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ON THE LATTICE DYNAMICS OF THE INTERSTITIAL IMPURITIES

D. Vamanu

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ABSTRACT

The interstitial impurities in a crystal are thought of as a system of harmonic oscillators coupled by the vibrations of their host lattice. The response function of an impurity is expressed by a host lattice and many-defect contributions. The interaction of the impurities is renormalized within an infinite-order perturbation theory, which provides the concept of "dressed defects". The procedure is tested on the problem of localized modes on impurities in a one-dimensional lattice.

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I. INTRODUCTION

Since the description by Montroll and Potts (1955) of the basic features of the interaction of the defects in a crystal, the Green's function formalism introduced the many-body concepts and techniques into common practice. Thus, the response function of a lattice with randomly distributed substitutional impurities was analysed in terms of diagrams accounting for the alterations by defects of the phonon propagation throughout the lattice (Langer 1961, Davies and Langer 1963, Ludwig 1967). A complementary approach concentrated on the one-defect response function. In this way the localized modes on a single interstitial impurity perturbed by its host lattice was investigated by Blaesser, Peretti and Toth (1968). The first aim of the present paper is to extend the partition technique as used by these authors to the case of a crystal with essentially many interstitial impurities.

The one-defect response function is found to be given by a Green's function of an Einstein harmonic oscillator along with a host lattice and many-defect contributions. Appropriate diagrams are designed to describe within an infinite-order perturbation theory the interaction of the defects through their host lattice. The interaction of each defect with the host lattice "dresses" the defect. The dynamic coupling of the "dressed" defects by host lattice vibrations is also affected by the alterations in the host lattice due to impurities. As a consequence both defects and their interaction are renormalized.

In the last section the "dressed" defects approximation is tested in searching for localized modes of vibration of impurities in a one-dimensional lattice.

II. RESPONSE FUNCTIONS OF INTERSTITIAL DEFECTS

Given a crystal with N lattice atoms and n interstitial impurities per cyclicity volume, the response function is defined (see, e.g. Ludwig 1967) as the $3(N + n) \times 3(N + n)$-sized matrix

$$R \equiv (\Phi - \omega^2 \mathcal{M})^{-1} , \qquad (1)$$

where Φ is the tensor of the coupling constants and $\mathcal{M}$ is the diagonal tensor of the atomic masses.

The matrix (1) can be subject to the following natural partition:

$$R = \begin{pmatrix} R_{LL} & R_{LD_1} & R_{LD_2} & \cdots & R_{LD_k} & \cdots & R_{LD_n} \\ R_{D_1L} & R_{D_1D_1} & R_{D_1D_2} & \cdots & R_{D_1D_k} & \cdots & R_{D_1D_n} \\ R_{D_2L} & R_{D_2D_1} & R_{D_2D_2} & \cdots & R_{D_2D_k} & \cdots & R_{D_2D_n} \\ \vdots & \vdots & \vdots & & \vdots & & \vdots \\ R_{D_kL} & R_{D_kD_1} & R_{D_kD_2} & \cdots & R_{D_kD_k} & \cdots & R_{D_kD_n} \\ \vdots & \vdots & \vdots & & \vdots & & \vdots \\ R_{D_nL} & R_{D_nD_1} & R_{D_nD_2} & \cdots & R_{D_nD_k} & \cdots & R_{D_nD_n} \end{pmatrix} \qquad (2)$$

The $3N \times 3N$ block matrix R_{LL} in the top left corner refers to all the atoms of the host lattice but to them only. It stands as the response function of the host lattice perturbed by the intrusion of interstitial impurities. The 3×3 matrices $R_{D_kD_k}$, $k = 1,2,\ldots,n$ along the diagonal of R stands as the response function of the individual interstitial impurities $D_1, D_2, \ldots, D_n$, perturbed by the surrounding lattice (the other interstitial impurities included).

The inverted response function can also be subject to a similar partition. Assuming that the density of defects and the range of the interatomic forces fit each other such that there is no straight coupling between any two interstitials, this matrix reads

$$R^{-1} = \Phi - \omega^2 \mathcal{M} =$$

$$\begin{pmatrix} (\Phi_{LL} - m_L\omega^2 I_{3N}) & \Phi_{LD_1} & \Phi_{LD_2} & \cdots & \Phi_{LD_k} & \cdots & \Phi_{LD_n} \\ \Phi_{D_1L} & (\Phi_{D_1D_1} - m_{D_1}\omega^2 I_3) & 0 & \cdots & 0 & \cdots & 0 \\ \Phi_{D_2L} & 0 & (\Phi_{D_2D_2} - m_{D_2}\omega^2 I_3) & \cdots & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & & \vdots & & \vdots \\ \Phi_{D_kL} & 0 & 0 & \cdots & (\Phi_{D_kD_k} - m_{D_k}\omega^2 I_3) & \cdots & 0 \\ \vdots & \vdots & \vdots & & \vdots & & \vdots \\ \Phi_{D_nL} & 0 & 0 & \cdots & 0 & \cdots & (\Phi_{D_nD_n} - m_{D_n}\omega^2 I_3) \end{pmatrix} \qquad (3)$$

with obvious notations for the lattice atoms and impurity masses, and for the unit matrices of appropriate sizes.

The 3×3 block matrices along the diagonal are, by construction, the inverted Green's functions of some interstitial harmonic oscillators embedded in a "frozen" lattice, which will read as follows:

$$\Phi_{D_k D_k} - m_{D_k} \omega^2 I_3 \equiv G^{-1}_{D_k D_k} \quad . \tag{4}$$

According to the requirement of invariance of the forces to bulk translations, the auto-force constants are given by

$$\Phi_{D_k D_k} = - \sum_{\ell} \Phi_{D_k \ell} \quad , \tag{5}$$

where, following the previous assumption, the sum extends only on host lattice atoms within the effective range of the coupling.

