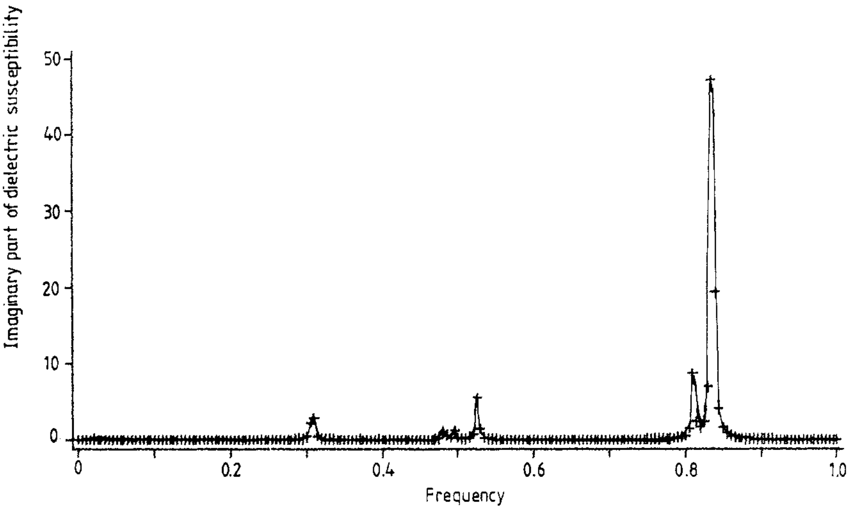

Figure 5. The imaginary part of the dielectric susceptibility obtained by the spectral moments method for a quasi-crystal with short- and long-range forces with 32 spectral moments.

modes are active in the scattering processes while, for a relatively large q, many low- and high-frequency modes become active. In the limit of the values of q concerned here, the behaviour of the inelastic cross section of a quasi-crystal is quite different from the behaviour of inelastic scattering of a periodic system.

4. Conclusion

In I, we showed that the spectral moments method is a powerful tool for determining the dielectric and light scattering properties of various systems. In this paper, we have

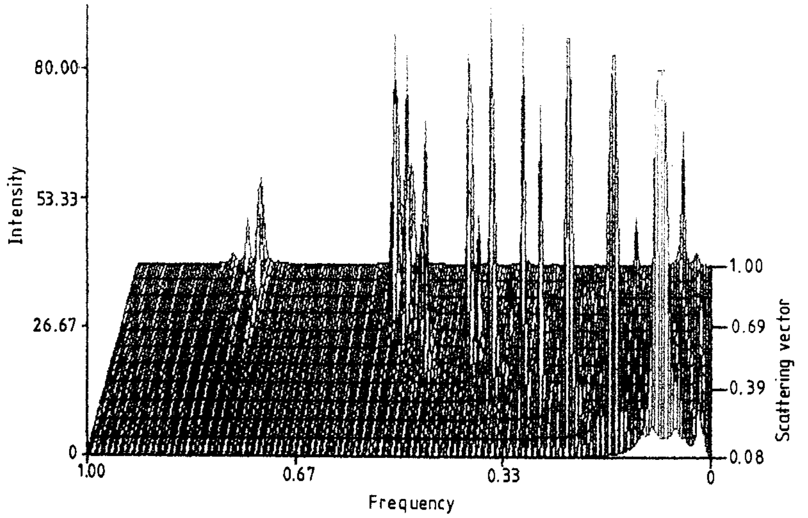

Figure 6. The inelastic neutron scattering cross section for 12 values of the scattering vector for a quasi-crystal with short- and long-range forces, with 32 spectral moments.

shown that the inelastic neutron cross section $\sigma(\omega, \boldsymbol{q})$ can be obtained very easily, directly from the dynamic matrix without any calculation of eigenfrequencies and eigenvectors. We have illustrated this method by determining the inelastic neutron scattering cross section for three models: the first model concerned the perfect chain and was used to test the accuracy of the calculation, and the second model was an application to a chain with defects, i.e. a soliton lattice. The results of the calculations are in complete agreement with the previous results concerning this type of model. The last application concerned quasi-crystals. This type of application is very interesting because the frequency distribution is a Cantor set and it is well known that in the presence of gaps the determination of the infinite tail of the continued fraction is difficult. However, with the spectral moments method the problem of determination of the infinite tail is not so critical and we have shown that the calculation of the scattering properties of a quasi-periodic structure could be easily performed. For this last example, we have shown that the Cantor-set-type spectrum is independent of the range of forces used and we have reported the infrared activity and the inelastic cross section of modes for several momentum transfers. The results show that, although the structure of the chain presents only two types of different bond, the dynamic properties are fundamentally different from the properties of periodic or disordered materials. It is evident that quasi-periodicity plays a central role in these systems.

References

Benoit C 1987 *J. Phys. C: Solid State Phys.* **20** 765
Blumstein C and Wheeler J C 1973 *Phys. Rev.* B **8** 1764
Brockhouse B N 1966 *Phonons in Perfect Lattices and in Lattices with Point Imperfections* ed. R W H Stevenson (Edinburgh: Oliver and Boyd)
Cyrot-Lackmann F 1967 *Adv. Phys.* **16** 393
Dean P 1960 *Proc. R. Soc.* A **254** 507
—— 1972 *Rev. Mod. Phys.* **44** 127
Dyson F J 1953 *Phys. Rev.* **92** 1331
Family F and Landau D P 1984 *Kinetics of Aggregation and Gelation* (Amsterdam: North-Holland)
Galtier M and Beniot C 1981 *Phys. Status Solidi* b **105** K61
Gaspard J P and Cyrot-Lackmann F 1973 *J. Phys. C: Solid State Phys.* **6** 3077
Haydock R 1980 *Solid State Phys.* **35** 215 (New York: Academic)
Haydock R, Heine V and Kelly M 1972 *J. Phys. C: Solid State Phys.* **5** 2845
Heine V 1980 *Solid State Phys.* **35** 1 (New York: Academic)
Isaacson E and Keller H B 1966 *Analysis of Numerical Methods* (New York: Wiley)
Ishii Y and Fujiwara T 1980 *J. Phys. F: Met. Phys.* **10** 2125
Jurczek E 1985 *Phys. Rev.* B **32** 4208
Kelly J M 1980 *Solid State Phys.* **35** 295 (New York: Academic)
Kohmoto M, Sutherland B and Tang C 1987 *Phys. Rev.* B **35** 1020
Lambin P H and Gaspard J P 1982 *Phys. Rev.* B **26** 4356
Lanczos C 1950 *J. Res. NBS* **45** 255
Luck J M 1986 *J. Physique Coll.* **47** C3 205
Mattis C and Lieb H 1966 *Mathematical Physics in One Dimension* (New York: Academic)
Montroll E W 1942 *J. Chem. Phys.* **10** 218
Peretti J and Jouanin C 1965 *Nuovo Cimento* **34** 293
Saad Y 1981 *Math. Comput.* **37** 105
Seitz F 1940 *The Modern Theory of Solids* (New York: McGraw-Hill)
Su W P, Schrieffer J R and Heeger A J 1980 *Phys. Rev.* B **22** 2099
Turchi P, Ducastelle F and Treglia G 1982 *J. Phys. C: Solid State Phys.* **15** 2891
Wheeler J C, Prais M G and Blumstein C 1974 *Phys. Rev.* B **10** 2429