Effect of Defects on Lattice Vibrations: Interaction of Defects and an Analogy with Meson Pair Theory*

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An analysis is given of the determination of additive functions of the frequencies of the normal mode vibrations of a lattice. The method is applied to the problem of calculating the self-energies and interaction energies of defects in lattices of any dimension. In particular results are derived for the self-energies and interaction energies of isotopes, holes, and "source" defects in simple cubic monatomic and diatomic lattices. For example it is shown that two holes in a simple cubic lattice attract each other, the energy of interaction being inversely proportional to the cube of the distance of separation. The general method is also applied to the problem of the interaction of lattice defects with the boundaries of the lattice. Finally, if the lattice approaches the limit of a continuum, it is shown that the energy of interaction between two holes is just that obtained by Wentzel for the interaction between two fixed nucleons according to the scalar meson pair theory.

INTRODUCTION

THE influence of defects such as impurities and holes on the physical properties of crystals has been one of the most studied phases of solid state physics in recent years. This paper is the third report of a detailed mathematical investigation of the effect of localized irregularities on lattice vibrations[1] (the first report will be referred to as D-1 and the second as D-2). Although the authors are interested in the general defect problem, they have decided that various suitable mathematical techniques can more easily be applied to perturbations of lattice vibrations than to other degrees of freedom in a solid and have elected to examine that problem first. The work of Koster and Slater[2] on the theory of semiconductors via Wannier wave functions parallels our analysis to some extent (as do the brief remarks of Lax and Smith[3] on lattice vibrations). Work is now in progress on the influence of defects on the spin wave, Ising, and spherical models of magnetic materials.

D-1 is mostly concerned with those vibrational modes which are localized around lattice defects. It is shown that under certain conditions discrete normal modes exist which are diplaced out of the continuum of modes of the unperturbed lattice. Only a few atoms in the immediate neighborhood of a defect participate in these modes. Generally motions of all atoms in a perfect monatomic crystal contribute equally to the energy in each normal mode. However, the atoms which participate in localized modes are responsible for more than their normal share of the internal energy of the crystal. Hence the region around a defect is equivalent to a "hot spot" in the lattice. A localized mode (either in the interior or on the surface of a crystal) might catalyze physical and chemical processes which would not normally occur at the existing temperature of the crystal. D-2 is concerned with localized modes in linear diatomic lattices.

It was also pointed out in D-1 that at low temperatures an attraction exists between "like" defects (for example a pair of isotopic impurities of the same mass) and a repulsion between "unlike" defects (for example, two isotopes of different mass, one heavier than a normal atom in the crystal and one lighter). This interaction is greatest at absolute zero. A consequence of the attraction between like defects would be a clustering tendency between atoms of like atomic weight in a mixed crystal of two isotopic species. Indeed one would expect a separation into two isotopic phases at $T=0$ (actually the equilibrium time for such a process might be very long). This effect has been discussed by Prigogine, Bingen, and Jeener.[4] It will be shown in Sec. 6 that light isotopes and holes are attracted to the free boundary of a crystal.

This paper is mainly concerned with the development of a formalism for the discussion of the effect of the interaction of defects on additive functions of the normal mode frequencies. The formalism will be applied to the calculation of the interaction energy between defects (as determined from the change in zero-point energy) and of that between defects and surfaces. Although thermodynamic quantities are additive functions of the frequencies, we shall postpone a discussion of their behavior until part 4 of this series. Detailed calculations are made here on simple cubic lattices with interactions (described through both central and noncentral forces) between nearest neighbors only. Both one- and two-component systems are analyzed.

Some remarks will be made concerning continuum field theory by letting our crystalline lattice spacings vanish. It was pointed out to the authors by Professor

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[1] E. W. Montroll and R. B. Potts, Phys. Rev. **100**, 525 (1955); Mazur, Montroll, and Potts, J. Wash. Acad. Sci. **46**, 2 (1956).
[2] G. F. Koster and J. C. Slater, Phys. Rev. **95**, 1167 (1954); G. F. Koster, Phys. Rev. **95**, 1436 (1954).
[3] M. Lax, Phys. Rev. **94**, 1391 (1954).
[4] Prigogine, Bingen, and Jeener, Physica **20**, 383 (1954); **20**, 516 (1954).

T. D. Lee that our methods are similar to those used by Wentzel[5] in his investigation of the meson pair theory of forces between nucleous. We show that pair theory is mathematically equivalent to the continuum limit of the theory of the interactions of holes in a crystal lattice.

The reader is referred to D-1 for a detailed discussion of the model[6] used here.

1. GENERAL FORMULAS FOR CALCULATION OF ADDITIVE FUNCTIONS OF NORMAL MODE FREQUENCIES

Let us suppose that the normal mode frequencies of a lattice are $\omega_1, \omega_2, \cdots$. Many quantities of interest can be expressed as sums of functions of the normal mode frequencies

$$S=\sum_j g(\omega_j). \tag{1.1}$$

For example, the zero-point energy of the lattice is given by S if $g(z)=\frac{1}{2}hz$. The characteristic function, $E(\exp i\alpha\omega^2)$, whose Fourier transform is the frequency distribution function, corresponds to

$$g(z)=N^{-1}\exp(i\alpha z^2),$$

where N is the number of degrees of freedom of the lattice. Thermodynamic quantities are generally of the form of (1.1).

Let us also assume that the frequencies are roots of a characteristic equation

$$D(\omega)=0.$$

It was pointed out in D-1 that if $g(z)$ is an analytic function inside of a closed counter-clockwise contour C and if $D(z)$ has all of its zeros but no poles inside the contour, then[7]

$$S=\sum_j g(\omega_j)=\frac{1}{2\pi i}\int_C g(z)\frac{d}{dz}\{\log D(z)\}dz. \tag{1.2}$$

We represent the function whose zeros are normal mode frequencies of a perfect lattice by $D_0(z)$, and represent the corresponding function associated with a lattice with defects enumerated by $\alpha, \beta, \cdots$ by $D(\alpha,\beta,\cdots;z)$.

The change in an additive function S which results from a single defect, α, is

$$\begin{aligned}\Delta S_\alpha&=\frac{1}{2\pi i}\int_C g(z)\frac{d}{dz}\{\log D(\alpha;z)-\log D_0(z)\}dz\\&=\frac{1}{2\pi i}\int_C g(z)\frac{d}{dz}\log\{D(\alpha;z)/D_0(z)\}dz.\end{aligned} \tag{1.3}$$

This quantity might be referred to as the self-S of the lattice. The "interaction-S" of a defect pair (α,β) is defined as the difference between the S of a system of two interacting defects and that of a pair of isolated defects and is given by

$$\Delta S_{\alpha,\beta}=\frac{1}{2\pi i}\int_C g(z)\frac{d}{dz}\times\log\{D(\alpha,\beta;z)D_0(z)/D(\alpha;z)D(\beta;z)\}dz. \tag{1.4}$$

If $\epsilon_\alpha, \epsilon_\beta, \cdots$ are the parameters which characterize defects $\alpha, \beta, \cdots$, and $D(\alpha;z)$ is of the form

$$D(\alpha;z)=D_0(z)[1+\epsilon_\alpha h_\alpha(z)] \tag{1.5a}$$

(as we shall show to be the case in a wide variety of situations), and

$$D(\alpha,\beta;z)=D_0(z)[1+\epsilon_\alpha h_\alpha(z)+\epsilon_\beta h_\beta(z)+\epsilon_\alpha\epsilon_\beta h_{\alpha\beta}(z)], \tag{1.5b}$$

we find

$$\Delta S_\alpha=\frac{\epsilon_\alpha}{2\pi i}\int_C\frac{h_\alpha'(z)g(z)dz}{1+\epsilon_\alpha h_\alpha(z)}, \tag{1.6a}$$

where the prime denotes the derivative with respect to the argument. Also

$$\Delta S_{\alpha\beta}=\frac{1}{2\pi i}\int_C g(z)\frac{d}{dz}\log\left\{1+\frac{\epsilon_\alpha\epsilon_\beta(h_{\alpha\beta}-h_\alpha h_\beta)}{(1+\epsilon_\alpha h_\alpha)(1+\epsilon_\beta h\beta)}\right\}dz, \tag{1.6b}$$

so that as ϵ_α and $\epsilon_\beta\to 0$

$$\Delta S_{\alpha\beta}\sim-\frac{\epsilon_\alpha\epsilon_\beta}{2\pi i}\int_C g(z)[h_\alpha(z)h_\beta(z)-h_{\alpha\beta}(z)]'dz$$

and the interaction S is of second order in $\epsilon_\alpha, \epsilon_\beta$ in the limit of "weak defects."

The total interaction S due to a large number of defects is $\sum\Delta S_{\alpha\beta}$ over all defect pairs and is a quadratic form in $\epsilon_\alpha, \epsilon_\beta, \cdots$ in the limit of weak defects, but cubic and higher order terms occur when "strong" defects (large ϵ's) exist.

2. ON THE GENERAL FORM OF THE CHARACTERISTIC EQUATIONS OF NORMAL MODE FREQUENCIES

The normal mode frequencies $\{\omega_j\}$ of a set of coupled harmonic oscillators are zeros of the characteristic determinant

$$D_0(\omega)=\begin{vmatrix}a_{11}+M_1\omega^2 & a_{12} & a_{13} & \cdots\\ a_{21} & a_{22}+M_2\omega^2 & a_{23} & \cdots\\ a_{31} & a_{32} & a_{33}+M_3\omega^2 & \cdots\\ \cdots & \cdots & \cdots & \cdots\end{vmatrix}. \tag{2.1}$$

Here the M_j's are particle masses and the a_{ij}'s are related to the force constants of the "springs." We shall assume that defects in a lattice alter the determinant through the introduction of a set of parameters $\delta_\alpha, \delta_\beta, \cdots$ at the αth, βth, $\cdots$ elements along the main

[5] G. Wentzel, Helv. Phys. Acta **15**, 111 (1942).

[6] See also E. W. Montroll, Third Berkeley Symposium on Statistics and Probability, 1955.

[7] See E. C. Titchmarsh, *Theory of Functions* (Oxford University Press, Oxford, 1932), p. 116.

diagonal so that these elements become $a_{\alpha\alpha}+M_\alpha\omega^2+\delta_\alpha$, etc. (Although it is sometimes necessary to perturb off-diagonal terms as well, the analysis of such cases is essentially the same as that given below.)

In the case of a single defect, the determinant can be expanded by the αth row in the usual manner to yield

$$D(\alpha;\omega)=D_0(\omega)+\delta_\alpha A_{\alpha\alpha}, \tag{2.2a}$$

where $A_{\alpha\alpha}$ is the cofactor of $a_{\alpha\alpha}+\omega^2M_\alpha$ in the determinant $D_0(\omega)$. It is well known that if $\{a_{ij}^{(-1)}(\omega)\}$ is the set of elements of the inverse of the matrix of $D_0(\omega)$, then

$$A_{\alpha\alpha}=D_0(\omega)a_{\alpha\alpha}^{(-1)}(\omega), \tag{2.2b}$$

and

$$D(\alpha;\omega)=D_0(\omega)[1+\delta_\alpha a_{\alpha\alpha}^{(-1)}(\omega)], \tag{2.3}$$

which is of the form (1.5a) where h_α is to be identified with $a_{\alpha\alpha}^{(-1)}$.

