Coupled Electron-Phonon System*

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The coupled electron-phonon system is considered for phonon spectra of Einstein and Debye forms. The single-particle electron Green's function G is calculated in a nonperturbative manner in both models, and its spectral weight function is examined to determine the validity of a quasiparticle picture. The weight function and the poles of G both lead to several branches of excitations rather than a single "dressed" electron. The asymptotic time dependence of the G is found, and the effect of multiphonon processes on the electron decay rate is discussed. The electronic polarizability, P of the interacting system is calculated with the aid of a generalized Ward's identity for the electron-phonon vertex. This identity, which is a consequence of electronic charge conservation, is derived in an Appendix. The calculation of P is carried out in the limit that the Fermi velocity is small compared with the phase velocity of the polarization field. An Appendix on the formal development of the Green's function equations is included.

INTRODUCTION

We investigate the coupled electron-phonon system using a field-theoretic scheme[1,2] that goes beyond lowest order processes. Two model phonon spectra of the coupled system are studied; these are the Einstein and Debye models.[3] We view these models as two limiting cases, neither of which is realized in practice. The Einstein model is a reasonable approximation for short-wavelength phonons while the Debye model is preferable for processes emphasizing long-wavelength phonons.

We begin with the Einstein model in Sec. I. By approximating the electron-phonon vertex function Γ by unity and the free electron density of states in energy by a constant, the integral equation for the electronic self-energy Σ can be trivially solved. This approximation of Γ for the Debye model has been discussed by Migdal[4] who argues that the error thereby introduced is of the order of the square root of the electron to ion mass ratio $(m/M)^{1/2}$ for normal metals and is therefore negligible. His argument also applies to short-wavelength modes in the Einstein model but fails when the phonon's phase velocity is of the order or greater than the Fermi velocity.

The poles of the electron Green's function are given in several figures. Several branches of excitations appear. The quasiparticle picture is examined for this model and found to be inappropriate except very near to or far from the Fermi surface. In Sec. II, the result for $G(\mathbf{p},p_0)$ is used to calculate the asymptotic behavior of $G(\mathbf{p},t)$ as $t\to\infty$.

In Sec. I, it is found that the electronic decay rate shows no anomalies near the thresholds for multiple-phonon emission. The constant density of states approximation is relaxed in Sec. III, and such anomalies appear. However, their relative magnitude is again of order $(m/M)^{1/2}$ and they are not to be trusted if vertex corrections are neglected.

The electronic polarizability $P(\mathbf{q},q_0)$ is discussed in Sec. IV with the aid of a generalized Ward's identity for the electron-phonon vertex which follows from charge conservation. This identity is derived in Appendix B. With the approximation of Sec. I for Σ, the Ward identity is satisfied by the ladder approximation for the vertex function which enters the expression for P. The polarizability is calculated to order $(\mathbf{q}v_F/q_0)^2$, where v_F is the Fermi velocity. This calculation allows one to investigate the long-wavelength phonon spectrum.

The Debye model is considered in Sec. V. Within the same approximations used for the Einstein model, the spectral function and poles of the electron Green's function are derived and plotted for the Debye case. Several branches are again found in the single-particle spectrum.

The definition of the Green's functions and the formal development of the equations determining these functions are given in Appendix A.

I. ELECTRON SPECTRUM IN THE EINSTEIN MODEL

The model we first consider is one in which the lattice is composed of independent oscillators, each having a single characteristic frequency. Thus, a phonon can carry only a fixed energy, ω, independent of its momentum. Since the phonon damping is expected

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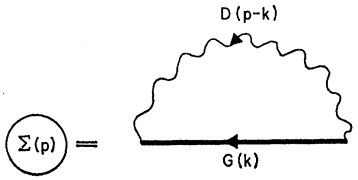

FIG. 1. Diagram corresponding to the approximation for the self-energy.

to be small, our initial choice is that of undamped oscillators.