As for the $3N \times 3N$ host lattice part in the top left corner of (3), it can be set in the form

$$\Phi_{LL} - m_L \omega^2 I_{3N} = \overset{\circ}{\Phi}_{LL} - H_{LL} - m_L \omega^2 I_{3N} = G^{-1}_{LL} - H_{LL} \quad . \tag{6}$$

Here the force tensor Φ_{LL} is split so as to exhibit a part $\overset{\circ}{\Phi}_{LL}$ which would correspond to the <u>ideal</u> host lattice and a part H_{LL} which is supposed to collect together all the alterations induced in the coupling scheme of the host lattice by the intrusion of interstitial impurities. The straightest of these alterations appear in the auto-force constants of the host lattice atoms falling within the co-ordination sphere of the interstitials; thus, one has

$$\Phi_{\ell\ell} = - \sum_{\substack{\ell' \\ \ell' \neq \ell}} \Phi_{\ell\ell'} - \sum_{k} \Phi_{\ell D_k} \quad . \tag{7}$$

Even apart from the changes in $\Phi_{\ell\ell'}$ by leakage of some of the point-group symmetries of the ideal host lattice when the interstitial impurities come into it, there is always the additional term $\sum_k \Phi_{\ell D_k}$ bringing the defects into play. By pointing out the ideal lattice tensor it became possible to identify in Eq.(6) the inverted Green's function of the ideal host lattice as

$$\overset{\circ}{\Phi}_{LL} - m_L \omega^2 I_{3N} \equiv G_{LL}^{-1} \quad . \tag{8}$$

In many problems the quantity of interest is the response function $R_{D_k D_k}$ of a given defect in the lattice. To get it here, one multiplies the k-th column of R (Eq.(2)) by all the lines of its inverse (Eq.(3)). After some manipulation one finds $R_{D_k D_k}$ in the form

$$R_{D_k D_k}^{-1} = G_{D_k D_k}^{-1} - \Phi_{D_k L} \left[(G_{LL}^{-1} - H_{LL}) - \sum_j{}' \Phi_{LD_j} G_{D_j D_j} \Phi_{D_j L} \right]^{-1} \Phi_{LD_k} , \tag{9}$$

where the sum in the right-hand side extends over all the n defects except for D_k itself.

Eq.(9) gives the response function of an arbitrary interstitial defect by an "unperturbed" part coming from the oscillating interstitial in a fictitiously "frozen" host lattice, a host lattice contribution, and a many-defect contribution. All the contributions are adduced to the defect under consideration by appropriate coupling tensors.

When dropping out from Eq.(9): i) the many-defect part $\sum_j{}' \Phi_{LD_j} G_{D_j D_j} \Phi_{D_j L}$ and ii) the host lattice alterations H_{LL}, the result of Blaesser et al. (1968) is refined. The response function R_{LL} of the host lattice can also be obtained from the multiplication table of R by its inverse. The case of vacancies and substitutional impurities can be derived straightforwardly following the concept of Blaesser et al. (1968).

III. THE INTERACTING DEFECTS

Using Eq.(9) in its raw form is difficult in general, because one has to invert a $3N \times 3N$ matrix in the right-hand side. One may obtain some advantage by an iterative expansion of this matrix, which makes Eq.(9) read:

$$R_{D_k D_k}^{-1} = G_{D_k D_k}^{-1} - \Phi_{D_k L} \left\{ (G_{LL}^{-1} - H_{LL})^{-1} + (G_{LL}^{-1} - H_{LL})^{-1} \sum_j{}' \Phi_{LD_j} G_{D_j D_j} \Phi_{D_j L} \times \right.$$

$$\left. \times \left[(G_{LL}^{-1} - H_{LL}) - \sum_j{}' \Phi_{LD_j} G_{D_j D_j} \Phi_{D_j L} \right]^{-1} \right\} \Phi_{LD_k} =$$

$$G^{-1}_{D_k D_k} - \Phi_{D_k L}(G^{-1}_{LL} - H_{LL})^{-1}\,\Phi_{LD_k} -$$

$$\sum_j{}' \Phi_{D_k L}\,(G^{-1}_{LL} - H_{LL})^{-1}\,\Phi_{LD_j} \cdot G_{D_j D_j} \cdot \Phi_{D_j L}\,(G^{-1}_{LL} - H_{LL})^{-1}\,\Phi_{LD_k} -$$

$$\sum_{j_1}{}' \sum_{j_2}{}' \Phi_{D_k L}\,(G^{-1}_{LL} - H_{LL})^{-1}\,\Phi_{LD_{j_1}} \cdot G_{D_{j_1} D_{j_1}} \cdot \Phi_{D_{j_1} L}\,(G^{-1}_{LL} - H_{LL})^{-1}\,\Phi_{LD_{j_2}} \cdot$$

$$\cdot G_{D_{j_2} D_{j_2}} \cdot \Phi_{D_{j_2} L}\,(G^{-1}_{LL} - H_{LL})^{-1}\,\Phi_{LD_k} - \ldots \qquad (10)$$

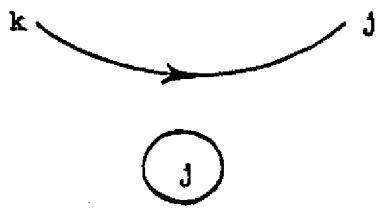
The terms in Eq.(10) are assigned to describe the dynamical interaction of the defects through the host lattice. Thus, one sees that the defect D_k interacts with the defect D_j through a lattice "propagator"

$$\Pi_{D_k D_j} \equiv \Phi_{D_k L}\,\Lambda_{LL}\,\Phi_{LD_j}\,, \qquad (11)$$

where

$$\Lambda_{LL} \equiv (G^{-1}_{LL} - H_{LL})^{-1} = (1 - G_{LL} H_{LL})^{-1} G_{LL}\,, \qquad (12)$$

and a defect D_j contributes to the response function of D_k by its Green's matrix $G_{D_j D_j}$ (Eq.(4)). These elements of the defect interaction can be denoted graphically as



$\Pi_{D_k D_j}$

$G_{D_j D_j}$. (13)

This convention provides a diagrammatic representation of all the terms in the iterative series (10). The technique is introduced in Fig.1. The first graph denotes a self-interaction of the defect D_k through the host lattice. It corresponds to a single propagator. Since no passing of the propagator line through any but the k-th defect is involved, this may be termed as a zero-th order contribution to the response function. The second diagram in the figure involves passing through an additional D_j defect, and therefore stands as a first-order contribution. When using this, a sum over j has

to gather all the first-order contributions. A second-order diagram can be drawn in two topologically non-equivalent ways , as shown by the following two graphs. The first depicts a double self-interaction of a single defect through the lattice, while the other denotes a "chain" interaction of two different defects. The remaining four graphs in Fig.1 are third-order topologically non-equivalent diagrams. Among them one notices the triple self-interaction through the lattice of a single defect.