Now let there be two defects, one at α and the other at β. Then, if we expand $D(\alpha,\beta;\omega)$ with respect to the βth row, we find

$$D(\alpha,\beta;\omega)=D(\alpha;\omega)+\delta_\beta A_{\beta\beta}(\alpha),$$

where $A_{\beta\beta}$ is the cofactor of the βth diagonal element of the determinant $D(\alpha;\omega)$. This is, however,

$$A_{\beta\beta}(\alpha)=A_{\beta\beta}+A\begin{Bmatrix}\alpha\alpha\\ \beta\beta\end{Bmatrix},$$

where $A\begin{Bmatrix}\alpha\alpha\\ \beta\beta\end{Bmatrix}$ is the second-order cofactor obtained by striking out the αth and βth rows and columns of $D_0(\omega)$. Since this cofactor is

$$A\begin{Bmatrix}\alpha\alpha\\ \beta\beta\end{Bmatrix}=D_0(\omega)\begin{vmatrix}a_{\alpha\alpha}^{(-1)} & a_{\alpha\beta}^{(-1)}\\ a_{\beta\alpha}^{(-1)} & a_{\beta\beta}^{(-1)}\end{vmatrix},$$

we have

$$\begin{aligned}D(\alpha,\beta;\omega)&=D_0(\omega)\Big\{1+\delta_\alpha a_{\alpha\alpha}^{(-1)}(\omega)+\delta_\beta a_{\beta\beta}^{(-1)}(\omega)\\&\qquad+\delta_\alpha\delta_\beta\begin{vmatrix}a_{\alpha\alpha}^{(-1)} & a_{\alpha\beta}^{(-1)}\\ a_{\beta\alpha}^{(-1)} & a_{\beta\beta}^{(-1)}\end{vmatrix}\Big\}\\&=D_0(\omega)\begin{vmatrix}1+\delta_\alpha a_{\alpha\alpha}^{(-1)} & (\delta_\alpha\delta_\beta)^{\frac12}a_{\alpha\beta}^{(-1)}\\ (\delta_\alpha\delta_\beta)^{\frac12}a_{\beta\alpha}^{(-1)} & 1+\delta_\beta a_{\beta\beta}^{(-1)}\end{vmatrix}.\end{aligned} \tag{2.4}$$

The reader can verify the three-defect formula,

$$D(\alpha,\beta,\gamma;\omega)=D_0(\omega)\begin{vmatrix}1+\delta_\alpha a_{\alpha\alpha}^{(-1)} & (\delta_\alpha\delta_\beta)^{\frac12}a_{\alpha\beta}^{(-1)} & (\delta_\alpha\delta_\gamma)^{\frac12}a_{\alpha\gamma}^{(-1)}\\ (\delta_\beta\delta_\alpha)^{\frac12}a_{\beta\alpha}^{(-1)} & 1+\delta_\beta a_{\beta\beta}^{(-1)} & (\delta_\beta\delta_\gamma)^{\frac12}a_{\beta\gamma}^{(-1)}\\ (\delta_\gamma\delta_\alpha)^{\frac12}a_{\gamma\alpha}^{(-1)} & (\delta_\gamma\delta_\beta)^{\frac12}a_{\gamma\beta}^{(-1)} & 1+\delta_\gamma a_{\gamma\gamma}^{(-1)}\end{vmatrix}, \tag{2.5}$$

and may generalize these results to any given number of defects.

Since the elements of the inverse matrices appear in all formulas independently of the specific nature of the defects, we derive formulas for these elements in the next section.

3. ELEMENTS OF INVERSE MATRIX FOR CERTAIN MODELS

We shall now find the elements of the inverse of the matrix D_0 which corresponds to one-component, n-dimensional simple cubic lattices with interactions between nearest neighbors only (and both central and noncentral forces). We assume the lattices to be cubes containing N^n lattice points. At the end of this section we discuss the case of a diatomic lattice.

The mechanics of these systems are discussed in detail in D-1 and in reference 6. A mathematically convenient (but physically somewhat unreal) feature of this model is the independence of the x, y, and z components of the motions of the lattice particles.

The equation of motion of the x component of the displacement of a particle at lattice point $(m_1,m_2,\cdots,m_n)$ is

$$\begin{aligned}M\ddot{x}(m_1,\cdots,m_n)=\sum_{j=1}^{n}\gamma_j[&x(m_1,\cdots,m_j-1,\cdots,m_n)\\&-2x(m_1,\cdots,m_n)+x(m_1,\cdots,m_j+1,\cdots,m_n)],\end{aligned} \tag{3.1a}$$

where γ_j is the force constant associated with displacements parallel to the jth coordinate axis. Similar equations exist for the other components of the displacement. We choose solutions of the form

$$x(m_1,\cdots,m_n)=e^{i\omega t}u(m_1,m_2,\cdots) \tag{3.1b}$$

and find D_0 to be the determinant of the coefficients of the u's in

$$\begin{aligned}\omega^2Mu(m_1,m_2,\cdots)+\sum_{j=1}^{n}\gamma_j[&u(\cdots,m_j-1,\cdots)\\&-2u(\cdots,m_j,\cdots)+u(\cdots,m_j+1,\cdots)]=0.\end{aligned} \tag{3.2a}$$

We first assume the existence of periodic boundary conditions; later we discuss the cases of free and rigid boundaries. The characteristic vectors of the matrix of the coefficients of $u(m)$ are of the form

$$u_s(m)=N^{-\frac12 n}\exp(2\pi i\mathbf{s}\cdot\mathbf{m}/N), \tag{3.2b}$$

where

$$\mathbf{s}=(s_1,\cdots,s_n),\quad \mathbf{m}=(m_1,m_2,\cdots,m_n)$$

and the characteristic values

$$\begin{aligned}\lambda(s_1,s_2,\cdots)&=M\omega^2-2\sum_{j=1}^{n}\gamma_j(1-\cos\varphi_j),\\&\varphi_j=2\pi s_j/N.\end{aligned} \tag{3.3}$$

The elements of our determinant can be expressed as

$$\begin{aligned}a(\mathbf{m};\mathbf{m}')=N^{-n}\sum_{s_1,s_2,\cdots=1}^{N}&\lambda(s_1,s_2,\cdots)\\&\times\exp\{2\pi i\mathbf{s}\cdot(\mathbf{m}-\mathbf{m}')/N\},\end{aligned} \tag{3.4}$$

while those of the inverse are

$$a^{(-1)}(\mathbf{m};\mathbf{m}')=N^{-n}\sum_s \lambda^{-1}(\mathbf{s}) \times\exp\{2\pi i\mathbf{s}\cdot(\mathbf{m}-\mathbf{m}')/N\}. \quad (3.5)$$

In the limit as $N\to\infty$,

$$a^{(-1)}(\mathbf{m};\mathbf{m}')=\left(\frac{1}{2\pi}\right)^n\int_0^{2\pi}\cdots\int \times\frac{\exp[i(\mathbf{m}-\mathbf{m}')\cdot\varphi]d^n\varphi}{[M\omega^2-2\sum_1^n\gamma_j(1-\cos\varphi_j)]}. \quad (3.6a)$$

These integrals are essentially the Green's functions discussed in D-1. In that notation,

$$a^{(-1)}(\mathbf{m};\mathbf{m}')=(\gamma_1+\gamma_2+\cdots+\gamma_n)^{-1}g(m-m'). \quad (3.6b)$$

In the one-dimensional case,

$$g(j)=\begin{cases}-\frac{1}{2}\operatorname{csch}y\exp(-|j|y) & \text{if } f^2<0\\ \frac{1}{2}\operatorname{csch}y\exp\{-|j|(y+\pi i)\} & \text{if } f^2>1,\end{cases} \quad (3.7)$$

where $f=\omega/\omega_L$ and

$$\cosh y=|2f^2-1|. \quad (3.7a)$$

The case $0<f^2<1$ corresponds to scattering problems and will not interest us here.

The elements of the inverse of the matrix for a two-dimensional square lattice has the form

$$a^{(-1)}(\mathbf{s}_1,\mathbf{s}_2)=\frac{\mu_{st}}{(2\pi)^2}\int_0^{2\pi}\int\frac{\exp(i\mathbf{s}\cdot\varphi)d\varphi_1d\varphi_2}{4b^2+2\gamma_1\cos\varphi_1+2\gamma_2\cos\varphi_2}, \quad (3.8)$$

where

$$\mu_{st}=\begin{cases}-1 & \text{if } f^2=(\omega/\omega_L)^2<0\\ (-1)^{s+t} & \text{if } f^2>1,\end{cases}$$

$$4b^2=|M\omega^2-2(\gamma_1+\gamma_2)|.$$

This integral can be expressed in terms of generalized hypergeometric functions of two variables.[6] This form is not particularly useful for our purpose. However, when $s_1=s_2=s$ a relatively simple expression exists for $a^{(-1)}(s,s)$:

$$a^{(-1)}(s,s)=\frac{\mu_{ss}}{(2\pi)^2}\int_0^\infty dx\int_0^{2\pi}\int \times\exp(-4b^2x-2x\gamma_1\cos\varphi_1-2x\gamma_2\cos\varphi_2) \times\exp(i\mathbf{s}\cdot\varphi)d\varphi_1d\varphi_2 \quad (3.9a)$$

$$=\frac{\mu_{ss}}{(2\pi)^2}\int_0^\infty\exp(-4b^2x)I_s(2x\gamma_1)I_s(2x\gamma_2)dx$$

$$=\frac{\beta\mu_{ss}}{(\gamma_1+\gamma_2)\pi}Q_{s-\frac{1}{2}}(1+2\beta^2f^2[f^2-1]),$$

where $Q_n(z)$ is the nth Legendre function of the second kind and

$$\beta=(\gamma_1+\gamma_2)/(\gamma_1\gamma_2)^{\frac{1}{2}}. \quad (3.9b)$$

An asymptotic expression for $a^{(-1)}(s_1,s_2)$ can be obtained when

$$s_1^2\gamma_1^{-1}+s_2^2\gamma_2^{-1}$$

is very large. However, since in the general case $a^{(-1)}(s_1,s_2,\cdots,s_n)$ can be considered as simply $a^{(-1)}(s_1,s_2)$, we proceed with the general case to find the asymptotic expression for $a^{(-1)}(s_1,s_2,\cdots,s_n)$ when

$$S=[s_1^2\gamma_1^{-1}+\cdots+s_n^2\gamma_n^{-1}]^{\frac{1}{2}} \quad (3.10)$$

is very large.