We start with the approximation to the self-energy (A19), illustrated in Fig. 1, which neglects vertex corrections

$$\Sigma(p)=ig^2\int\frac{d^4k}{(2\pi)^4}D(p-k)G(k)$$
$$=ig^2\int\frac{d^4k}{(2\pi)^4}\frac{1}{[(p_0-k_0)^2-\omega^2+i\delta]}\times\frac{1}{[k_0-\epsilon(\mathbf{k})-\Sigma(k)]},\quad\delta\to0^+\quad(1.1)$$

where

$$\epsilon(\mathbf{k})=k^2/2m-\mu\,.$$

Here μ is the chemical potential and g, the coupling constant, is chosen to be independent of wave vector. The propagator for the electron field is written in its most general form, (A9). The phonon propagator has the characteristics mentioned above and includes an infinitesimal imaginary part to insure temporal outgoing wave boundary conditions which is required by the definition given in (A4).

We see that for this model $\Sigma(p)$ is independent of $\mathbf{p}$; we therefore define

$$k_0-\Sigma(k_0)=k_0Z(k_0)\,.\quad(1.2)$$

To perform the d^3k integration, we approximate the free-electron density of states $N(\epsilon)=mk/2\pi^2$ by its value at the Fermi surface $mk_F/2\pi^2$. Furthermore, we maintain particle-hole symmetry by carrying out the ϵ integration symmetrically about the Fermi surface, $\epsilon=0$, and for convenience extend the limits of integration to infinity.

The justification for these approximations is that the major contribution to the self-energy integral comes from electron states with energies $\epsilon<\omega$, the Einstein energy, which is typically one hundredth of the Fermi energy.[3] Thus, we expect the characteristic features of our results to be insensitive to the changes of the integration region far from the Fermi surface. Within this approximation the electron self-energy may be written as

$$\Sigma(p_0)=ig^2N\int_{-\infty}^{\infty}\frac{dk_0}{2\pi}\times\int_{-\infty}^{\infty}d\epsilon\frac{1}{(p_0-k_0)^2-\omega^2+i\delta}\frac{k_0Z(k_0)}{(k_0Z)^2-\epsilon^2}.\quad(1.3)$$

$\Sigma(p_0)$ may now be completely determined if we use the relation

$$\mathrm{Im}k_0Z(k_0)>0\quad\text{for}\quad k_0>0$$
$$<0\quad\text{for}\quad k_0<0$$

which follows from the Fourier transform of the definition (A4). Closing the ϵ contour in the upper half-plane we obtain the expression

$$\Sigma(p_0)=\frac{g^2N}{2}\left\{\int_{\infty}^{0}dk_0-\int_{0}^{\infty}dk_0\right\}\frac{1}{(p_0-k_0)^2-\omega^2+i\delta},\quad(1.4)$$

valid for p_0 on the real axis.

It is interesting to investigate whether a simple quasiparticle picture of our model leads to a reasonable approximation for $G(p)$. A quasiparticle picture assumes that the weight function $A(\epsilon_p,p_0)\equiv(1/\pi)|\mathrm{Im}G(\mathbf{p},p_0)|$, which appears in the spectral representation

$$G(\mathbf{p},p_0)=\int_0^{\infty}dp_0'\frac{A(\epsilon_p,p_0')}{p_0-p_0'+i\delta}+\int_{-\infty}^{0}dp_0\frac{A(\epsilon_p,p_0')}{p_0-p_0'-i\delta},\quad(1.5)$$

can be well represented by a single Lorentzian function

$$A(\epsilon_p,p_0')=\frac{\alpha_p|\Gamma_p|/\pi}{(p_0'-E_p)^2+\Gamma_p{}^2}.$$

The quantities E_p and $2|\Gamma_p|$ are interpreted as the energy and decay rate of the quasiparticle. Were this picture exact, the quasiparticle peak would exhaust the sum rule

$$\int_{-\infty}^{\infty}A(\epsilon_p,p_0')dp_0'=1\,,\quad(1.6)$$

and the parameter α_p would be unity. In general, the weight function is given by

