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Self-Consistent Field Approximation for the Frequency Spectrum of a Disordered Chain*†

R. W. DAVIES AND J. S. LANGER
Carnegie Institute of Technology, Pittsburgh, Pennsylvania

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The frequency spectrum of a disordered one-dimensional chain is calculated using a self-consistent field approximation. By requiring that the phonon scattering amplitudes satisfy a certain requirement of analytic self-consistency, an implicit equation for the phonon self-energy function is obtained. This equation turns out to be exactly soluble, and leads to a spectral function which possesses no singularities and which exhibits a very flat, broad impurity band.

IN a previous publication one of the present authors (J.S.L.) discussed a multiple scattering technique for the calculation of the frequency spectrum of an isotopically disordered one-dimensional lattice.[1] It was shown that, for small impurity concentrations, the spectrum could be determined from the amplitudes for scattering of a phonon by a single impurity or small clusters of impurities. In the interesting case of light impurities, these scattering amplitudes contained poles associated with high-frequency localized modes, and these poles gave rise to new bands at the upper end of the frequency spectrum. Furthermore, these impurity bands turned out to be narrow and spikey, i.e., the spectral function contained a set of infinite discontinuities. However, certain mathematical features of the solution led the author to speculate that these singularities would not be present in a calculation in which the analytic properties of the scattering amplitudes were taken into account more nearly self-consistently. In this note we should like to describe a nontrivial self-consistent field approximation which satisfies these requirements of analyticity, which leads to exactly soluble equations for the one-dimensional model lattice, and which does, in fact, remove the unpleasant singularities from the frequency spectrum.

We begin with a brief review of the previous results. The spectral function is given by

$$g(\omega)=\lim_{N\to\infty}\frac{2\omega}{N}\sum_n\delta(\Omega_n{}^2-\omega^2)=\frac{2\omega}{\pi}\lim_{\substack{N\to\infty\\ \epsilon\to 0}}\frac{1}{N}\operatorname{Im}\operatorname{Tr}D(\omega^2+i\epsilon),\tag{1}$$

where the Ω_n are the normal mode frequencies of a chain of N atoms and D is the phonon Green's function. For any particular configuration of impurities, D may be written as a matrix in a wave number representation; i.e., in the representation whose basic states are the phonon eigenstates of the pure lattice. Upon averaging over all configurations of impurities we regain translational symmetry and D becomes diagonal. Thus, according to the analysis of I, we may write

$$\langle D_{k,k'}(\omega^2)\rangle_{\mathrm{av}}=D_k(\omega^2)\delta_{k,k'};$$

$$D_k(\omega^2)=\frac{1}{\omega_k{}^2-\omega^2+G_k(\omega^2)},\tag{2}$$

where the ω_k's are the eigenfrequencies of the unperturbed lattice and $G_k(\omega^2)$ is a self-energy function.

To lowest order in the concentration of impurities q, $G_k(\omega^2)$ turns out to be proportional to the forward scattering amplitude for a phonon incident on an isolated impurity. That is

$$G_k(\omega^2)=Nqt_{k,k}(\omega^2),\tag{3}$$

and $t_{k,k'}(\omega^2)$ satisfies the equation

$$t_{k,k'}(\omega^2)=\frac{\lambda\omega_{k'}{}^2}{N}-\frac{1}{N}\sum_{k''}\frac{\lambda\omega_{k''}{}^2}{\omega_{k''}{}^2-\omega^2}t_{k'',k'}(\omega^2).\tag{4}$$

Here $\lambda\equiv M/M'-1$, where M and M' are the masses of the host and impurity atoms, respectively. Notice that the quantity $\lambda\omega_k{}^2/N$ plays the role of the phonon-impurity interaction, and that the quantity $(\omega_k{}^2-\omega^2)^{-1}$ is the unperturbed propagator.

From very general principles, we know that the *exact* expressions for D and G have very similar analytic properties. In particular, both functions are analytic everywhere in the ω plane except along the real axis where there are branch cuts. These branch cuts occur wherever the spectral function $g(\omega)$ is nonzero. In the approximation described by Eqs. (2), (3), and (4), D and G both have branch cuts coinciding with the single acoustic band of the unperturbed lattice. If a local mode exists, however, $G_k(\omega^2)$ has a simple pole at the local mode frequency ω_0; $D_k(\omega^2)$ has a similar pole near ω_0, the exact position depending upon k; and $g(\omega)$ is nonzero in a narrow band in this region. In a more accurate approximation, we know that both D and G should have branch cuts coinciding with this impurity band.