Higher-order diagrams can be devised along these lines to depict many-defect contributions to the response function of a given defect. It is already clear that in any order the self-interaction of a single defect is always met among the topologically non-equivalent diagrams. The order of a diagram is given by the total number of passings through the Green's "nuclei" of the defects involved. A reading convention can be assigned to higher-order diagrams, i.e. to read the inner lines first.

The diagrammatic language facilitates renormalization of the interaction of the defects within the infinite series (10). This is particularly desirable when the coupling of the interstitial impurities to the host lattice is comparable or even stronger than the mutual coupling of the host lattice atoms, in which case no straight cut-off in the iterative series (10) would be a dependable approach. The renormalization requires summing up to the infinite order of all graphs denoting self-interaction of the interatitials through the host lattice. It starts as

$$R^{-1}_{D_k D_k} = G^{-1}_{D_k D_k} - k \;\bigcirc$$

$$- \sum_j{}' \Big\{ k \;\bigcirc\!\!-\!\!\bigcirc\; j + k \;\bigcirc\!\!=\!\!\bigcirc\; j + k \;\bigcirc\!\!\equiv\!\!\bigcirc\; j + \ldots \Big\} - \ldots =$$

$$= (G^{-1}_{D_k D_k} - \Pi_{D_k D_k}) - \sum_j{}' \Pi_{D_k D_j} \Big[G_{D_j D_j} + G_{D_j D_j} \Pi_{D_j D_j} G_{D_j D_j} +$$

$$+ G_{D_j D_j} \Pi_{D_j D_j} G_{D_j D_j} \Pi_{D_j D_j} G_{D_j D_j} + \ldots \Big] \Pi_{D_j D_k} - \ldots \qquad (14)$$

Thus each defect "dressed" by its multiple self-interaction through the host lattice provides a renormalized Green's nucleus

$$\mathcal{G}_{DD} \equiv (G^{-1}_{DD} - \Pi_{DD})^{-1} \quad . \qquad (15)$$

Graphically the renormalization can be fixed in all diagrams by the substitution

(16)

which implies elimination of all diagrams involving self-interaction parts. The "dressed defects" series starts now as shown in Fig.2, and the response function series reads

$$R^{-1}_{D_k D_k} = \mathcal{G}^{-1}_{D_k D_k} - \sum_{j}{}' \Pi_{D_k D_j} \mathcal{G}_{D_j D_j} \Pi_{D_j D_k} - \sum_{j_1}{}' \sum_{\substack{j_2 \\ j_1 \neq j_2}}{}' \Pi_{D_k D_{j_1}} \mathcal{G}_{D_{j_1} D_{j_1}} \Pi_{D_{j_1} D_{j_2}} \mathcal{G}_{D_{j_2} D_{j_2}} \Pi_{D_{j_2} D_k} - \ldots \tag{17}$$

Further improvements of the convergence of the response function series are hardly expected in a general frame. That is, answering the questions: i) how many defects surrounding a given one are to be taken into account? and ii) to what order is the series to be cut off? requires inspection of the physical problem under consideration. However, there are at least two advantageous circumstances to be pointed out. Thus it can be seen by inspection that the series can be restricted to only low-order diagrams if the coupling of the interstitials to the host lattice surrounding is much weaker than the mutual coupling of the host lattice atoms. On the other hand, one can limit oneself to only a small number of defects, if only frequencies exceeding the top frequency of the lattice are considered (localized modes); it comes from the fact that for $\omega > \omega^{max}_{lattice}$ the ideal lattice Green's function G_{LL} involved in the propagators $\Pi_{DD'}$ induces an exponential decay of the interaction with increasing distance between the defects D, D' .

A circumstance which may eventually restrict the versatility of the "dressed defects" approach is that the matrix Λ_{LL} (12) can hardly be obtained in general in a closed form. The matrix Λ_{LL} may be considered to describe the phonon propagation through the host lattice from defect to defect. Had the host lattice remained identical to the ideal one, the phonon propagation would be described by the Green's function G_{LL} of the ideal lattice, as usual. But, since the host lattice "feels" the defects by the

matrix H_{LL} the phonon propagation occurs renormalized in the form Λ_{LL}. For a low density of defects and short-ranged forces it may be possible to handle Λ_{LL} in closed form, as shown in the final section. To handle the problem in general one may use the fact that H_{LL} can always be written as a superposition of one-defect contributions, in the form $H_{LL} = \sum_k H_{LL}^{D_k}$, where $H_{LL}^{D_k}$ comes from only the defect D_k. Consequently an iterative expansion of Λ_{LL} can be set up

$$\Lambda_{LL} = \left(G_{LL}^{-1} - \sum_j H_{LL}^{D_j} \right)^{-1} = G_{LL} + \sum_j G_{LL} H_{LL}^{D_j} G_{LL} + \sum_{j_1} \sum_{j_2} G_{LL} H_{LL}^{D_{j_1}} G_{LL} H_{LL}^{D_{j_2}} G_{LL} + \ldots \qquad (18)$$

It can be treated in terms of Langer-like diagrams, as shown in Fig.3. All Langer's techniques can now be used analogously for the present purpose. A comprehensive account in this respect was given by Ludwig (1967). The zeroth order approximation of the phonon propagator $\Lambda_{LL} \approx G_{LL}$, which is most convenient in practice, stands only if the alterations H_{LL} induced by the interstitial defects in the host lattice are negligibly small. According to Eq.(7) it would imply at least that the interstitial-lattice coupling is much weaker than the lattice-lattice coupling.

IV. APPLYING THE DRESSED-DEFECTS APPROACH

In a single-defect approach of a lattice with defects the response function R_{DD} is found in a closed form as

$$R_{DD} = \boxed{D} = \mathcal{G}_{DD} , \qquad (19)$$

where the right-hand side is given by Eq.(15). One may hopefully try to get the phonon propagator Λ_{LL} in its closed form (12). For a single defect the result (19) is therefore exact.

A closed result for the response function is also found in the two-defect approach of the defect interaction. One gets

$$R^{-1}_{D_1D_1} = \boxed{1}^{-1} - 1 \bullet \text{(loop)} \boxed{2} =$$

$$= \mathcal{G}^{-1}_{D_1D_1} - \Pi_{D_1D_2}\, \mathcal{G}_{D_2D_2}\, \Pi_{D_2D_1} \quad . \qquad (20)$$

From two defects onward, approaching Λ_{LL} in a closed form requires considerable effort. The approximation (18) can be used as far as the problem suggests it.