$$A(\epsilon_p,p_0)=\frac{1}{\pi}\frac{|\Sigma_I(p)|}{[p_0-\epsilon_p-\Sigma_R(p)]^2+\Sigma_I{}^2(p)},\quad(1.7)$$

where Σ_R and Σ_I are the real and imaginary parts of Σ, respectively. It follows from (1.4) that for real p_0

$$\Sigma_I(p_0)=-\frac{g^2N\pi}{4\omega}\int_0^{\infty}dk_0\{\delta(p_0-k_0-\omega)+\delta(p_0-k_0+\omega)-\delta(p_0-k_0-\omega)-\delta(-p_0-k_0-\omega)\}$$
$$=-\frac{g^2N\pi}{2\omega}\,\mathrm{sgn}p_0\quad\text{for}\quad|p_0|>\omega$$
$$=0\quad\text{for}\quad|p_0|<\omega\,.\quad(1.8)$$

Thus, within our approximation Σ_I is a constant for energies above the threshold for phonon emission. Were we to include damping of the phonons, due to their interaction with electrons, Σ_I would be nonzero for $|p_0|<\omega$. However, its value in this region is very small compared to the value of Σ_I above the phonon

emission thresnold. The real part of Σ for real p_0 is

$$\Sigma_R(p_0)=-\frac{g^2N}{2\omega}\ln\left|\frac{p_0+\omega}{p_0-\omega}\right|. \tag{1.9}$$

Due to the assumed particle-hole symmetry we find $\Sigma_R(0)=0$, so that the chemical potential is unaffected by the interactions. On combining (1.7), (1.8), and (1.9), one finds the weight function is

$$\begin{aligned}\frac{1}{\pi}|\mathrm{Im}G(\mathbf{p},p_0)| &= \delta(p_0-\epsilon_\mathbf{p}+(g^2N/2\omega)\ln|(p_0+\omega)/(p_0-\omega)|) \quad \text{for} \quad |p_0|<\omega \\ &= \frac{g^2N/2\omega}{[p_0-\epsilon_\mathbf{p}+(g^2N/2\omega)\ln|(p_0+\omega)/(p_0-\omega)|]^2+|\pi g^2N/2\omega|^2} \quad \text{for} \quad |p_0|>\omega.\end{aligned} \tag{1.10}$$

This function is plotted for several values of $\epsilon_\mathbf{p}$ in Figs. 2 through 5. For electrons injected in momentum states just above the Fermi surface ($\omega\gg\epsilon_\mathbf{p}>0$) a "quasiparticle peak," here a delta function, occurs at the energy

$$E_\mathbf{p}=\epsilon_p/(1+g^2N/\omega^2) \tag{1.11}$$

with a strength

$$\alpha_\mathbf{p}=1/(1+g^2N/\omega^2). \tag{1.12}$$

For large g^2N/ω^2 the major contribution to the sum rule (1.6) comes from the continua above the phonon emission threshold $|p_0|=\omega$. The maximum value of the weight function in the continuum occurs at $p_0=\omega(1+g^2N/\omega^2)^{1/2}$. The continuum for $p_0<0$ enters only when an electron is extracted from state $\mathbf{p}$ (i.e., hole injection) and describes a dressed hole and a phonon being excited.

As $\epsilon_\mathbf{p}$ increases, the delta-function peak moves toward ω, approaching ω asymptotically as $\epsilon_\mathbf{p}\to\infty$. If we continue to interpret this peak as a quasiparticle even for $\epsilon_\mathbf{p}\gg\omega$, this branch of the excitation spectrum exponentially approaches a constant energy, ω, at large momentum. The strength of the peak decreases however as $\exp[-2\epsilon_\mathbf{p}\omega/g^2N]$, as $\epsilon_\mathbf{p}\to\infty$.