First let $\omega^2<0$. Then

$$a^{(-1)}(s_1,s_2,\cdots)=-\frac{1}{(2\pi)^n}\int_{-\pi}^{\pi}\cdots\int \times\frac{\exp(i\mathbf{s}\cdot\varphi)d^n\varphi}{-M\omega^2+2(\gamma_1+\cdots)-2\gamma_1\cos\varphi_1-\cdots}. \quad (3.11)$$

When S is large, the integrand oscillates very rapidly except in the region of $|\varphi|$ close to the origin. Hence we can expand each of the cosines as a power series in φ and retain only the first few terms. Also, since the remote regions in φ space contribute practically nothing to the integral, after this expansion is made we can integrate over the entire φ space without significantly changing the integral (in the limit as $S\to\infty$). Hence

$$a^{(-1)}(s_1,s_2,\cdots)\simeq-\frac{1}{(2\pi)^n}\int_{-\infty}^{\infty}\cdots\int \times\frac{\exp i[(s_1\gamma_1^{-\frac{1}{2}}\cdot\varphi_1\gamma_1^{\frac{1}{2}})+\cdots]d\varphi_1\cdots d\varphi_n}{-M\omega^2+\gamma_1\varphi_1^2+\cdots+\gamma_n\varphi_n^2}. \quad (3.12)$$

If we introduce new coordinates $x_j=\varphi_j\gamma_j^{\frac{1}{2}}$, the integral becomes an n-fold Fourier transform of a function of $r^2=x_1^2+\cdots+x_n^2$. Such integrals have been discussed by Bochner[8] and lead to the following result after a transformation to polar coordinates:

$$a^{(-1)}(s_1,s_2,\cdots)\simeq-\frac{(2\pi)^{\frac{1}{2}n}}{(2\pi)^n(\gamma_1\gamma_2\cdots\gamma_n)^{\frac{1}{2}}S^{\frac{1}{2}(n-2)}} \times\int_0^\infty r^{\frac{1}{2}n}[r^2+(-M\omega^2)]^{-1}J_{\frac{1}{2}(n-2)}(Sr)dr. \quad (3.13)$$

Here the J function is a Bessel function of order $\frac{1}{2}(n-2)$, while the integral is a Hankel transform which

[8] S. Bochner, *Vorlesungen über Fouriersche Integral* (Chelsea Publishing Company, New York, 1948), p. 187.

is well known.[9] One finds

$$a^{(-1)}(s_1,s_2,\cdots)\simeq-\frac{(-M\omega^2)^{\frac{1}{4}(n-2)}}{(\gamma_1\cdots\gamma_n)^{\frac{1}{2}}(2\pi)^{\frac{1}{2}n}S^{\frac{1}{2}(n-2)}}\times K_{\frac{1}{2}(n-2)}([-M\omega^2]^{\frac{1}{2}}S), \quad (3.14)$$

where $K_\nu(z)$ is that Bessel function which is commonly referred to as the K function. In particular,

$$K_{\frac{1}{2}}(z)=(\pi/2z)^{\frac{1}{2}}e^{-z},$$

while as $z\to\infty$

$$K_\nu(z)\sim(\pi/2z)^{\frac{1}{2}}e^{-z}$$

for all positive ν if $|\arg z|<\frac{3}{2}\pi$. Finally as $S\to\infty$ (with $\omega^2<0$), we have, when $n\geqslant 3$,

$$a^{(-1)}(s_1,s_2,\cdots)\sim-\frac{(-M\omega^2)^{\frac{1}{4}(n-3)}}{(2\pi)^{\frac{1}{2}n}(\gamma_1\cdots\gamma_n)^{\frac{1}{2}}}\frac{(\frac{1}{2}\pi)^{\frac{1}{2}}}{S^{\frac{1}{2}(n-1)}}\times\exp\{-(-M\omega^2)^{\frac{1}{2}}S\}. \quad (3.15)$$

One can determine $a^{(-1)}(s_1,s_2,\cdots)$ in a similar manner when $(2f^2-1)>1$. We replace the φ_j's by $\varphi_j+\pi$ to obtain

$$a^{(-1)}(s_1,s_2,\cdots)=\frac{(-1)^{s_1+\cdots+s_n}}{(2\pi)^n}\int_{-\pi}^{\pi}\cdots\int\times\frac{\exp(i\boldsymbol{\varphi}\cdot\mathbf{s})d^n\varphi}{M\omega^2-2(\gamma_1+\gamma_2+\cdots)-2\gamma_1\cos\varphi_1+\cdots}$$

and (when $\omega^2>\omega_L^2$)

$$a^{(-1)}(s_1,s_2,\cdots)\sim\frac{[M(\omega^2-\omega_L^2)]^{\frac{1}{4}(n-2)}}{(\gamma_1\gamma_2\cdots\gamma_n)^{\frac{1}{2}}(2\pi)^{\frac{1}{2}n}S^{\frac{1}{2}(n-2)}}\times K_{\frac{1}{2}(n-2)}([M(\omega^2-\omega_L^2)]^{\frac{1}{2}}S), \quad (3.16)$$

by using the arguments given in the foregoing.

It is to be noted that if we let

$$as=r, \quad k=\varphi/a,$$

a being the lattice spacing, (3.11) becomes

$$a^{(-1)}(r_1,r_2,\cdots)=-\frac{a^n}{(2\pi)^n}\int_{-\pi/a}^{\pi/a}\cdots\int\times\frac{\exp(i\mathbf{r}\cdot\mathbf{k})d^nk}{-M\omega^2+2(\gamma_1+\cdots)-\sum 2\gamma_j\cos ak_j},$$

so that, as $a\to 0$ in the continuum limit, (3.14) corresponds to an *exact* rather than asymptotic expression and

$$a^{(-1)}(r_1,\cdots,r_n)=-\frac{a^{\frac{1}{2}(n-2)}(-M\omega^2/\gamma_1)^{+\frac{1}{4}(n-2)}\gamma_1{}^{n/2}}{(\gamma_1\cdots\gamma_n)^{\frac{1}{2}}R^{\frac{1}{2}(n-2)}(2\pi)^{\frac{1}{2}n}}\times K_{\frac{1}{2}(n-2)}([-M\omega^2/\gamma_1]^{\frac{1}{2}}R/a), \quad (3.17a)$$

where now we define R (with units of length) by

$$R=[r_1{}^2+r_2{}^2(\gamma_1/\gamma_2)+\cdots+r_n{}^2(\gamma_1/\gamma_n)]^{\frac{1}{2}}. \quad (3.17b)$$

Section 6 will be devoted to a discussion of the interaction of defects with crystal boundaries. For this purpose we shall record the inverses $a^{(-1)}(m,m')$ which correspond to rigid and free boundaries. We shall sketch the manner in which results were obtained by examining one-dimensional chains.

Let us consider a chain of $N+2$ masses with the end two held fixed at their equilibrium positions (the rigid boundary case). This corresponds to boundary conditions of (3.2a) (with $n=1$):

$$u(0)=u(N+1)=0.$$

The components of the jth characteristic vector of the matrix whose elements are the coefficients of the u's in (3.2a) are

$$u_j(m)=[2/(N+1)]^{\frac{1}{2}}\sin[mj\pi/(N+1)],$$

the associated characteristic value being

$$\lambda_j=M\omega^2-2\gamma\{1-\cos[j\pi/(N+1)]\}.$$

Hence the elements of the required inverse matrix are

$$a^{(-1)}(m;m')=\frac{2}{N+1}\sum_{j=1}^{N}\frac{\sin[mj\pi/(N+1)]\sin[m'j\pi/(N+1)]}{M\omega^2-2\gamma\{1-\cos[j\pi/(N+1)]\}}. \quad (3.18a)$$

The n-dimensional "rigid boundary" inverse is

$$a^{(-1)}(m;m')=\left(\frac{2}{N+1}\right)^n\sum_{s_1=1}^{N}\cdots\sum_{s_n=1}^{N}\times\frac{\prod_{k=1}^{n}\left\{\sin\frac{m_ks_k\pi}{N+1}\sin\frac{m_k's_k\pi}{N+1}\right\}}{M\omega^2-2\sum_1{}^n\gamma_k\{1-\cos[s_k\pi/(N+1)]\}}. \quad (3.18b)$$

The boundary conditions at a free boundary are

$$u(1)-u(0)=u(N)u-(N+1)=0.$$

This is obtained by noting that the equation appropriate for an end-particle displacement $u(1)$ is

$$u(1)[M\omega^2-\gamma]+\gamma u(2)=0,$$

or

$$u(1)[M\omega^2-2\gamma]+\gamma u(2)+\gamma u(0)=0,$$

the standard form if

$$u(1)-u(0)=0.$$

[9] Erdelyi, Magnus, Oberhettinger, and Tricomi, *Tables of Integral Transforms* (McGraw-Hill Book Company, Inc., New York, 1954), Vol. 2, p. 23.

The characteristic vectors which satisfy the boundary conditions have components

$$u_0(m)=(1/N)^{\frac{1}{2}},$$
$$u_j(m)=(2/N)^{\frac{1}{2}}\cos[(2m-1)\pi j/2N] \quad \text{if} \quad j=1, 2, \cdots, N-1.$$

with characteristic values

$$\lambda_j=M\omega^2-2\gamma[1-\cos(\pi j/N)], \quad j=0, 1, \cdots, N-1.$$

The elements of the required inverse are

$$a^{(-1)}(m; m')=\frac{2}{N}\sum_{j=1}^{N-1} \times\frac{\cos[(2m-1)\pi j/2N]\cos[(2m'-1)\pi j/2N]}{M\omega^2-2\gamma[1-\cos(\pi j/N)]}+\frac{1}{NM\omega^2}, \tag{3.19a}$$

with an n-dimensional generalization

$$a^{(-1)}(m; m')=\left(\frac{2}{N}\right)^n\sum_{s_1=1}^{N-1}\sum_{s_1=1}^{N-1}\frac{\prod_1^n\{\cos[(2m_k-1)\pi s_k/2N]\cos[(2m_k'-1)\pi s_k/2N]\}}{M\omega^2-2\sum_1^n\gamma_k[1-\cos(\pi s_k/N)]}+O\left(\frac{1}{N}\right). \tag{3.19b}$$

The elements of the inverse matrix $a^{(-1)}(m; m')$ associated with a two-component system with nearest-neighbor interactions only can be discussed in a similar manner. The one-dimensional case will be developed in detail and the results merely stated for the general n-dimensional lattice. We postulate the even-numbered particles on our chain to be of mass M and the odd-numbered ones of mass m. Then the analog of (3.2a) is two sets of equation

$$\gamma u(2j+1)+(M\omega^2-2\gamma)u(2j)+\gamma u(2j-1)=0, \tag{3.20a}$$
$$\gamma u(2j+2)+(m\omega^2-2\gamma)u(2j+1)+\gamma u(2j)=0. \tag{3.20b}$$

If we let

$$v(2j)=(M\omega^2-2\gamma)^{\frac{1}{2}}u(2j), \tag{3.21}$$
$$v(2j+1)=(m\omega^2-2\gamma)^{\frac{1}{2}}u(2j+1), \tag{3.22}$$

we obtain the more compact single set of equations:

$$\gamma v(j-1)+(M^*\omega^2-2\gamma)v(j)+\gamma v(j+1)=0, \tag{3.23}$$

where the mass M^* is defined by

$$\omega^2M^*=2\gamma+[(M\omega^2-2\gamma)(m\omega^2-2\gamma)]^{\frac{1}{2}}. \tag{3.24}$$

Clearly, if $m=M$ these equations reduce to the one-component ones and $M^*=M$.