We may automatically satisfy the requirement of

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[1] J. S. Langer, J. Math. Phys. 2, 584 (1961). Hereafter referred to as I.

analytic self-consistency by modifying Eq. (4) to read

$$t_{k,k'}(\omega^2)=\frac{\lambda\omega_{k'}^2}{N}-\frac{1}{N}\sum_{k''}\lambda\omega_{k''}^2D_{k''}(\omega^2)t_{k'',k'}(\omega^2). \tag{5}$$

According to Eq. (2), this means

$$t_{k,k'}(\omega^2)=\frac{\lambda\omega_{k'}^2}{N}-\frac{\lambda}{N}\sum_{k''}\frac{\omega_{k''}^2}{\omega_{k''}^2-\omega^2+G_{k''}(\omega^2)}t_{k'',k'}(\omega^2). \tag{6}$$

The kernel of this equation is separable; thus, it may be solved easily, with the result

$$t_{k,k'}(\omega^2)=\lambda N\omega_{k'}^2\bigg/\left(1+\frac{\lambda}{N}\sum_{k''}\frac{\omega_{k''}^2}{\omega_{k''}^2-\omega^2+G_{k''}(\omega^2)}\right). \tag{7}$$

Then, because $G_k(\omega^2)=Nqt_{k,k}(\omega^2)$, we find the following implicit equation for the self-energy function:

$$G_k(\omega^2)=q\lambda\omega_k^2\bigg/\left(1+\frac{\lambda}{N}\sum_{k''}\frac{\omega_{k''}^2}{\omega_{k''}^2-\omega^2+G_{k''}(\omega^2)}\right). \tag{8}$$

Equation (8) may be compared with the corresponding result obtained from Eq. (4), which is

$$G_k(\omega^2)=q\lambda\omega_k^2\bigg/\left(1+\frac{\lambda}{N}\sum_{k''}\frac{\omega_{k''}^2}{\omega_{k''}^2-\omega^2}\right). \tag{8$'$}$$

In diagrammatical language, we may say that, in Eq. (8), we have replaced the unperturbed Green's function by the exact one in each of the phonon lines of the diagrams which contributed to (8′). The solution of (8) is thus equivalent to the summation of a very large class of diagrams.

We may solve Eq. (8) quite easily because $G_k(\omega^2)$ depends on k only through the factor ω_k^2. Therefore, if we write

$$G_k(\omega^2)=\gamma(\omega^2)\omega_k^2, \tag{9}$$

then $\gamma(\omega^2)$ satisfies

$$\gamma(\omega^2)=q\lambda\bigg/\left(1+\frac{\lambda}{N}\sum_{k}\frac{\omega_k^2}{\omega_k^2(1+\gamma)-\omega^2}\right). \tag{10}$$

It is convenient to rewrite (10) in the form

$$\gamma(\omega^2)=q\lambda\bigg/\left(1+\frac{\lambda}{(1+\gamma)}+\frac{\lambda\omega^2}{(1+\gamma)}\frac{1}{N}\sum_{k=1}\frac{1}{\omega_k^2(1+\gamma)-\omega^2}\right). \tag{11}$$

In the limit $N\rightarrow\infty$, the sum in this expression becomes an integral and is readily evaluated (see I):

$$\lim_{\substack{N\rightarrow\infty\\ \epsilon\rightarrow 0}}\frac{1}{N}\sum_k\frac{1}{\omega_k^2(1+\gamma)-\omega^2-i\epsilon}=\frac{i}{\omega[\omega_m^2(1+\gamma)-\omega^2]^{1/2}}, \tag{12}$$

where ω_M is the maximum frequency of the unperturbed chain. Thus, γ is determined by the purely algebraic equation,

$$\gamma(\omega^2)=\frac{q\lambda(1+\gamma)}{1+\gamma+\lambda+i\omega\lambda/[\omega_m^2(1+\gamma)-\omega^2]^{1/2}}. \tag{13}$$

Finally, the averaged spectral function is given by

$$\bar{g}(\omega)=\lim_{\substack{N\rightarrow\infty\\ \epsilon\rightarrow 0}}\frac{2\omega}{\pi}\operatorname{Im}\frac{1}{N}\sum_k\frac{1}{\omega_k^2-\omega^2+G_k(\omega^2)}. \tag{14}$$

According to (9) and (12), (14) becomes

$$\bar{g}(\omega)=\frac{2}{\pi}\operatorname{Re}\frac{1}{[\omega_m^2(1+\gamma)-\omega^2]^{1/2}}, \tag{15}$$

where $\gamma(\omega^2)$ is the solution of (13).