There is an important change in the continuum as $\epsilon_\mathbf{p}$ increases beyond ω in that the simple peak occurring for $\epsilon_\mathbf{p}<\omega$ splits into two maxima, the lower energy maximum approaching ω asymptotically from above as $\epsilon_\mathbf{p}\to\infty$, while the upper peak approaches the free-particle energy as $\epsilon_\mathbf{p}\to\infty$. Since the upper peak almost completely exhausts the sum rule for large $\epsilon_\mathbf{p}$, it appears natural to call this peak the quasiparticle peak for large $\epsilon_\mathbf{p}$.

Therefore, the quasiparticle representation of $G(p)$ is reasonable in the regions $|\epsilon_\mathbf{p}|\gg\omega$, however for $|\epsilon_\mathbf{p}|\sim\omega$ the picture is clearly incorrect.

Another procedure often used to define quasiparticles[2] is to seek poles of the analytic continuation of G into the lower (upper) half-plane of the complex p_0 plane for $p_0>0$ ($p_0<0$). If a simple pole is the only singularity of this function near the real axis, the asymptotic time dependence of $G(\mathbf{p},t)$ in the limit $t\to\infty$ will contain the term $\alpha_\mathbf{p}e^{-iE_\mathbf{p}t}e^{-|\Gamma_\mathbf{p}|t}$, where the pole is located at $p_0=E_\mathbf{p}+i\Gamma_\mathbf{p}$, with residue $\alpha_\mathbf{p}$. In our problem, the analytic structure of G is complicated by the branch cut due to the logarithm in Σ_R. While poles do occur on the second Riemann sheet, the branch point at $p_0=\omega$ leads to contributions to $G(\mathbf{p},t)$ which cannot be neglected as $t\to\infty$.

The analytic continuation of G across the cut from ω to ∞ and from $-\infty$ to $-\omega$ is accomplished by subtracting from $\Sigma_I(\mathbf{p},p_0)$ the jump in its value as p_0 crosses the real axis from above to below for $p_0>0$ and vice versa for $p_0<0$. Defining $p_0=E+i\Gamma$, we have the continued expressions

$$\Sigma_R(E+i\Gamma)=\frac{-g^2N}{4\omega}\ln\left|\frac{(E+\omega)^2+\Gamma^2}{(E-\omega)^2+\Gamma^2}\right| \tag{1.13a}$$

$$\Sigma_I(E+i\Gamma)=\frac{g^2N}{2\omega}\tan^{-1}\frac{2\omega\Gamma}{E^2+\Gamma^2-\omega^2}\,\mathrm{sgn}E. \tag{1.13b}$$

To define the energy spectrum of the quasiparticles by this approach we look for zeros of $G^{-1}(p)=p_0-\epsilon_\mathbf{p}-\Sigma(p_0)$. The solutions of this equation are presented in Figs. 6 and 7 and were obtained by numerically solving the transcendental equation for Γ as a function of E, then plotting E as a function of $E-\Sigma_R(E+i\Gamma)=\epsilon$. Typical values of g^2N/ω^2 range from $\frac{1}{4}$ to $\frac{1}{2}$ in metals. Figures 6 and 7 have been drawn for $g^2N/\omega^2=\frac{1}{2}$. The branch labeled I arises from the delta-

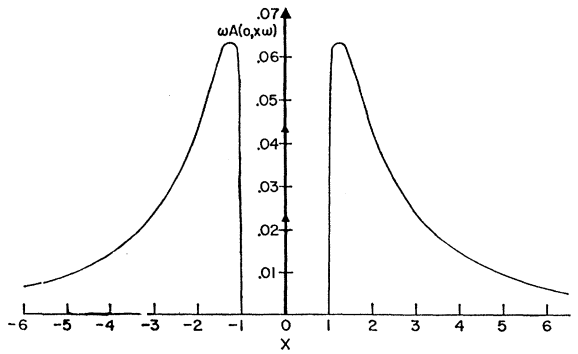

FIG. 2. Spectral weight function $A(\epsilon_\mathbf{p},x\omega)$ appropriate to the electron Green's function for $\epsilon_\mathbf{p}=0$, $g^2N/\omega^2=\frac{1}{2}$. There is a delta-function contribution at $x=0$.