It can be shown that in the n-dimensional case the new single set of equations is the same form as (3.2a) with the mass replaced by M^*, with

$$\omega^2M^*=2(\gamma_1+\cdots+\gamma_n)+[(M\omega^2-2\gamma_1-\cdots-2\gamma_n)\times(m\omega^2-2\gamma_1-\cdots-2\gamma_n)]^{\frac{1}{2}}. \tag{3.25}$$

The normal mode frequencies of an n-dimensional monatomic lattice are

$$M\omega^2=2\sum\gamma_j(1-\cos\varphi_j), \quad \varphi_j=2\pi s_j/N,$$

the s_j's being integers. In our diatomic lattice

$$M^*\omega^2=2\sum\gamma_j(1-\cos\varphi_j). \tag{3.26}$$

If we substitute (3.22) into this equation and solve for ω^2, we find two branches:

$$\omega^2=(\gamma_1+\cdots+\gamma_n)(M+m)/Mm \pm(mM)^{-1}[(\gamma_1+\cdots+\gamma_n)^2(M-m)^2+4mM(\textstyle\sum_j\gamma_j\cos\varphi_j)^2]^{\frac{1}{2}}. \tag{3.27}$$

If $M>m$, the largest frequency ω_L^2 is given by

$$\omega_L^2=2(\gamma_1+\cdots+\gamma_n)(M+m)/Mm. \tag{3.28a}$$

The top edge of the lower band is at

$$\omega_1^2=2(\gamma_1+\cdots+\gamma_n)/M, \tag{3.28b}$$

while the lower edge of the top band is at

$$\omega_2^2=2(\gamma_1+\cdots+\gamma_n)/m. \tag{3.28c}$$

The Green's function (3.15) is valid for the diatomic lattice if $\omega^2<0$ and M is replaced by M^*.

4. CHARACTERIZATION OF DEFECTS

As in D-1, we shall be concerned mainly with changes in masses and force constants but not in equilibrium positions. If the mass of the particle at lattice point $\alpha=(\alpha_1,\alpha_2,\cdots,\alpha_n)$ is changed from M to M_α, Eq. (3.2a) with $m=\alpha$ can be put in the appropriate form by adding the term

$$\omega^2(M_\alpha-M)u(\alpha_1,\alpha_2,\cdots)$$

to the left-hand side. Then, we set (see 2.2a)

$$\delta_\alpha=-\omega^2M\epsilon_\alpha, \tag{4.1}$$

where we define

$$\epsilon_\alpha=1-(M_\alpha/M). \tag{4.2}$$

The single mass defect function $D(\alpha;\omega)$ is then

$$D(\alpha;\omega)=D_0(\omega)\{1-\omega^2M\epsilon_\alpha a^{(-1)}(\alpha,\alpha)\}. \tag{4.3}$$

The characterization of a mass defect in a diatomic lattice is obtained from (3.20). Let the heavy mass M be replaced by M_α. Then Eq. (3.20a) has a correction term

$$\omega^2(M_\alpha-M)u(\alpha).$$

After the transformation (3.21) is made the new equation in $v(\alpha)$ has the term

$$-M\omega^2\epsilon_\alpha(m\omega^2-2\gamma)^{\frac{1}{2}}/(M\omega^2-2\gamma)^{\frac{1}{2}}$$

added to the left-hand side of (3.23).

In general, the mass defect function is

$$D(\alpha;\omega)=D_0(\omega)\{1-\omega^2a^{(-1)}(\alpha;\alpha)\times M\epsilon_\alpha[(m\omega^2-2\gamma)/(M\omega^2-2\gamma)]^{\frac{1}{2}}\} \tag{4.4}$$

if M is normal mass at α, and

$$D(\alpha;\omega)=D_0(\omega)\{1-\omega^2 a^{(-1)}(\alpha;\alpha) \times m\epsilon_\alpha[(M\omega^2-2\gamma)/(m\omega^2-2\gamma)]^{\frac{1}{2}}\} \quad (4.5)$$

if m is normally at α. Generally,

$$\epsilon_\alpha=\left(1-\frac{\text{defect mass at }\alpha}{\text{normal mass at }\alpha}\right). \quad (4.6)$$

The defect in force constant as well as mass is first discussed in the one-dimensional monatomic case. Let the force constant associated with the interaction of α with $\alpha+1$ and $\alpha-1$ be changed from γ to γ'. Then (3.2a) becomes (in the cases $m=\alpha-1$, α, $\alpha+1$):

$$[\omega^2M-(\gamma'+\gamma)]u(\alpha-1)+\gamma' u(\alpha)+\gamma u(\alpha-2)=0,$$
$$[\omega^2M_\alpha-2\gamma']u(\alpha)+\gamma' u(\alpha-1)+\gamma' u(\alpha+1)=0,$$
$$[\omega^2M-(\gamma'+\gamma)]u(\alpha+1)+\gamma' u(\alpha)+\gamma u(\alpha+2)=0.$$

If we replace $u(\alpha)$ by a new variable $(\gamma/\gamma')v(\alpha)$, the determinant of the coefficients of the u's and v is of the form (2.1) with additions to elements along the main diagonal:

$$\delta_{\alpha-1}=\delta_{\alpha+1}=-\gamma\tau_\alpha/(1-\tau_\alpha), \quad (4.7a)$$

$$\delta_\alpha=M\omega^2[(1-\epsilon_\alpha)(1-\tau_\alpha)^2-1]+2\gamma\tau_\alpha, \quad (4.7b)$$

where

$$\tau_\alpha=1-(\gamma/\gamma'). \quad (4.8)$$

If both the mass and the force constant are changed, three consecutive diagonal elements are changed in D_0.

If defects exist at α, β, $\cdots$, the appropriate value of the new M's and γ's are substituted into (4.1–4.5) at the appropriate diagonal elements in (2.1).

Equation (4.7) is still valid in the n-dimensional case when $\gamma_1=\gamma_2=\gamma_3=\cdots$ and when the force constants between the αth particle and its nearest neighbors are all changed to γ'. However, if $\gamma_1\neq\gamma_2, \gamma_3, \cdots$, and only force constants in the m_1 direction are changed, the normal mode determinant (2.1) is changed in several off-diagonal elements as well as along the main diagonal. The functions (2.4) and (2.5) are somewhat more complicated but can be easily found.

In the n-dimensional case, with $\gamma_1=\gamma_2=\cdots$, a defect at $(\alpha,\beta,\cdots)$ yields

$$\delta_{\alpha,\beta,\ldots}=M\omega^2[(1-\epsilon_{\alpha,\beta\ldots})(1-\tau_{\alpha,\beta\ldots})^2-1] +2n\gamma\tau_{\alpha,\beta\ldots}, \quad (4.9)$$

$$\delta_{\alpha\pm1,\beta,\ldots}=\delta_{\alpha,\beta\pm1,\ldots}=\cdots=-\gamma\tau_{\alpha\beta\ldots}/(1-\tau_{\alpha\beta\ldots}), \quad (4.10)$$

where the defect mass at $(\alpha,\beta,\cdots)$ is $M_{\alpha,\beta,\ldots}$ and

$$\epsilon_{\alpha,\beta,\ldots}=(1-M^{-1}M_{\alpha,\beta,\ldots}), \quad (4.11)$$

while a change of the force constant to $\gamma_{\alpha,\beta,\ldots}$ between $(\alpha,\beta,\cdots)$ and its nearest neighbor yields

$$\tau_{\alpha,\beta,\ldots}=(1-\gamma\gamma_{\alpha,\beta,\ldots}{}^{-1}). \quad (4.12)$$

A defect which we shall discuss later, but which corresponds to neither a mass nor force constant change, is the defect "source" at α which we characterize by

$$\delta_\alpha=\kappa\gamma=\text{constant independent of }\omega.$$

5. SELF-ENERGY AND INTERACTION ENERGY OF DEFECTS

In this section, the formulas derived above will be applied to the calculation of the self-energy and interaction energies of various defects in monatomic and and diatomic lattices.

The simplest type of defect is the source defect described by (4.13). Although it does not correspond to any attainable defect in a crystal lattice, we shall discuss it first to demonstrate the ideas involved in making more complicated calculations. We shall show at the end of this section that source defects are mathematically equivalent to holes in lattices if one is concerned with the interaction of holes separated by many lattice spacings.

The self-energy of a source defect of strength $\kappa\gamma$ is given by

$$\Delta E_S=\frac{\hbar}{4\pi i}\int_C \omega d\log[1+\kappa\gamma a^{(-1)}(\alpha,\alpha;\omega)], \quad (5.1)$$

where use has been made of (1.6a) and (4.13). From (3.6a),

$$a^{(-1)}(\alpha,\alpha;\omega)=\frac{1}{(2\pi)^n}\int_0^{2\pi}\cdots\int\frac{d^n\varphi}{M\omega^2-2\sum_1^n\gamma_j(1-\cos\varphi_j)}.$$

The contour C has to contain the positive real axis of ω since the frequencies of interest are positive real numbers; it may be chosen to be the counter-clockwise contour about the right half-plane. Then the only non-vanishing contribution to (5.1) is the integration down the imaginary axis. Since the integrand is an even function, the logarithmic term being a function of ω^2, the integral reduces to

$$\Delta E_S=-\frac{\hbar}{2\pi}\int_0^\infty \omega d\log[1+\kappa\gamma a^{(-1)}(\alpha,\alpha;i\omega)].$$

In the case of the one-dimensional lattice, this integral can be evaluated in terms of elementary functions. The inverse $a^{(-1)}(\alpha,\alpha;i\omega)$ is given by $-1/\{4\gamma f(1-f^2)^{\frac{1}{2}}\}$ (where $f=\omega/\omega_L$), so that

$$\Delta E_S=-\frac{\hbar\omega_L}{2\pi}\int_0^\infty f d\log\{1-\tfrac{1}{4}\kappa[1/f(1-f^2)^{\frac{1}{2}}]\}.$$