Any many-defect approach of a lattice with defects requires a careful inspection of the physical problem. Such elements as the density and the distribution of the defects, the strength and range of different types of coupling, the nature of the investigated modes (resonance modes, localized modes) now become essential in deciding upon the type and order of diagrams to be taken into account. Let us take as an example a three-defect approach in two characteristic cases.

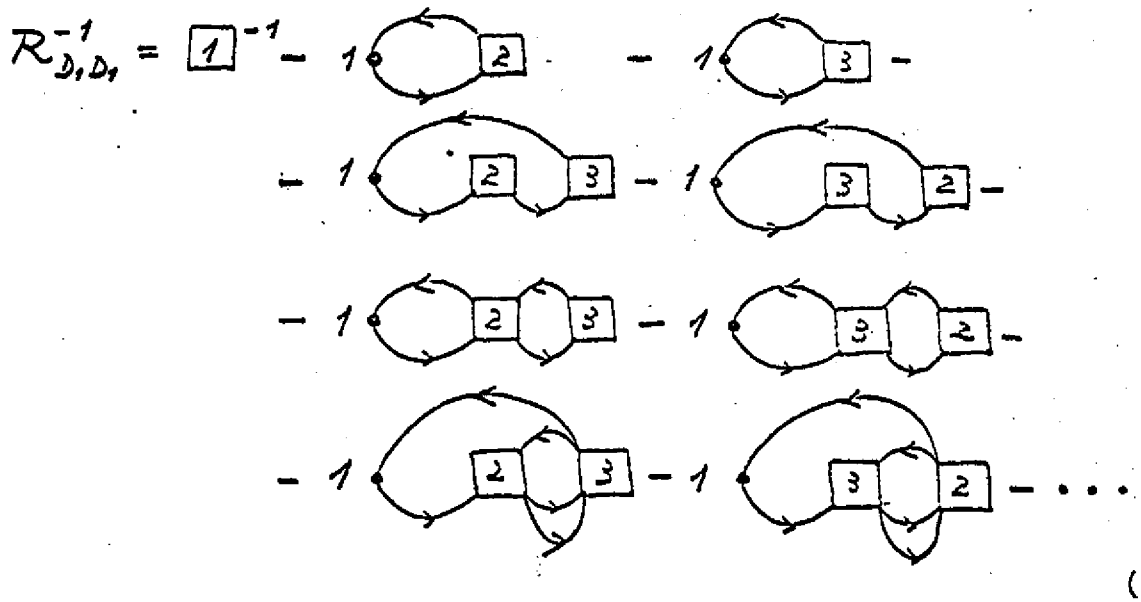
i) Suppose one searches for the localized vibrations of the central defect in the configuration of Fig.4a of three identical defects (identical defects have a renormalized Green's nucleus $\mathcal{G}_{DD}$ independent of the defect site in the lattice). In this case a dependable enough approach of the response function should be

$$R^{-1}_{D_1D_1} \approx \boxed{1}^{-1} - 1 \bullet \text{(loop)} \boxed{2} - 1 \bullet \boxed{3} \approx \boxed{1}^{-1} - 2 \times \bullet \text{(loop)} \boxed{2} =$$

$$= \mathcal{G}^{-1}_{DD} - 2 \times \Pi_{D_1D_2}\, \mathcal{G}_{D_2D_2}\, \Pi_{D_2D_1} \quad . \qquad (21)$$

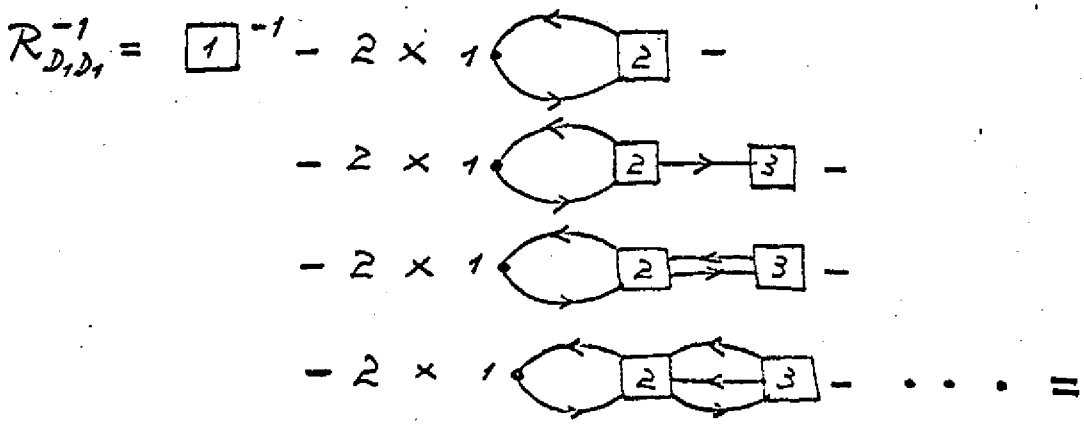
The exponential decay of the propagators with the increasing distance between defects has been used twice in this equation: to get rid of higher-order diagrams implying interactions of the exceedingly distant extreme defects, and to take as equal the contributions of the extreme defects (see also the previous section).

ii) Suppose now one looks for localized vibrations of the defect D_1 in the configuration of Fig.4b of three identical defects. The response function series now starts as



(22)

By similar arguments the following approximation seems realistic:

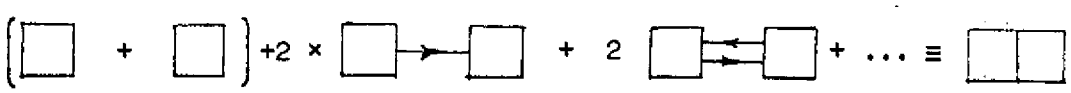


$$= \mathcal{G}^{-1}_{DD} - 2 \times \Pi_{D_1D_2} (\mathcal{G}_{DD} + \mathcal{G}_{DD}\Pi_{D_2D_3}\mathcal{G}_{DD} + \mathcal{G}_{DD}\Pi_{D_2D_3}\mathcal{G}_{DD}\Pi_{D_3D_2}\mathcal{G}_{DD} + \ldots)\Pi_{D_2D_1}$$

$$= \mathcal{G}^{-1}_{DD} - \Pi_{D_1D_2}\mathcal{K}^{D_3}_{D_2}\Pi_{D_2D_1} \quad , \qquad (\Pi_{DD'} = \Pi_{D'D}) \ .$$