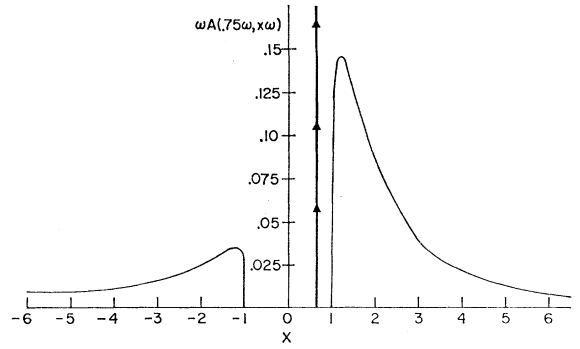

FIG. 3. The spectral weight function $A(\epsilon_p,x\omega)$ for $\epsilon_p=0.75\omega$ and $g^2N/\omega^2=\frac{1}{2}$. The heavy vertical line represents a delta-function contribution.

function term in the weight function. Branch II arises from a pole on the second sheet. It should be emphasized that a quasiparticle picture based on these two branches alone does not give an accurate representation of $G(\mathbf{p},p_0)$, as is clear from the plots of the weight function. This physical statement is true since $G(p_0)$ is not meromorphic but has branch-point singularities at energies $p_0=\pm\omega$ which cannot be neglected in determining the time dependence of G.

The origin of the two branches or alternatively of the peaks in the spectral weight function might be partially clarified by considering the soluble problem of N pairs of coupled harmonic oscillators. Consider the Hamiltonian

$$H=\tfrac{1}{2}\sum_{n=1}^{N}(p_n^2+\lambda_n^2q_n^2+P_n^2+\Lambda_n^2Q_n^2)+\sum_{n=1}^{N}g_nq_nQ_n. \quad (1.14)$$

The Green's function for the operator q_n, defined by

$$G_{q_n}(E)=i\int_{-\infty}^{\infty}dte^{iEt}\langle 0|\{T(q_n(t)q_n(0)\}|0\rangle \quad (1.15)$$

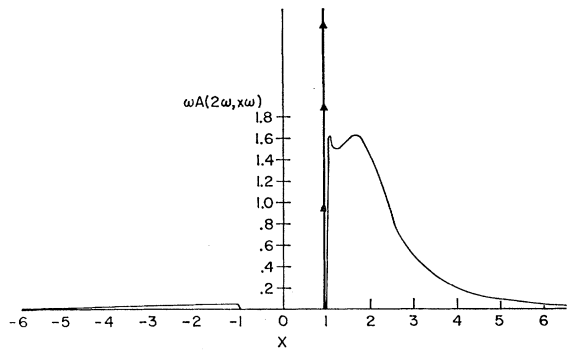

FIG. 4. The spectral weight function $A(\epsilon_p,x\omega)$ for $\epsilon_p=2\omega$ and $g^2N/\omega^2=\frac{1}{2}$. The heavy vertical line represents a delta-function contribution.

has poles at the characteristic frequencies ω_n and Ω_n of the coupled system.

$$\Omega_n^2=\frac{\lambda_n^2+\Lambda_n^2}{2}+\tfrac{1}{2}[(\lambda_n^2-\Lambda_n^2)^2+g_n^2]^{1/2},$$
$$\omega_n^2=\frac{\lambda_n^2+\Lambda_n^2}{2}-\tfrac{1}{2}[(\lambda_n^2-\Lambda_n^2)^2+g_n^2]^{1/2}. \quad (1.16)$$