If we let $f=\tan\vartheta$, we obtain after some manipulation:

$$\Delta E_S=-\frac{\hbar\omega_L}{2\pi}\left\{\frac{\pi}{2}-\alpha\int_0^{\pi/2}\frac{d\vartheta}{\alpha-\sin\vartheta}-\int_0^{\pi/2}\frac{d\vartheta}{1+\alpha\sin\vartheta}\right\}, \quad (5.2a)$$

where α is related to κ by

$$\kappa=4\alpha/(1-\alpha^2), \quad -1<\alpha<1, \quad (5.2b)$$

so that by letting α range from -1 to $+1$, κ ranges from $-\infty$ to $+\infty$. Hence

$$\Delta E_S=-\frac{\hbar\omega_L}{2\pi}\left\{\frac{\pi}{2}+\frac{\alpha}{(1-\alpha^2)^{\frac{1}{2}}}\log\left|\frac{1+(1-\alpha^2)^{\frac{1}{2}}}{\alpha}\right|-(1-\alpha^2)^{-\frac{1}{2}}\cos^{-1}\alpha\right\}. \quad (5.3a)$$

The interaction energy between two source defects separated by a great distance can be obtained as follows for all numbers of dimensions $\geqslant 3$. The case $n<3$ must be handled in a slightly different manner and will be omitted here. We consider the special case $\gamma_1+\gamma_2=\cdots=\gamma$. If one defect of strength κ is at $m=(m_1,m_2,\cdots)$ and the other κ' at $m'=(m_1',m_2',\cdots)$ we find

$$\Delta E_I=-\frac{\hbar}{2\pi}\int_0^\infty \omega d\log\left\{1-\frac{\kappa\kappa'\gamma^2 a^{(-1)}(m,m';i\omega)a^{(-1)}(m',m;i\omega)}{[1+\gamma\kappa a^{(-1)}(m,m;i\omega)][1+\gamma\kappa' a^{(-1)}(m',m';i\omega)]}\right\}. \quad (5.3b)$$

As $|m-m'|\to\infty$, $a^{(-1)}(m,m';i\omega)\to 0$ so that at great distances we obtain (after integrating by parts), in the weak defect limit as κ and $\kappa'\to 0$,

$$\Delta E_I\simeq-\frac{\hbar\kappa\kappa'}{2\pi}\int_0^\infty \gamma^2 a^{(-1)}(m,m';i\omega)a^{(-1)}(m',m;i\omega)d\omega. \quad (5.3c)$$

Since

$$a^{(-1)}(m,m';i\omega)=a^{(-1)}(m',m;i\omega)\sim(M\omega_L^2)^{\frac{1}{4}(n-3)}\times f^{\frac{1}{2}(n-3)}(\tfrac{1}{2}\pi)^{\frac{1}{2}}(2\pi\gamma)^{-\frac{1}{2}n}S^{\frac{1}{2}(n-1)}\exp\{-(M\omega_L^2)^{\frac{1}{2}}fS\},$$

where

$$S=\gamma^{-\frac{1}{2}}[s_1^2+s_2^2+\cdots+s_n^2]^{\frac{1}{2}},$$

$$s_j=m_j'-m_j, \quad \text{and} \quad M\omega_L^2=4n\gamma$$

we find

$$\Delta E_I\sim-\frac{\hbar\kappa\kappa'\gamma^2}{4(2\pi\gamma)^n}\frac{M^{\frac{1}{2}(n-3)}\omega_L{}^{n-2}}{s^{n-1}}\int_0^\infty f^{n-3}\times\exp(-2M^{\frac{1}{2}}\omega_L Sf)df \quad (5.4)$$

$$=-\frac{\hbar\omega_L\kappa\kappa'(n-3)!}{2(4\pi)^n n^{\frac{1}{2}}|m'-m|^{2n-3}}.$$

In particular, if $n=3$,

$$\Delta E_I\simeq-\hbar\omega_L\kappa\kappa'/2(4\pi)^3\sqrt{3}\,|m'-m|^3; \quad (5.5)$$

or, if we let a be our lattice spacing and $R=a|m'-m|$, then

$$\Delta E_I\simeq-\hbar\omega_L\kappa\kappa' a^3/2(4\pi)^3\sqrt{3}R^3. \quad (5.6)$$

Two sources or "sinks" (we call the case $\kappa<0$ a sink) attract each other, while a source and sink repel each other, with an energy of interaction inversely proportional to R^3.

A more realistic example is that of the isotopic defects in a lattice. We examine the behavior of such defects in both monatomic and diatomic lattices.

(a) Monatomic Lattice

The self-energy of an isotope of mass $(1-\epsilon_\alpha)M$ is given by

$$\Delta E_S=\frac{\hbar}{4\pi i}\int_C \omega d\log[1-\epsilon_\alpha M\omega^2 a^{(-1)}(\alpha,\alpha;\omega)]. \quad (5.7)$$

As in the previous case, our integration can be carried from 0 to ∞:

$$\Delta E_S=-\frac{\hbar}{2\pi}\int_0^\infty \omega d\log[1+\epsilon_\alpha M\omega^2 a^{(-1)}(\alpha,\alpha;i\omega)]. \quad (5.8)$$

In the case of the one-dimensional lattice, this integral can be evaluated explicitly; in fact using (3.7), (5.8) becomes

$$\frac{\Delta E_S}{\frac{1}{2}\hbar\omega_L}=-\frac{1}{\pi}\int_0^\infty fd\log[1-\epsilon f(1+f^2)^{-\frac{1}{2}}] \quad (5.9a)$$

$$=\tfrac{1}{2}[(1-\epsilon^2)^{-\frac{1}{2}}-1]+\pi^{-1}(1-\epsilon^2)^{-\frac{1}{2}}\sin^{-1}\epsilon, \quad (5.9b)$$

in agreement with D-1, Eq. (4.15).

A similar analysis gives for the more interesting case of the interaction of two isotopes the formula

$$\Delta E_I=-\frac{\hbar}{2\pi}\int_0^\infty \omega d\log\left[1-\epsilon_\alpha\epsilon_\beta M^2\omega^4\left\{\frac{a^{(-1)}(\beta,\alpha;i\omega)a^{(-1)}(\alpha,\beta;i\omega)}{[1+\epsilon_\alpha M\omega^2 a^{(-1)}(\alpha,\alpha;i\omega)][1+\epsilon_\beta M\omega^2 a^{(-1)}(\beta,\beta;i\omega)]}\right\}\right]; \quad (5.10)$$

or, for ϵ_α, $\epsilon_\beta\to 0$ (in the general case the integration is more difficult but can be carried out either numerically or through various series expansions),

$$\Delta E_I\simeq\frac{\hbar\epsilon_\alpha\epsilon_\beta}{2\pi}\int_0^\infty \omega d[M^2\omega^4 a^{(-1)}(\alpha,\beta;i\omega)a^{(-1)}(\beta,\alpha;i\omega)], \quad (5.11)$$

which after integrating by parts simplies to

$$\Delta E_I\approx-\frac{\hbar\epsilon_\alpha\epsilon_\beta}{2\pi}\int_0^\infty M^2\omega^4 a^{(-1)}(\alpha,\beta;i\omega)a^{(-1)}(\beta,\alpha;i\omega)d\omega. \quad (5.12)$$

For the one-dimensional lattice, (5.12) gives

$$\frac{\Delta E_I}{\frac{1}{2}\hbar\omega_L}\approx-\frac{\epsilon_\alpha\epsilon_\beta}{\pi}\int_0^\infty\frac{[(1+f^2)^{\frac{1}{2}}-f]^{2|\alpha-\beta|}}{f^2(1+f^2)} \quad (5.13)$$

$$=-\frac{\epsilon_\alpha\epsilon_\beta}{2\pi}\left\{\frac{4|\alpha-\beta|}{16(\alpha-\beta)^2-\frac{1}{4}}-\psi(\tfrac{3}{4}+2|\alpha-\beta|)+\psi(\tfrac{1}{4}+2|\alpha-\beta1)\right\} \quad (5.14)$$

in agreement with D-1 (5.31).

Of more interest is the expression for the interaction energy for large distances. Then (3.15) may be inserted in (5.12) to yield

$$\Delta E_I \sim \frac{\hbar\epsilon_\alpha\epsilon_\beta}{2\pi}\int_0^\infty M^2\omega^4 \frac{(M\omega^2)^{\frac{1}{2}(n-3)}}{(2\pi)^n(\gamma_1\gamma_2\cdots\gamma_n)}\frac{\pi}{2}S^{1-n} \times\exp(-2\omega M^{\frac{1}{2}}S)d\omega \quad (5.15)$$

or

$$\frac{\Delta E_I}{\frac{1}{2}\hbar\omega_L} \sim \frac{-\epsilon_\alpha\epsilon_\beta}{4(\gamma_1+\cdots+\gamma_n)^{\frac{1}{2}}(2\pi)^n(\gamma_1\gamma_2\cdots\gamma_n)S^{n-1}} \times\int_0^\infty k^{n+1}e^{-2kS}dk = \frac{-\epsilon_\alpha\epsilon_\beta(n+1)\,!S^{-(2n+1)}}{16(\gamma_1+\cdots+\gamma_n)^{\frac{1}{2}}(\gamma_1\gamma_2\cdots\gamma_n)(4\pi)^n}. \quad (5.16)$$

For the case $\gamma_1=\gamma_2=\cdots=\gamma_n=\gamma$,

$$\gamma^{\frac{1}{2}}S=(s_1^2+s_2^2+\cdots+s_n^2)^{\frac{1}{2}}=R/a$$

and the energy of interaction is given by

$$\frac{\Delta E_I}{\frac{1}{2}\hbar\omega_L}\sim-\frac{\epsilon_\alpha\epsilon_\beta(n+1)\,!a^{2n+1}}{16n^{\frac{1}{2}}(4\pi)^nR^{2n+1}}. \quad (5.17)$$

For one dimension, $\Delta E_1\propto R^{-3}$ as derived in D-1. For two dimensions $\Delta E_1\propto R^{-5}$ and for three dimensions $\Delta E_1\propto R^{-7}$.

An attraction exists when both M_α and M_β are larger or smaller than M (like defects), while a repulsion appears when $M_\alpha>M>M_\beta$ or $M_\alpha<M<M_\beta$ (unlike defects).