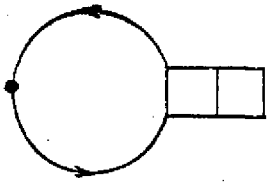
(23)

The notation $\mathcal{K}^{D_3}_{D_2}$ was assigned to the expression within the brackets, which is thought to denote a "clustering interaction" of the pair D_2 , D_3 . In closed form the "renormalized" pair interaction reads $\mathcal{K}^{D_3}_{D_2} \equiv 2 \times (\mathcal{G}^{-1}_{DD} - \Pi_{D_2D_3})^{-1}$. Its graphical equivalent should be



(24)

so that one has

$$R^{-1}_{D_1 D_1} \approx \mathcal{G}^{-1}_{DD} - 1$$  . (25)

These examples are intended to hint the way the dressed-defects approach can be used. Specific ways are yet to be devised for any particular problem.

It can readily be shown that the problem of the localized vibrations of an interstitial D can be solved in terms of the response function R_{DD}. Suppose the equation of motion

$$(\Phi - \omega^2 \mathcal{M})\ u = 0 \qquad (26)$$

is expanded according to the partition (2). It implies partition of u as a column vector of components $(u_L)_{3N\times 1}$, $(u_{D_k})_{3\times 1}$, $k = 1,2,\ldots,n$. After some manipulation one finds that the 3×1 part u_{D_k} assigned to the defect D_k is ruled by the 3×3 homogeneous system of equations

$$R^{-1}_{D_k D_k} \cdot u_{D_k} = 0 \quad , \qquad (27)$$

which has non-trivial solutions only for a vanishing determinant. Therefore, for D_k a necessary condition for localized modes to exist is

$$\det\ (R^{-1}_{D_k D_k}) = 0 \quad . \qquad (28)$$

The one-dimensional problem is discussed in the next section.

V. LOCALIZED VIBRATIONS OF DRESSED INTERSTITIALS. ONE-DIMENSIONAL LATTICE

The way of coupling the atoms stands in the following for the only mark of the interstitial character of the impurities in a one-dimensional lattice, their positions being irrelevant in this respect. One assumes one sort of impurities of mass m_D spread over the "interstitials" of a linear chain of atoms of mass m_L. The coupling of the nearest host lattice atoms is given the coupling constant γ ($\gamma < 0$) whereas the interstitial-lattice

coupling is denoted by δ ($\delta < 0$) (Fig.5). A lattice constant $a = 1$ is taken as reference length.

The unperturbed Green's function of a single interstitial is obviously the same for all the identical interstitials:

$$G_{DD} = \left(2\,|\delta| - m_D\,\omega^2\right)^{-1} \quad . \tag{29}$$

The Green's function of the ideal lattice can be set in a closed form (e.g. Ludwig 1964):

$$G_{\ell,\ell'}(z) = -(1/|\gamma|)\; z^{|\ell-\ell'|}/(z - 1/z) \;, \tag{30}$$

where, for localized modes, one has $z = -e^{-\sigma}$ and

$$\omega^2 = 2|\gamma|/m\;(1 + \mathrm{ch}\,\sigma) \quad . \tag{31}$$

Let D_0 be a single defect in the lattice (Fig.5a). Then the eigenfrequency of the localized mode comes from Eqs.(28), (19) which now read

$$\mathcal{G}_{DD}^{-1} = 0 \quad . \tag{32}$$

This should give the exact eigenfrequency provided the phonon propagator (12) is calculated exactly. Since the perturbation in the host lattice by the intrusion of the interstitial is confined to the atoms -1 and 0 one has

$$H_{\ell\ell'} = -\,|\delta| \cdot \Delta_{\ell,\ell'} \cdot (\Delta_{\ell',-1} + \Delta_{\ell',0}) \;, \tag{33}$$

($\Delta_{\ell,\ell'}$ is the Krönecker symbol), which indeed allows an exact calculation of Λ_{LL}. After some algebra one gets to the following exact expression of the self-propagator $\Pi_{D_0D_0}$ (see Eq.(11)):

$$\Pi_{D_0D_0} = -2|\gamma|\;K^2\;(e^{\sigma} + 1 - K)^{-1} \quad . \tag{34}$$

Here σ is the momentum of the localized mode (Eq.(31)) and $K \equiv |\delta|/|\gamma|$. Combining now Eqs.(15), (29), (34), the renormalized Green's nucleus representing the "dressed" defect is found to be

$$\mathcal{G}(\sigma) = (2|\gamma|)^{-1}\,[K + K^2(e^{\sigma} + 1 - K)^{-1} - 2M\,\mathrm{ch}^2(\sigma/2)]^{-1} \;, \tag{35}$$

where $M \equiv m_D/m_L$. Accordingly, the momentum equation is

$$\mathrm{ch}^2\left(\frac{\sigma}{2}\right) - \frac{K}{2M} = \frac{K^2}{2M}\,\frac{1}{e^{\sigma} + 1 - K} \quad . \tag{36}$$

It can be subject to a graphical solution for different values of the parameters K and M involved.

Eq.(36) can now be compared with the momentum equation emerging from the straightforward solution of the equations of motion of the chain. This is found by fitting a <u>symmetric localized</u> wave of the form

$$u_\ell = A(-1)^\ell\, e^{-\sigma|\ell + 1/2|} \tag{37}$$

in the "boundary" equations for the atoms $\ell = -1$ and D_0 . One gets the same equation (36), as is expected.

Suppose one takes now for the phonon propagator Λ_{LL} the zeroth-order approach, i.e. $H_{LL} \approx 0$, and then $\Lambda_{LL} \approx G_{LL}$. In the present case it would come from a weak coupling of the impurity to its surrounding ($K << 1$), which allows one to neglect in the auto-force constants $\Phi_{-1,-1}$ and $\Phi_{0,0}$ the constant δ as compared with γ . The only consequence of this approximation concerns the propagator (34), which now reads

$$\Pi_{D_0D_0} = -2|\gamma|\, K^2\, (e^{\sigma} + 1)^{-1} \quad . \tag{38}$$

Accordingly, the momentum equation (36) turns into

$$\mathrm{ch}^2\left(\frac{\sigma}{2}\right) - \frac{K}{2M} = \frac{K^2}{2M}\,\frac{1}{e^{\sigma} + 1} \quad , \tag{39}$$

which <u>is</u> indeed the weak coupling limit of Eq.(36).