The general features of the spectral function $\bar{g}(\omega)$ now may be deduced from an examination of the roots of the algebraic equation (13). First, we make the following transformation of variables:

$$\eta(x)=\frac{i}{[1+\gamma-x^2]^{1/2}},\quad x\equiv\frac{\omega}{\omega_m}. \tag{16}$$

Then

$$\omega_m\bar{g}(x)=\frac{2}{\pi}\operatorname{Im}\eta(x) \tag{17}$$

and

$$\gamma(x)=x^2-1-\frac{1}{\eta^2}=\frac{q\lambda(x-1/\eta)}{x-1/\eta+\lambda\eta}. \tag{18}$$

Equation (18) has been derived from (13) by making the substitution (16) and factoring out $(x+1/\eta)$ in the numerator and denominator of the right-hand side. We are left with a quartic equation with real coefficients.

In the case of vanishingly small q, we know that (18) must have a solution which approaches the spectral function for the unperturbed lattice, i.e.,

$$\omega_m\bar{g}_0(x)=\frac{2}{\pi}\frac{1}{[1-x^2]^{1/2}},\quad x<1$$
$$=0,\qquad x>1. \tag{19}$$

Accordingly, we regroup the terms in (18) as follows:

$$f(\eta)=[(1-x^2)\eta^2+1][\lambda\eta^2+x\eta-1]+q\lambda\eta^2(x\eta-1)=0. \tag{20}$$

At $q=0$, $f(\eta)$ always has two real roots at

$$\lambda\eta^2+x\eta-1=0. \tag{21}$$

For $x<1$, the other two roots are pure imaginary; for $x>1$ they are real, and Eq. (19) follows immediately. The function $f(\eta)$ relevant to this unperturbed situation is drawn in Fig. 1. Next consider small but finite values

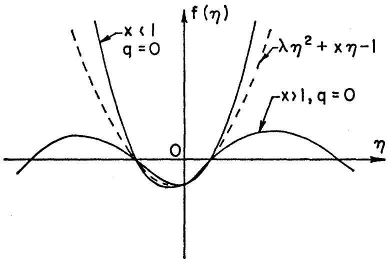

FIG. 1. Behavior of quartic equation for $q=0$.

of q. As long as we are far from the band edge, i.e., x is less than and not too close to unity, the picture drawn in Fig. 1 remains qualitatively correct and $\bar{g}(x)$ will not be much different from $\bar{g}_0(x)$. For sufficiently small values of $1-x^2$, however, there will be some region along the negative η axis where the cubic term in (20) will be stronger than the quartic term. The resulting curve will look something like Fig. 2. Notice that we have drawn four real roots of $f(\eta)$ for $x<1$. In other words, for sufficiently small q, $\bar{g}(x)$ may go to zero below the edge of the unperturbed acoustic band. The new band edge will occur at that value of x where the roots A and B merge in Fig. 2.

If q is small (and λ is not too small), both roots A and B will occur at large negative values of η, whereas C and D will remain relatively close to $\eta=0$. In this case we may investigate the behavior of $\bar{g}(x)$ near the new band edge by assuming that the roots C and D are still given accurately by (21) and factoring them out of (20). The resulting quadratic equation

$$2y\eta^2+q\eta+1-q\left(1+\frac{1}{\lambda}\right)\cong 0,\quad y\equiv 1-x \qquad (22)$$

has the roots

$$\eta_{A,B}\cong -\frac{q}{4y}\pm\frac{1}{4y}\left[q^2-8y\left(1-q-\frac{q}{\lambda}\right)\right]^{1/2}. \qquad (23)$$