(b) Diatomic Lattice

The self-energy of an isotopic defect in a diatomic lattice of alternating masses m and M is given (by a derivation similar to that for the monatomic lattice) by

$$\Delta E_S=-\frac{\hbar}{2\pi}\int_0^\infty \omega d\,\log[1-D(\alpha;i\omega)a^{(-1)}(\alpha,\alpha;i\omega)], \quad (5.18)$$

where D is given by (4.4) or (4.5) and for the one-dimensional lattice

$$a^{(-1)}(\alpha,\alpha;i\omega)=-[(m\omega^2+2\gamma)(M\omega^2+2\gamma)-4\gamma^2]^{\frac{1}{2}}. \quad (5.19)$$

For an isotope of mass $(1-\epsilon_\alpha)m$, this integral becomes

$$\frac{\Delta E_S}{\frac{1}{2}\hbar\omega_L}=-\frac{1}{\pi\omega_L}\int_0^\infty \omega d \times\log\left[1-\frac{\epsilon m\omega^2\{(m\omega^2+2\gamma)(M\omega^2+2\gamma)\}^{\frac{1}{2}}}{(m\omega^2+2\gamma)\{(m\omega^2+2\gamma)(M\omega^2+2\gamma)-4\gamma^2\}^{\frac{1}{2}}}\right]. \quad (5.20)$$

This integral has been evaluated in D-2 for two special cases, namely, when $M=m(1+\eta)$, η small and $M=\zeta^2m$, ζ small. In the first case,

$$\frac{\Delta E_S}{\frac{1}{2}\hbar(4\gamma/m)^{\frac{1}{2}}}=-\frac{1}{2}+\frac{1}{\pi(1-\epsilon^2)}[\tfrac{1}{2}\pi+\sin^{-1}\epsilon] +\frac{\epsilon\eta}{4\pi}\left[\frac{\sqrt{2}}{1+\epsilon^2}\log(1+\sqrt{2})-\frac{\epsilon\pi\sqrt{2}}{2(1+\epsilon^2)}+\frac{\pi}{2\epsilon} -\frac{(1-\epsilon^2)^{\frac{1}{2}}}{\epsilon(1+\epsilon^2)}\{\tfrac{1}{2}\pi+\sin^{-1}\epsilon\}\right]+O(\eta^2) \quad (5.21)$$

and in the second case,

$$\frac{\Delta E_S}{\frac{1}{2}\hbar(2\gamma/m)^{\frac{1}{2}}}=-\frac{1}{2}+\frac{1}{\pi(1-\epsilon^2)^{\frac{1}{2}}}\{\tfrac{1}{2}\pi+\sin^{-1}\epsilon\}+\frac{\zeta\epsilon}{4(1-\epsilon)} -\zeta^2\left[\frac{\epsilon}{2\pi(1-\epsilon^2)^{\frac{1}{2}}}+\frac{\epsilon^2}{2\pi(1-\epsilon^2)^{\frac{3}{2}}}\{\tfrac{1}{2}\pi+\sin^{-1}\epsilon\}\right]+O(\zeta^3). \quad (5.22)$$

For the interaction energy between two isotopes,

$$\Delta E_I\approx-\frac{\hbar}{2\pi}\int_0^\infty \delta_\alpha(i\omega)\delta_\beta(i\omega)[a^{(-1)}(\alpha,\beta;i\omega)]^2d\omega, \quad (5.23)$$

where δ_α and δ_β are given by (4.4) or (4.5).

If

$$u^2=[(m\omega^2+2\gamma)(M\omega^2+2\gamma)]^{\frac{1}{2}}-2\gamma, \quad (5.24)$$

then the asymptotic expression for the element of the inverse matrix can be inserted in (5.23), giving

$$\Delta E_I\simeq-\frac{\hbar}{2\pi}\int_0^\infty \delta_\alpha(i\omega)\delta_\beta(i\omega)\frac{\pi}{2(2\pi)^n} \times\frac{u^{n-3}\exp(-2uS)}{(\gamma_1\gamma_2\cdots\gamma_n)S^{n-1}}\frac{d\omega}{du}du. \quad (5.25)$$

But, from (5.24),

$$\omega^2=\frac{2}{m+M}u^2+O(u^4) \quad (5.26)$$

and

$$\delta_\alpha(i\omega)\delta_\beta(i\omega)=\frac{4\sigma_\alpha\sigma_\beta}{(m+M)^2}u^4+O(u^6), \quad (5.27)$$

where $\sigma=\epsilon m$ or ϵM is the change in mass of the isotope from the normal mass. As above, the integration can be carried out with the final result:

$$\frac{\Delta E_I}{\frac{1}{2}\hbar\omega_L}\simeq-\frac{\sigma_\alpha\sigma_\beta(mM)^{\frac{1}{2}}}{2(m+M)^3} \times\frac{(n+1)\,!S^{-(2n+1)}}{(4\pi)^n(\gamma_1\gamma_2\cdots\gamma_n)(\gamma_1+\gamma_2+\cdots+\gamma_n)^{\frac{1}{2}}}. \quad (5.28)$$

If $m=M$, then

$$\sigma_\alpha\sigma_\beta(mM)^{\frac{1}{2}}/2(m+M)^3=\epsilon_1\epsilon_2/16 \tag{5.29}$$

and (5.28) is obtained.

For $\gamma_1=\gamma_2=\cdots=\gamma_n$, $\gamma^{\frac{1}{2}}S=R/a$, (5.24) becomes

$$\frac{\Delta E_I}{\frac{1}{2}\hbar\omega_L}\simeq-\frac{\sigma_\alpha\sigma_\beta(mM)^{\frac{1}{2}}}{2(m+M)^3}\frac{(n+1)!\,a^{2n+1}}{(4\pi)^n n^{\frac{1}{2}}R^{2n+1}}. \tag{5.30}$$

In particular, when $n=3$ our interaction energy varies inversely as the 7th power of the distance.

An interesting consequence of (5.30) is obtained if we consider a pair of defects whose masses lie between M and m. If these defects move on the same sublattice (the lattice of M's or m's), an attraction between the defects results; whereas, if in their motion one defect remains on one sublattice and one on the other sublattice, a continuing repulsion exists.

The interaction of two impurities (or holes) which do not distort the lattice equilibrium positions can be discussed in the same manner as that of the isotopic defects. We examine for simplicity the special case $\gamma_1=\gamma_2=\cdots=\gamma$ which corresponds to equal central and noncentral force constants.

Consider two similar defects, one at lattice point (0,0,0) and the other at (l,m,n), characterized by a mass M' and springs with force constants γ' connecting these lattice points to their nearest neighbors. The determinant $D(\omega)$ is changed by the addition of

$$\delta_1=\gamma-\gamma' \tag{5.31}$$

to the diagonal elements $(-1,0,0)$, $(1,0,0)$, $(0,-1,0)$, $(0,1,0)$, $(0,0,-1)$, $(0,0,1)$, $(l-1,m,n)$, $(l+1,m,n)$, $(l,m-1,n)$, $(l,m+1,n)$, $(l,m,n-1)$, $(l,m,n+1)$ and by the addition of

$$\delta_2=(\omega/\gamma')^2(M'\gamma^2-\gamma'^2)+(6\gamma/\gamma')(\gamma'-\gamma) \tag{5.32}$$

to diagonal elements (0,0,0) and (l,m,n). The energy of interaction between two defects is

$$\Delta E_I=-\frac{\hbar}{2\pi}\int_0^\infty \omega d\log\left\{\begin{vmatrix}A & B\\ B & A\end{vmatrix}|A|^{-2}\right\}, \tag{5.33}$$

where A and B are 7×7 matrices given in Appendix I. The product of the determinants can be simply expressed as

$$|I-(A^{-1}B)^2|$$

and this can be easily evaluated by taking account of the symmetry of A and B. However, the resulting expression is rather complicated and will not be exhibited here. It simplifies considerably if only the first term in the expansion in inverse powers of the distance r between the defects is required. In this approximation, A can be taken as the unit matrix and (5.33) becomes

$$\Delta E_I=-\frac{\hbar}{2\pi}\int_0^\infty \mathrm{Trace}B^2d\omega. \tag{5.34}$$

The first term in $\mathrm{Tr}(B^2)$ is

$$[(6/\gamma')(\gamma'-\gamma^2)]^2[a^{(-1)}(0,l;i\omega)]^2, \tag{5.35}$$

so that E_I is precisely the expression (5.36) obtained for the interaction energy between two source defects with

$$\kappa=(6/\gamma\gamma')(\gamma'-\gamma)^2. \tag{5.36}$$

We have used the invariance relation $a^{(-1)}(m,m';i\omega)=a^{(-1)}(0,l;i\omega)$ if $l=m-m'$. It is to be noted that to this first order of approximation the interaction energy is independent of M'. When we set $M'=0$, our defects become holes in the lattice. We then find that the interaction energy of two holes is attractive and varies as the inverse third power of the separation distance (5.5). Furthermore, the discussion of the interaction of a pair of holes is equivalent to that between a pair of source defects when the source strength κ is defined by (5.36).

6. INTERACTION OF DEFECTS WITH BOUNDARIES

As a first example of the interaction of a defect with a boundary, we consider an isotopic impurity m lattice spacings from the end of a chain. In the case of a *rigid boundary* (end of chain held fixed) the characteristic determinant for normal modes is obtained by combining (4.3), (3.18a), and (2.3):

$$D(m;\omega)=D_0(\omega)\left[1-2\omega^2M\epsilon N^{-1}\sum_{j=1}^{N}\left\{\sin^2\left(\frac{m\pi j}{N+1}\right)\right\}\Big/\left\{M\omega^2-2\gamma\left[1-\cos\left(\frac{\pi j}{N+1}\right)\right]\right\}\right],$$

which, in the limit as $N\to\infty$, becomes for the case $f^2<0$:

$$D(m;\omega)=D_0(\omega)\{1-\epsilon(\tanh\tfrac{1}{2}z)(1-e^{-2mz})\},\qquad\text{rigid boundary,}\quad(6.1)$$

with $\cosh z=1-2f^2$. As usual, $\epsilon=1-(M'/M)$ with M' being the impurity mass. The corresponding determinant in the case of a free boundary is obtained by combining (3.19a) with (2.3) and (4.3)

$$D(m;\omega)=D_0(\omega)\{1-\epsilon(\tanh\tfrac{1}{2}z)(1+e^{-(2m-1)z})\},\qquad\text{free boundary.}\quad(6.2)$$

It is to be noted that as the defect recedes from the boundary the m dependent exponentials vanish and (6.1) and (6.2) reduce to the ordinary single-defect result:

$$D(\infty;\omega)=D_0(\omega)[1-\epsilon\tanh\tfrac{1}{2}z]. \tag{6.3}$$

Furthermore, the sign of the interaction terms are such that if a defect is attracted to a free boundary it is repelled from a rigid boundary and vice versa. The interaction is of $O(\epsilon)$ rather than ϵ^2; hence interactions of isotopes with boundaries are not of the "image" type

which exist in electrostatics and hydrodynamics. The ratio $D(m;\omega)/D(\infty;\omega)$, which is to be substituted into (1.3) to find the interaction, is then

$$\frac{D(m;\omega)}{D(\infty;\omega)}=\begin{cases}1+\dfrac{\epsilon e^{-2mz}\tanh\frac{1}{2}z}{1-\epsilon\tanh\frac{1}{2}z}, & \text{rigid boundary}\\[2ex] 1-\dfrac{\epsilon e^{-(2m+1)z}\tanh\frac{1}{2}z}{1-\epsilon\tanh\frac{1}{2}z}, & \text{free boundary.}\end{cases} \tag{6.4}$$

Then the interaction with a free boundary is

$$\Delta E_{\mathrm{FB}}=-\frac{\hbar\omega_L}{2\pi}\int_0^\infty fd\log\left\{1-\frac{\epsilon e^{-(2m+1)z}\tanh\frac{1}{2}z}{1-\epsilon\tanh\frac{1}{2}z}\right\}, \tag{6.5a}$$

while that with a rigid boundary is

$$\Delta E_{\mathrm{RB}}=-\frac{\hbar\omega_L}{2\pi}\int_0^\infty fd\log\left\{1+\frac{\epsilon e^{-2mz}\tanh\frac{1}{2}z}{1-\epsilon\tanh\frac{1}{2}z}\right\}. \tag{6.5b}$$