It can be shown graphically (Fig.6) that both Eqs.(36) and (39) yield <u>one</u> localized mode of momentum σ_{loc} which, according to Eq.(37), corresponds to a <u>symmetric</u> wave localized on the impurity. The amplitude of the impurity is given by

$$u_{D_0} = \frac{K/(2M)}{K/(2M) - \mathrm{ch}^2(\sigma_{loc}/2)}\, u_0 \quad . \tag{40}$$

The case of two impurities can be handled similarly, starting with Eq.(20). Suppose the impurities are distributed as in Fig.5b. One must compare the <u>exact</u> momentum equation

$$ch^2\left(\frac{\sigma}{2}\right) - \frac{K}{2M} = \frac{K^2}{4M}\ \frac{2 \pm (1 - e^{\sigma})\, e^{-\sigma h}}{(1 + e^{\sigma}) - K(1 \pm e^{-\sigma h})} \qquad (41)$$

which is found either by using the correct phonon propagator Λ_{LL} in the dressed-defects approach or by straightforwardly solving the equations of motion, with the approximate momentum equation

$$ch^2\left(\frac{\sigma}{2}\right) - \frac{K}{2M} = \frac{K^2}{4M}\ \frac{2 \pm (1 - e^{\sigma})\, e^{-\sigma h}}{1 + e^{\sigma}}\ , \qquad (42)$$

found in the weak coupling limit ($\Lambda_{LL} \approx G_{LL}$) of the phonon propagator. Both Eqs.(41) and (42) provide essentially the same physical information, which consists in revealing the breaking of the degeneracy of the eigenfrequencies by defects interaction. A graphical solution of Eqs.(41) and (42) in the cases of closest possible and infinitely far apart defects is shown in Fig.6. In the limit $h \to \infty$ Eqs.(41) and (42) turn into Eqs.(36) and (39), as expected, and the degeneracy reappears. It turns out from the equations of motion that the low-energy mode (lower momentum mode in Fig.6) corresponds to a symmetric localized wave, whereas the high-energy mode (higher momentum in Fig.6) is antisymmetric and reads:

$$u_{\ell} = A\left[(-1)^{\ell}\, e^{-\sigma_a^s|\ell+1/2|} \pm (-1)^{(\ell-h)}\, e^{-\sigma_a^s|\ell-h+1/2|}\right]\ ,$$

$$u_{D_0} = \frac{K/(2M)}{K/(2M) - ch^2\,(\sigma_{loc}^s/2)} \cdot \frac{u_{-1} + u_0}{2}\ ,$$

$$u_{D_h} = \frac{K/(2M)}{K/(2M) - ch^2\,(\sigma_{loc}^s/2)} \cdot \frac{u_{h-1} + u_h}{2}\ . \qquad (43)$$

In the cases (39), (42) discussed above, localized modes exist only if the condition $M \leq K/2 - K^2/4$ for the atomic masses is fulfilled.

VI. CONCLUSION

The partition technique has been used to express the response function of an interstitial impurity in a crystal in terms of host lattice and many-defect contributions. Both the phonon propagation throughout the lattice and

the defects contributions to the response function were renormalized, which turned the picture of the interacting defects into a picture of interacting "dressed" defects, according to the standard many-body concepts.

As usual the convergence of the procedure and the way of using its facilities depend essentially on the physical problem approached. Hints were given on how the procedure works in the problem of localized vibrations of interstitial impurities. The one-dimensional lattice served as an example.

The dressed-defects approach may turn out to be useful in all problems involving correlation properties in the phonon field of the crystals, such as X-ray and neutron diffraction, and Mössbauer effect.

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FIGURE CAPTIONS

Fig.1 Interacting defects. Diagrammatic representation of the starting terms in the expansion of the response function.

Fig.2 Interacting "dressed" defects. Diagrammatic representation of the starting terms in the renormalized expansion of the response function. No self-interaction parts.

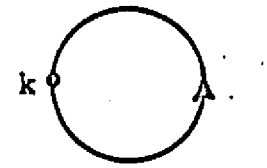
Fig.3 Langer's-like diagrams to approach the phonon propagator Λ_{LL} (Eq.(12)).

Fig.4 Two peculiar configurations of three interacting defects:
a) The extreme defects are very far apart from each other and almost equally distant from the defect in between.
b) The two defects in the right wing feature a "cluster" far apart from the defect on the left,

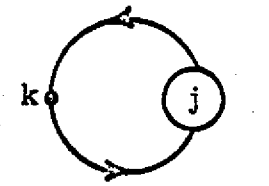
Fig.5 "Interstitial" impurities in a one-dimensional lattice:
a) Single interstitital.
b) Two interacting interstitials.

Fig.6 Graphical solution for the momentum equations (36), (39), (41) and (42), for the localized modes on interstitials in a one-dimensional lattice. The cases $h = 1$ and $h \to \infty$. The characteristic parameters are $K = 0.5$, $M = 0.05$. In heavy lines - the right-hand side of the exact Eqs.(36) and (41). In broken lines - the right-hand side of the approximate Eqs. (39) and (42).

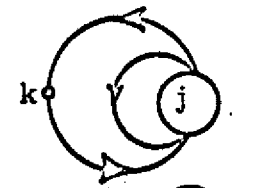
Fig.1



$\Pi_{D_k D_k}$ zeroth orde



$\Pi_{D_k D_j} G_{D_j D_j} \Pi_{D_j D_k}$ first orde



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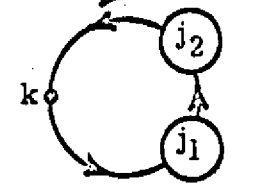

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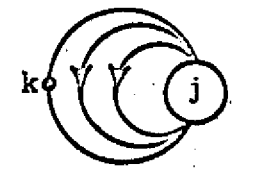
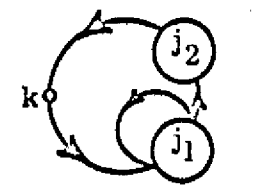
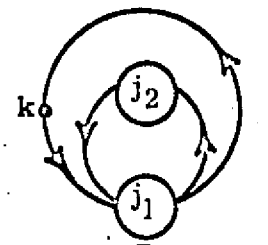