Thus, the new band edge ($\eta_A=\eta_B$) occurs at

$$y_{\min}\cong\frac{q^2}{8(1-q-q/\lambda)} \qquad (24)$$

and for $y>y_{\min}$ we have

$$\omega_m\bar{g}(y)\cong\frac{1}{2\pi y}[8y(1-q-q/\lambda)-q^2]^{1/2}. \qquad (25)$$

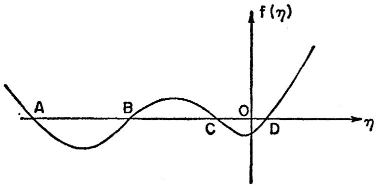

FIG. 2. Behavior of quartic near unperturbed band edge for small but finite concentration of impurities.

It is apparent that the self-consistent spectral function peaks and then goes to zero with infinite slope instead of becoming singular at the top of the band. Detailed numerical calculations confirm that, for small q, Eq. (25) is a very accurate representation of $\bar{g}$ near the band edge (see Fig. 4).

As was pointed out in I, the band gap must disappear for large enough values of the concentration q. We now may see in some detail how this happens. Consider values of x so close to unity (the unperturbed band edge) that root A in Fig. 2 is very far out along the negative η axis. Then $f(\eta)$ will be well approximated by a cubic expression obtained by setting $x=1$ in (20). As we have seen, this cubic will have three real roots B, C, and D for small q. As q increases, however, roots B and C merge and then become complex. In the case of a three-to-one mass ratio ($\lambda=2$), for example, the critical value of q is about 0.22. For concentrations greater than the critical q, $\bar{g}(x)$ will be nonzero throughout the region near $x=1$.

The complete spectral function for the case $M/M'=3$, $q=\frac{1}{10}$ is shown in Fig. 3. We have obtained this curve by direct numerical solution of Eqs. (17) and (18). That is, we have found two real roots of (18) numerically, factored these out, and then solved the remaining quadratic equation.[2]

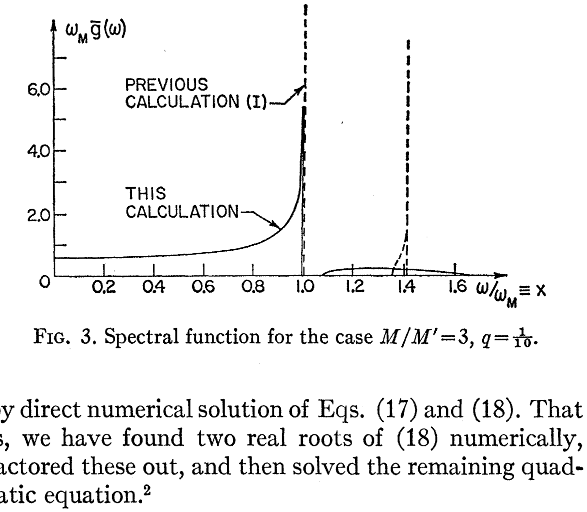

FIG. 3. Spectral function for the case $M/M'=3$, $q=\frac{1}{10}$.

In Fig. 3, we have plotted for comparison the spectrum computed in I for the same choice of parameters q and λ. As discussed above, the low-frequency acoustic bands are identical except in the very immediate neighborhood of the band edge. The function near the band edge is shown in more detail in Fig. 4. In our new approximation, however, the impurity band has become quite broad and flat. It seems likely that the broad band is an accurate representation of the average energy distribution of the impurity modes. On the other hand, having omitted all higher order effects associated

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[2] For the parameters chosen it turns out that $f(\eta)$ always does have two real roots and that the complex roots do, in fact, occur on what we might call the "physical sheet" of the function $\eta(x)$. That this is not always true may be seen by examining $f(\eta)$ for any negative value of λ, in which case $\eta(x)$ has an unphysical branch cut which must not be included in the spectral function $\bar{g}$.

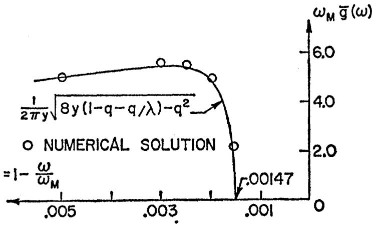

FIG. 4. Spectral function near the band edge for the case $M/M'=3$, $q=\frac{1}{10}$.

with clusters of impurities, we cannot hope to duplicate the detailed structure which we expect to exist at the high-frequency end of the spectrum.[3] In other words, the present calculation probably gives a $\bar{g}(x)$ which is suitable for calculation of the specific heat but which is not adequate for, say, transport calculations where the detailed dynamics of the system may be more important.