If we integrate by parts in the rigid boundary case, we find

$$\begin{aligned}\Delta E_{\mathrm{RB}}&=\frac{\hbar\omega_L}{4\pi}\int_0^\infty(\cosh\tfrac{1}{2}z)\log\left[1+\frac{\epsilon e^{-2mz}\tanh\frac{1}{2}z}{1-\epsilon\tanh\frac{1}{2}z}\right]dz\\ &\simeq\epsilon\frac{\hbar\omega_L}{4\pi}\int_0^\infty e^{-2mz}\sinh\tfrac{1}{2}z\,dz\quad\text{as}\quad m\to\infty\\ &=\epsilon\hbar\omega_L/32\pi m^2,\end{aligned} \tag{6.6a}$$

while as $m\to\infty$ in the free boundary case

$$\Delta E_{\mathrm{FB}}\sim-\epsilon\hbar\omega_L/32\pi m^2. \tag{6.6b}$$

Hence, in both the free boundary and rigid boundary cases, the interaction energy is inversely proportional to the square of the distance of the defect from the boundary. The interaction is one of attraction if

$$\begin{aligned}M<M'<\infty\quad&\text{for rigid boundary,}\\ 0<M'<M\quad&\text{for free boundary;}\end{aligned}$$

while it is repulsive if

$$\begin{aligned}0<M'<M\quad&\text{for rigid boundary,}\\ M<M'<\infty\quad&\text{for free boundary.}\end{aligned}$$

This is qualitatively expected. An interaction of an isotope with a rigid boundary is equivalent to that between the isotope and a particle of infinite mass. If both are heavier than a normal lattice atom, an attraction exists; when the isotopic defect is lighter, it interacts with the "infinite mass" boundary and a repulsion ensues. On the other hand, a free boundary is equivalent to a very light impurity at the end of the chain. Our above results are consistent with Eq. (5.16).

These qualitative results are valid in three dimensions as well. Without any extra difficulty we can discuss the isotopic defect in an n-dimensional lattice. We postulate it to be m lattice spacings in the m_1 direction (x direction when $n=3$) from a rigid surface. It is easy to show from (3.18b) by choosing $m_1=m$, $m_2=m_3=\cdots=\frac{1}{2}(N+1)$ and letting $N\to\infty$, that the generalization of the rigid boundary equation (6.4) becomes (after replacing ω by $i\omega$)

$$\frac{D(m,i\omega)}{D(\infty,i\omega)}=1-\frac{\omega^2M\epsilon I(m,i\omega)}{1+M\epsilon\omega^2I(\infty,i\omega)}, \tag{6.7}$$

where

$$I(m,i\omega)=-\left(\frac{1}{2\pi}\right)^n\int_{-\pi}^{\pi}\cdots\int\frac{\exp i\mathbf{s}\cdot\boldsymbol{\varphi}d\varphi_1\cdots d\varphi_n}{M\omega^2+2\sum\gamma_k(1-\cos\varphi_k)},$$

$$S=\gamma_1^{-\frac{1}{2}}(2m,0,0\cdots,0).$$

When m is fairly large, (3.15) is applicable with ω replaced by $i\omega$. Then the analog of (6.5b) which is appropriate here yields

$$\begin{aligned}\Delta E_{\mathrm{RB}}&\simeq-\frac{\hbar}{2\pi}\int_0^\infty\omega d\\ &\times\log\left\{1+\frac{\epsilon(M\omega^2)^{\frac{1}{2}(n+1)}(\frac{1}{2}\pi)^{\frac{1}{2}}\exp[-S(M\omega^2)^{\frac{1}{2}}]}{(2\pi)^{\frac{1}{2}n}(\gamma_1\cdots\gamma_n)^{\frac{1}{2}}S^{\frac{1}{2}(n-1)}}\right\}\\ &\sim\frac{\hbar\omega_L\epsilon(\frac{1}{2}\pi)^{\frac{1}{2}}[\frac{1}{2}(n+1)]!}{(\gamma_1\cdots\gamma_n)^{\frac{1}{2}}S^{n+1}(2\pi)^{\frac{1}{2}(n+2)}(M\omega_L^2)^{\frac{1}{2}}},\end{aligned} \tag{6.8}$$

with $S=2m/\gamma_1^{\frac{1}{2}}$. It is easily verified that the case $n=1$ is exactly the same as (6.6a).

The isotopic defect in a three-dimensional lattice is repelled from a rigid boundary when $\epsilon>0$ (light isotopic defect) and

$$\Delta E_{\mathrm{RB}}\sim\frac{\hbar\omega_L\epsilon(\gamma_1/m\omega_L^2)^{\frac{1}{2}}}{(\gamma_2\gamma_3/\gamma_1^2)^{\frac{1}{2}}(2\pi)^2(2m)^4}. \tag{6.9}$$

A free boundary attracts a light isotopic defect with a force of the same magnitude but opposite in sign.

We therefore find that not only should an ordering process exist at absolute zero[1,4] temperature but that a coating or "frosting" of light isotope should develop in a solid isotopic mixture, leaving the heavier atomic species inside. It would be interesting to leave a hydrogen-deuterium mixture in a liquid helium bath at low temperatures for a long period to observe whether the separation process would require days or years. Note that the energy of the boundary attraction diminishes as the inverse fourth power of the distance while the interatomic attraction energy [Eq. (5.17)] varies as the inverse seventh power.

If the state of perfect order is to exist at low temperatures, we should expect holes in a lattice to be attracted to a free boundary and hence expelled from a crystal. A repulsion from a rigid boundary should also exist. We consider these effects by using the source defect model. This defect was shown in the last section

to be equivalent to a hole when one deals with the interaction of a pair of holes separated by a distance large compared to a lattice spacing. We can also expect the model to apply to the interaction of a hole with a distant boundary. We restrict our discussion to the case $\gamma_1=\gamma_2=\cdots=\gamma$ and first analyze the effect of a rigid boundary.

We recall from (4.13) that a source defect is characterized by $\delta=\kappa\gamma$ and an isotopic defect by $\delta=-\omega^2M\epsilon$. If $\omega\to i\omega$, this becomes $\omega^2M\epsilon$ so that the expression equivalent to (6.7) for a source defect is

$$\frac{D(m,i\omega)}{D(\infty,i\omega)}=1-\frac{\kappa\gamma I(m,i\omega)}{1+\kappa\gamma I(\infty,i\omega)}.$$

The analog of (6.8) is

$$\Delta E_{\mathrm{RB}}\simeq-\frac{\hbar}{2\pi}\int_0^\infty \omega d$$

$$\times\log\left\{1+\frac{\kappa\gamma(M\omega^2)^{\frac{1}{2}(n-3)}(\tfrac{1}{2}\pi)^{\frac{1}{2}}\exp[-S(M\omega^2)^{\frac{1}{2}}]}{(2\pi\gamma)^{\frac{1}{2}n}S^{\frac{1}{2}(n-1)}}\right\}$$

$$\sim\frac{\hbar}{2\pi}\frac{\kappa\gamma(\frac{1}{2}\pi)^{\frac{1}{2}}}{(2\pi\gamma)^{\frac{1}{2}n}S^{\frac{1}{2}(n-1)}}\int_0^\infty(M\omega^2)^{\frac{1}{2}(n-3)}\exp[-(M\omega^2)^{\frac{1}{2}}S]d\omega$$

$$=\frac{\hbar\kappa\gamma(\pi/2M)^{\frac{1}{2}}[\frac{1}{2}(n-3)]!}{2\pi(2\pi\gamma)^{\frac{1}{2}n}S^{n-1}},\quad(6.10)$$

with $S=2m\gamma^{-\frac{1}{2}}$ and $M\omega_L{}^2=4n\gamma$. The sign is changed when the interaction is with a free boundary. In the three-dimensional case,

$$\Delta E=\begin{cases}+3^{-\frac{1}{2}}\hbar\omega_L\kappa/(8\pi m)^2, & \text{rigid boundary}\\ -3^{-\frac{1}{2}}\hbar\omega_L\kappa/(8\pi m)^2, & \text{free boundary.}\end{cases}\quad(6.11)$$

The hole corresponds to $\kappa\gamma=6(\gamma'-\gamma)^2/\gamma'$ and is attracted to a free boundary as was expected.

7. REMARKS ON THE CONTINUUM LIMIT AND ANALOGIES WITH QUANTUM FIELD THEORY

We shall now observe some consequences of letting our lattice spacings vanish and show the similarity of the continuum limit of a lattice with holes to Wentzel's[5] pair theory of the interaction of neutrons and protons.

One generally starts an analysis of a quantum field with the introduction of the proper Hamiltonian. Let us consider the Hamiltonian of a continuous medium of density ρ with propagation velocity c and a set of fixed point source defects of strength $\lambda_1,\lambda_2,\cdots$ at $r_1,r_2,\cdots$.

$$H=\frac{1}{2}\rho\int\dot\varphi^2d\tau+\frac{1}{2}\rho c^2\int(\nabla\varphi)^2d\tau+\frac{1}{2}\frac{m^2e^4}{\hbar^2}\rho\int\varphi^2d\tau$$

$$+\frac{1}{2}c^2\sum_{\alpha=1}^{n}\lambda_\alpha\int\delta(r-r_\alpha)\varphi^2(r)d\tau.\quad(7.1)$$

Here a mass m is associated with quanta propagated from one source to another. The λ_α's (which have units of length) represent the coupling strengths of the defects with the medium in which they are immersed. The δ function is defined by the property

$$\int\delta(r)f(r)d\tau=\rho f(0).$$

If we divide our continuum into a simple cubic lattice with unit cell cube edges a, introduce a mass M with a single degree of freedom into the center of each cell, couple it to its nearest neighbors by a spring of spring constant γ, associate each coupling constant γ_α to a dimensionless constant κ_α, and finally relate γ, M, and κ_α to the constants of the medium and sources ρ, c, and λ_α by

$$\rho=M/a^3,\quad c^2=\gamma a^2/M,\quad\text{and}\quad\lambda_\alpha=\kappa_\alpha a,\quad(7.2)$$

we obtain

$$H=\tfrac{1}{2}M\sum\dot\varphi^2(l,m,n)$$

$$+\tfrac{1}{2}\gamma a^2\sum\{[\varphi(l+1,m,n)-\varphi(l,m,n)]^2/a^2+\cdots\}$$

$$+\frac{1}{2}\frac{m^2c^4}{\hbar^2}M\sum\varphi^2(l,m,n)+\frac{\gamma}{2}\sum_\alpha\kappa_\alpha u^2(l_\alpha,m_\alpha,n_\alpha),\quad(7.3)$$

where all summations except the last extend over all lattice points. Once the conjugate momentum

$$p(l,m,n)=M\dot\varphi(l,m,n)$$

is associated with $\varphi(l,m,n)$, the application of Hamilton's equations of motion yield

$$M\ddot\varphi(l,m,n)+\frac{m^2c^4}{\hbar^2}M\varphi(l,m,n)$$

$$=-\gamma\sum_{\substack{\epsilon_1,\epsilon_2,\epsilon_3=0,1\\ \epsilon_1+\epsilon_2+\epsilon_3=1}}[\varphi(l+\epsilon_1,m+\epsilon_2,n+\epsilon_3)$$

$$-2\varphi(l,m,n)+\varphi(l-\epsilon_1,m-\epsilon_2,n-\epsilon_3)]\quad(7.4)$$

except at $(l,m,n)=(l_\alpha,m_\alpha,n_\alpha)$ in which case the terms $\gamma\kappa_\alpha\varphi(l_\alpha,m_\alpha,n_\alpha)$ are added to right-hand side.