$\Pi_{D_k D_j} G_{D_j D_j} \Pi_{D_j D_j} G_{D_j D_j} \Pi_{D_j D_j} G_{D_j D_j} \Pi_{D_j D_k}$



$\Pi_{D_k D_{j_1}} G_{D_{j_1} D_{j_1}} \Pi_{D_{j_1} D_{j_1}} G_{D_{j_1} D_{j_1}} \Pi_{D_{j_1} D_{j_2}} G_{D_{j_2} D_{j_2}} \Pi_{D_{j_2} D_k}$



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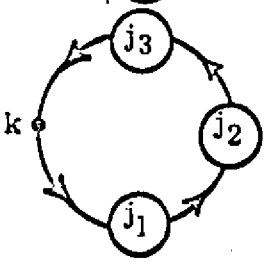
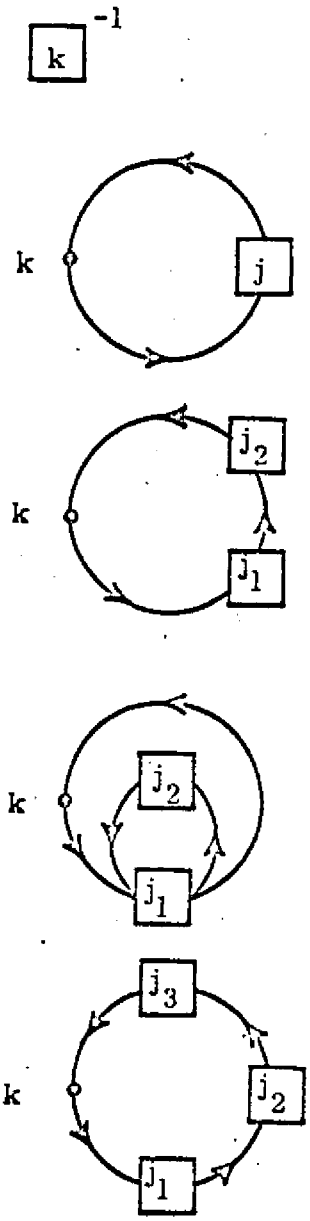


$\Pi_{D_k D_{j_1}} G_{D_{j_1} D_{j_1}} \Pi_{D_{j_1} D_{j_2}} G_{D_{j_2} D_{j_2}} \Pi_{D_{j_2} D_{j_3}} G_{D_{j_3} D_{j_3}} \Pi_{D_{j_3} D_k}$

Fig.2



$$\mathcal{G}^{-1}_{D_k D_k}$$

$$\Pi_{D_k D_j}\ \mathcal{G}_{D_j D_j}\ \Pi_{D_j D_k}$$

$$\Pi_{D_k D_{j_1}}\ \mathcal{G}_{D_{j_1} D_{j_1}}\ \Pi_{D_{j_1} D_{j_2}}\ \mathcal{G}_{D_{j_2} D_{j_2}}\ \Pi_{D_{j_2} D_k}$$

$$\Pi_{D_k D_{j_1}}\ \mathcal{G}_{D_{j_1} D_{j_1}}\ \Pi_{D_{j_1} D_{j_2}}\ \mathcal{G}_{D_{j_2} D_{j_2}}\ \Pi_{D_{j_2} D_{j_1}}\ \mathcal{G}_{D_{j_1} D_{j_1}}\ \Pi_{D_{j_1} D_k}$$

$$\Pi_{D_k D_{j_1}}\ \mathcal{G}_{D_{j_1} D_{j_1}}\ \Pi_{D_{j_1} D_{j_2}}\ \mathcal{G}_{D_{j_2} D_{j_2}}\ \Pi_{D_{j_2} D_{j_3}}\ \mathcal{G}_{D_{j_3} D_{j_3}}\ \Pi_{D_{j_3} D_k}$$