Apropos of the broad impurity band, we should mention that Flinn, Maradudin, and Weiss[4] have found a spectrum in remarkably good agreement with Fig. 3 using a completely different method. Also, it appears to be characteristic of the self-consistent field approximation to broaden the spectrum of allowed eigenvalues from that obtained using (4) or its analog. Klauder[5] has found this to be the case in his study of electron spectra in disordered metals.

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[3] P. Dean, Proc. Roy. Soc. (London) **260**, 263 (1961).

[4] P. A. Flinn, A. A. Maradudin, and G. H. Weiss, Westinghouse Research Report (unpublished).

[5] J. R. Klauder, Ann. Phys. (N.Y.) **14**, 43 (1961).

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Field Emission in a Magnetic Field*

F. J. BLATT

Physics Department, Michigan State University, East Lansing, Michigan

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An expression for the field-emission current in a longitudinal magnetic field is derived in the zero-temperature limit. Two cases are considered, corresponding to constant Fermi energy (A) and constant electron density (B). In both cases the calculated current density contains an oscillatory contribution periodic in $1/H$, as well as a term which decreases as the square of the magnetic field. In case B, however, an oscillatory contribution appears that is absent in case A. Since the two oscillatory terms in case B differ in phase and their amplitudes depend on different powers of H, it should be possible to distinguish between cases A and B. The current-decrease quadratic in H has its origin in the steady diamagnetism of the electron gas. Using accepted values of effective mass, Fermi energy, and work function, we find that for bismuth the predicted variations of the emission current with magnetic field should be readily observable.

INTRODUCTION

THE effects of a strong magnetic field upon the physical properties of metals, semimetals, and semiconductors have received considerable attention in recent years.[1] Much of the impetus derived from the lucid exposition of Lifshitz and co-workers[2] who demonstrated the far-reaching inferences that could be drawn from measurements of magnetoresistance and Hall effect on pure single crystals at low temperatures. At the same time, Harrison's work[3] provided a simple link between de Haas–van Alphen data and what had appeared to be very complicated band structures of most polyvalent metals. Finally, improved techniques of crystal purification and growth, the attainment of magnetic fields of better than 10^5 G by pulse techniques, and the development of improved experimental techniques account for the rapid accretion in recent years of de Haas–van Alphen, Shubnikov–de Haas, cyclotron resonance, and related data on a host of conductors.[4]

Application of a magnetic field to a free-electron gas gives rise to highly degenerate energy levels separated by $\hbar\omega=\beta^*H=e\hbar H/m^*c$ as well as to regular singularities in the density-of-states function, thereby exerting a profound influence on any physical property either directly or indirectly related to the electronic system. Variations of the magnetic susceptibility, of the specific heat, and of the transport properties periodic in H^{-1} are the direct effects most frequently investigated. The only indirect effect that has been studied is the influence of a magnetic field on the velocity of sound.[5]

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[1] *High Magnetic Fields* (John Wiley & Sons, Inc., New York, and Tech Press, Cambridge, Massachusetts, 1962), cf. particularly Part III.

[2] I. M. Lifshitz and V. G. Peschanskii, Zh. Eksperim. i Teor. Fiz. **35**, 1251 (1958); **38**, 180 (1960) [translations: Soviet Phys.—JETP **8**, 875 (1959); **11**, 131 (1960)]. N. E. Alekseevskii, Yu. P. Gaidukov, I. M. Lifshitz, and V. G. Peschanskii, *ibid.* **39**, 1201 (1960) [translation: *ibid.* **12**, 837 (1961)].

[3] W. A. Harrison, Phys. Rev. **126**, 497 (1962); **118**, 1190 (1960); **116**, 555 (1959).

[4] *The Fermi Surface*, edited by W. A. Harrison and M. B. Webb (John Wiley & Sons, Inc., New York, 1960).

[5] M. J. Harrison, Phys. Rev. Letters **9**, 299 (1962); J. J. Quinn and S. Rodriguez, *ibid.* **9**, 145 (1962).