If we let

$$\varphi(l,m,n)=u(l,m,n)e^{i\omega t}\quad(7.5)$$

and define ω^* by

$$(\omega^*)^2=\omega^2-m^2c^4\hbar^{-2},\quad(7.6)$$

the resulting equations are the same as (3.2a) when ω in (3.2) is replaced by ω^*, that is, if the lattice phonons are given a mass m.

It was shown at the end of Sec. 5 that the source defect is equivalent to a hole in the lattice if one considers the interaction of defects separated by a large number of lattice spacings. As the lattice spacing diminishes, this number increases for holes a fixed

distance apart. Hence the Hamiltonian (7.1) can be interpreted either as that of the continuum limit of a set of holes in a simple cubic lattice (with nearest-neighbor interactions due to central and noncentral forces of equal magnitude) or of a set of particles interacting through a meson pair field.

When the mass m is included, our inverse

$$a^{(-1)}(r_1,r_2,r_3;i\omega)$$

given by (3.17a) must have ω replaced by ω^*. Then

$$a^{(-1)}(r_1,r_2,r_3;i\omega)=a^{(-1)}(R;i\omega)$$
$$=-\frac{a}{\gamma R(2\pi)^3}\left(\frac{\pi}{2}\right)^{\frac{1}{2}}\exp\{-a^{-1}R[(\omega^2+\mu^2c^2)M/\gamma]^{\frac{1}{2}}\},\quad(7.7)$$

where

$$R^2=r_1^2+r_2^2+r_3^2\quad\text{and}\quad\mu=mc/\hbar.\qquad(7.8)$$

The interaction energy between two defects κ and κ' at two points separated by a distance $R=a|m-m'|$ is given by substituting (7.7) into (5.3c). This reduces the calculation of the interaction energy to quadratures *for all degrees of coupling*. In the weak coupling limit we can rederive Wentzel's result as follows:

$$\Delta E_I\sim-\frac{\hbar\kappa\kappa'}{(2\pi)^4}\frac{a^2}{R^2}\left(\frac{\pi}{2}\right)\int_0^\infty$$
$$\times\exp\{-2a^{-1}R[(\omega^2+\mu^2c^2)M/\gamma]^{\frac{1}{2}}\}d\omega.\quad(7.9)$$

This integral can be expressed in terms of the modified Bessel function of the third kind, K_1. If we let

$$\omega=\mu c\sinh x$$

and use the formula

$$K_1(z)=\int_0^\infty\exp(-z\cosh x)\cosh x\,dx,$$

we find

$$\Delta E_I\sim-\frac{\hbar\kappa\kappa'a^2\mu c}{4(2\pi)^3R^2}K_1(2Ra^{-1}\mu c[M/\gamma]^{\frac{1}{2}}),$$

or after employing (7.8) and (7.2) we find

$$\Delta E_I\sim-\frac{\lambda\lambda'mc^2}{32\pi^3R^2}K_1(2R\mu).\qquad(7.10)$$

This is exactly Wentzel's[5] result (with the exception of a factor of $\frac{1}{2}$ which was left out of his paper since he set $E=\sum\hbar\omega$ rather than $\sum\frac{1}{2}\hbar\omega$). The two limiting results follow:

$$\Delta E_I\sim-\frac{\lambda\lambda'\hbar c}{64\pi^3R^3}\quad\text{if}\quad R\ll\mu^{-1},\qquad(7.11)$$

$$\Delta E_I\sim-\frac{\lambda\lambda'\hbar c}{64\pi^{5/2}}\left(\frac{\mu}{R}\right)^{\frac{1}{2}}\frac{e^{-2\mu R}}{R^2}\quad\text{if}\quad R\gg\mu^{-1}.\qquad(7.12)$$

These finite convergent results are unique to a three-dimensional space. If we employ our n-dimensional inverse [Eq. (5.4)], we can show that in the n-dimensional case the weak-coupling approximation yields

$$\Delta E_I=-\frac{\hbar\lambda\lambda'a^{2n-6}}{(2\pi)^{n+1}R^{n-2}}\int_0^\infty[c^{-2}(\omega^2+\mu^2c^2)]^{\frac{1}{2}(n-2)}$$
$$\times K_{\frac{1}{2}(n-2)^2}[Rc^{-1}(\omega^2+\mu^2c^2)^{\frac{1}{2}}]d\omega,$$

so that the lattice spacing a occurs only as a coefficient a^{2n-6} while all other parameters in the equation represent macroscopic properties of the medium or defect. When $n<3$, the continuum limit $a\to0$ gives an infinite interaction energy at all separation distances between sources. On the other hand, when $n>3$ the interaction vanishes identically in the limit. Hence, if one were to take pair theory of nucleon forces seriously, one would have to conclude that only a three-dimensional universe could contain condensations of nucleons as we know them in atomic nuclei.

The continuum theory of the interaction of point defects in solids has been discussed by Eshelby.[10]

APPENDIX I. THE MATRICES A AND B OF EQ. (5.33)

$$A=\begin{bmatrix}
1+\delta_1(0,0,0) & \delta_1(2,0,0) & \delta_1(1,1,0) & \delta_1(1,1,0) & \delta_1(1,0,1) & \delta_1(1,0,1) & (\delta_1\delta_2)^{\frac{1}{2}}(1,0,0)\\
\delta_1(2,0,0) & 1+\delta_1(0,0,0) & \delta_1(1,1,0) & \delta_1(1,1,0) & \delta_1(1,0,1) & \delta_1(1,0,1) & (\delta_1\delta_2)^{\frac{1}{2}}(1,0,0)\\
\delta_1(1,1,0) & \delta_1(1,1,0) & 1+\delta_1(0,0,0) & \delta_1(0,2,0) & \delta_1(0,1,1) & \delta_1(1,0,1) & (\delta_1\delta_2)^{\frac{1}{2}}(0,1,0)\\
\delta_1(1,1,0) & \delta_1(1,1,0) & \delta_1(0,2,0) & 1+\delta_1(0,0,0) & \delta_1(0,1,1) & \delta_1(0,1,1) & (\delta_1\delta_2)^{\frac{1}{2}}(0,1,0)\\
\delta_1(1,0,1) & \delta_1(1,0,1) & \delta_1(0,1,1) & \delta_1(0,1,1) & 1+\delta_1(0,0,2) & \delta_1(0,0,2) & (\delta_1\delta_2)^{\frac{1}{2}}(0,0,1)\\
\delta_1(1,0,1) & \delta_1(1,0,1) & \delta_1(0,1,1) & \delta_1(0,1,1) & \delta_1(0,0,2) & 1+\delta_1(0,0,0) & (\delta_1\delta_2)^{\frac{1}{2}}(0,0,1)\\
(\delta_1\delta_2)^{\frac{1}{2}}(1,0,0) & (\delta_1\delta_2)^{\frac{1}{2}}(1,0,0) & (\delta_1\delta_2)^{\frac{1}{2}}(0,1,0) & (\delta_1\delta_2)^{\frac{1}{2}}(0,1,0) & (\delta_1\delta_2)^{\frac{1}{2}}(0,0,1) & (\delta_1\delta_2)^{\frac{1}{2}}(0,0,1) & 1+\delta_2(0,0,0)
\end{bmatrix}.$$

$$B=\begin{bmatrix}
\delta_1(l-2,m,n) & \delta_1(l,m,n) & \delta_1(l-1,m-1,n) & \delta_1(l-1,m+1,n) & \delta_1(l-1,m,n-1) & \delta_1(l-1,m,n+1) & (\delta_1\delta_2)^{\frac{1}{2}}(l-1,m,n)\\
\delta_1(l,m,n) & \delta_1(l+2,m,n) & \delta_1(l+1,m-1,n) & \delta_1(l+1,m+1,n) & \delta_1(l+1,m,n-1) & \delta_1(l+1,n,n+1) & (\delta_1\delta_2)^{\frac{1}{2}}(l+1,m,n)\\
\delta_1(l-1,m-1,n) & \delta_1(l+1,m-1,n) & \delta_1(l,m-2,n) & \delta_1(l,m,n) & \delta_1(l,m-1,n-1) & \delta_1(l,m-1,n+1) & (\delta_1\delta_2)^{\frac{1}{2}}(l,m-1,n)\\
\delta_1(l-1,m+1,n) & \delta_1(l+1,m+1,n) & \delta_1(l,m,n) & \delta_1(l,m+2,n) & \delta_1(l,m+1,n-1) & \delta_1(l,m+1,n+1) & (\delta_1\delta_2)^{\frac{1}{2}}(l,m+1,n)\\
\delta_1(l-1,m,n-1) & \delta_1(l+1,m,n-1) & \delta_1(l,m-1,n-1) & \delta_1(l,m+1,n-1) & \delta_1(l,m,n-2) & \delta_1(l,m,n) & (\delta_1\delta_2)^{\frac{1}{2}}(l,m,n-1)\\
\delta_1(l-1,m,n+1) & \delta_1(l+1,m,n+1) & \delta_1(l,m-1,n+1) & \delta_1(l,m+1,n+1) & \delta_1(l,m,n) & \delta_1(l,m,n+2) & (\delta_1\delta_2)^{\frac{1}{2}}(l,m,n+1)\\
(\delta_1\delta_2)^{\frac{1}{2}}(l-1,m,n) & (\delta_1\delta_2)^{\frac{1}{2}}(l+1,m,n) & (\delta_1\delta_2)^{\frac{1}{2}}(l,m-1,n) & (\delta_1\delta_2)^{\frac{1}{2}}(l,m+1,n) & (\delta_1\delta_2)^{\frac{1}{2}}(l,m,n-1) & (\delta_1\delta_2)^{\frac{1}{2}}(l,m,n+1) & \delta_2(l,m,n)
\end{bmatrix}.$$

$$(l,m,n)\equiv a^{(-1)}(0,0,0;l,m,n;i\omega).$$

[10] J. D. Eshelby, Acta Metallurgica **3**, 487 (1955).