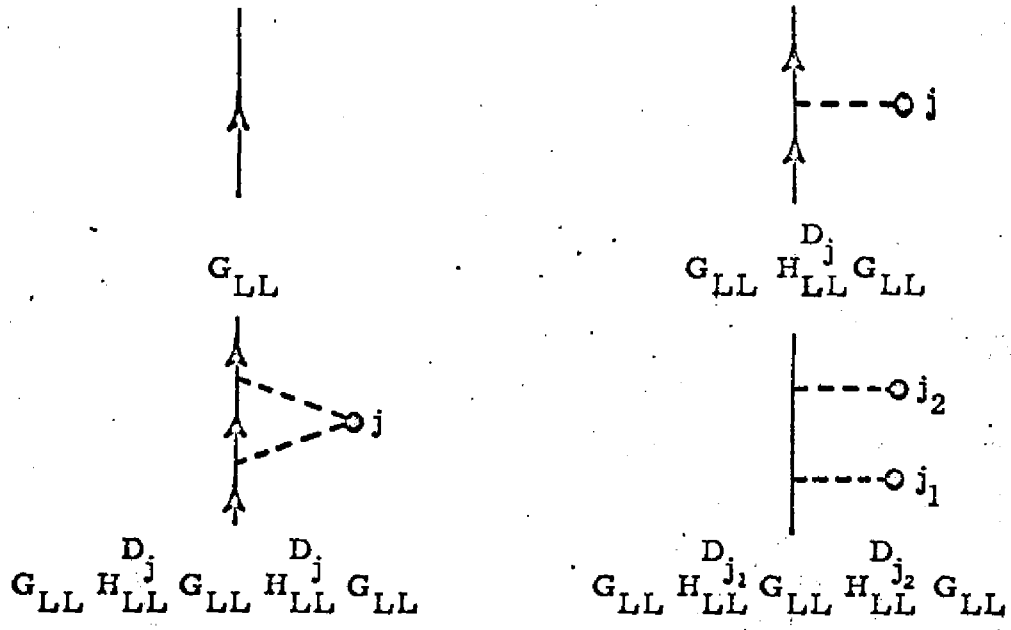


Fig. 3

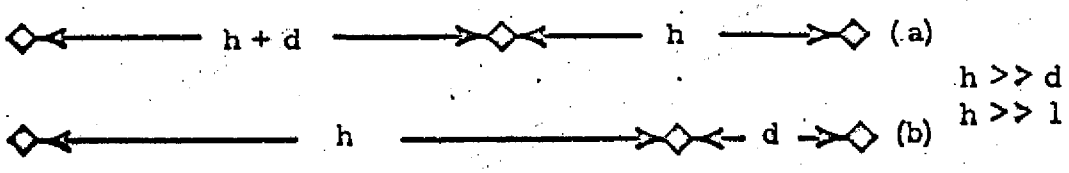


Fig.4

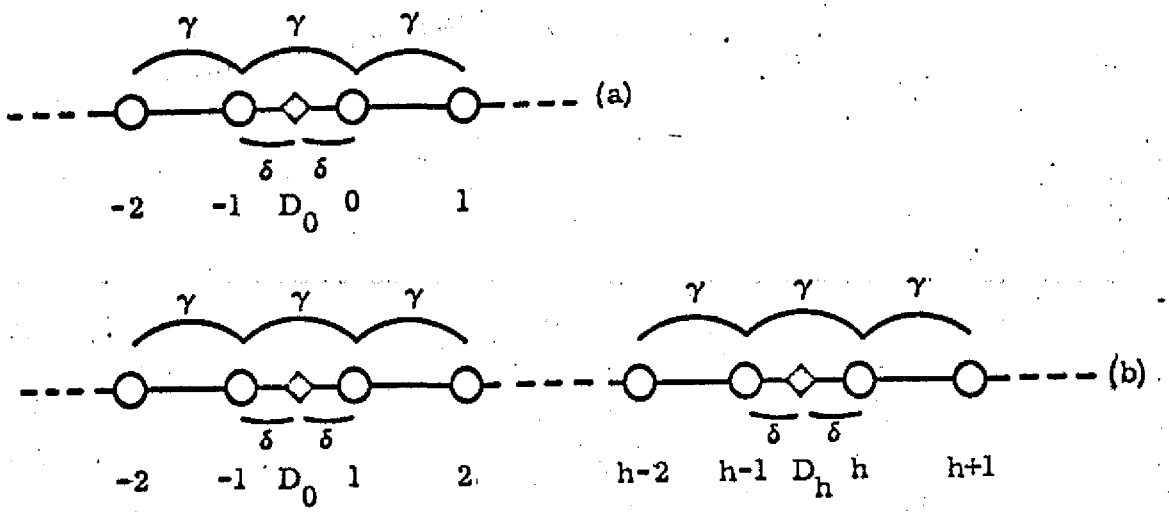


Fig. 5

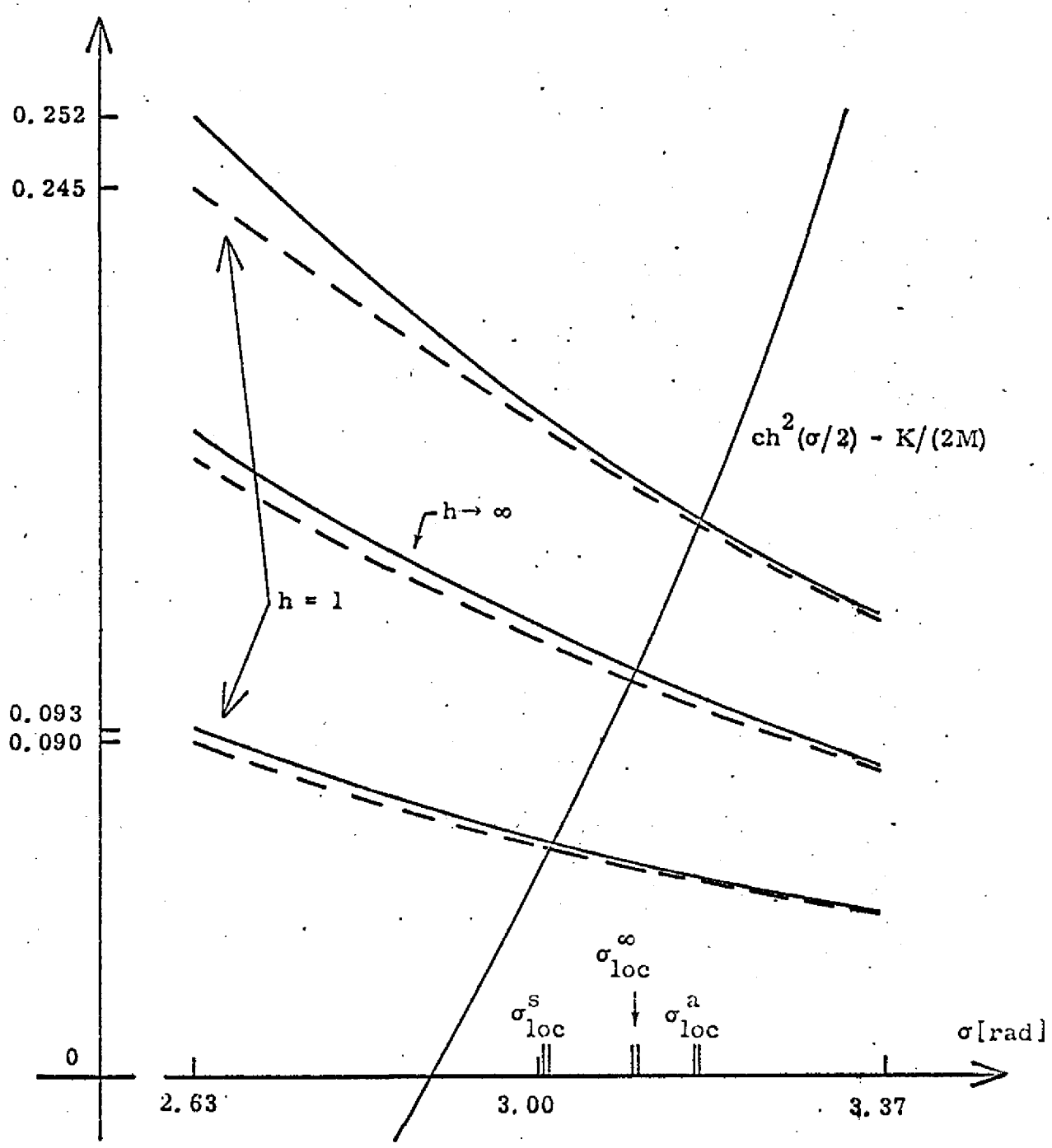

0. 252
0. 245
0. 093
0. 090
0
2. 63
3. 00
3. 37
σ[rad]
$ch^2(\sigma/2) - K/(2M)$
h → ∞
h = 1
σ^{∞}_{loc}
σ^{s}_{loc}
σ^{a}_{loc}

Fig. 6