If the starting Hamiltonian is positive-definite the system is stable, and both ω_n^2 and Ω_n^2 are positive. In a similar manner, our approximation for the electron Green's function has manifestations of two types of single-particle excitations. Roughly speaking, the peak at $E_p=\epsilon_p/(1+g^2N/\omega^2)$ corresponds to an electron "clothed" by a cloud of phonons analogous to a polaron in insulators, while the positive energy continuum for fixed momentum represents a clothed electron and a phonon being excited, the sum of their momenta being

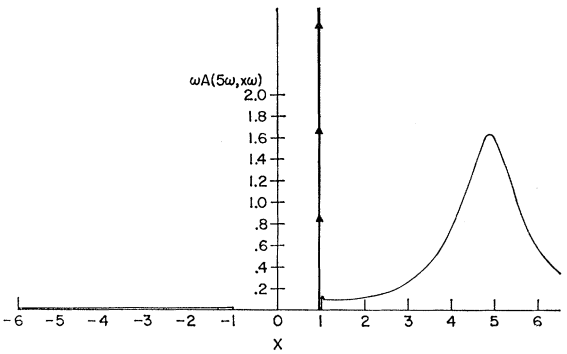

FIG. 5. The spectral weight function $A(\epsilon_p,x\omega)$ for $\epsilon_p=5\omega$ and $g^2N/\omega^2=\frac{1}{2}$. The heavy vertical line represents a delta-function contribution.

p. We note that for large ϵ_p the poles of $G(p_0)$ on the first and second sheets have the bare phonon-like behavior on branch I and the bare electron-like behavior on branch II.

Within the approximations made we have a result which is only of order the coupling constant squared. Our approximation for the self-energy contains implicitly the possibility for multiple phonon processes. Why is their effect not seen? The reason for these processes not contributing may be understood most simply by examining the relevant diagrams in the perturbation expansion. For example, consider double-phonon emission shown in Fig. 8:

$$\Sigma^{(4)}\propto\int d^4k_1d^4k_2D(k_1)D(k_2)G_0(p-k_1)^2G_0(p-k_1-k_2).$$

This expression contains as a factor

$$\int\frac{d^3k'}{(2\pi)^3}G_0^2(k')=N\int_{-\infty}^{\infty}d\epsilon\frac{1}{(\epsilon-k_0')^2}=0,$$

since

$$\oint dz\frac{1}{(z-\alpha)^2}=0$$

by Cauchy's theorem. Thus, we see we may even include some "phonon line crossing" diagrams which would arise from inclusion of the full vertex function; as long as there are two symmetrically placed electron lines, the contribution will be zero. In Sec. III we will consider the effects of multiple-phonon emission.

II. EVALUATION OF $G(\epsilon,t)$ FOR LARGE t

We now consider the evaluation of $G(\epsilon,t)$ for large positive t. The Fourier transform of $G(\epsilon,p_0)$ gives us the amplitude for a particle which is placed in the system at time zero with kinetic energy, ϵ, remaining in the same state after a time, t.

$$G(\epsilon,t)=\int\frac{dz}{2\pi}e^{-izt}G(\epsilon,z)$$
$$=\int\frac{dz}{2\pi}e^{-izt}\frac{1}{z-\epsilon+\dfrac{g^2N}{4\omega}\ln\left[\left(\dfrac{\omega+z}{\omega-z}\right)^2\right]}. \quad (2.1)$$

The integral is to be closed in the lower half-plane. For $\epsilon>\omega$ we choose the contour of integration as in Fig. 9. The result of the integration may be written as

$$G(\epsilon,t)=-i\frac{\exp(-iE_{\rm I}t)}{1+g^2N/(\omega^2-E_{\rm I}^2)}$$
$$-i\frac{\exp(-iE_{\rm II}t-\Gamma_{\rm II}t)}{1+g^2N/[\omega^2-(E_{\rm II}+i\Gamma_{\rm II})^2]}$$
$$+\int_L\frac{dz}{2\pi}\frac{\exp(-izt)}{z-\epsilon+\dfrac{g^2N}{4\omega}\ln\left[\left(\dfrac{\omega+z}{\omega-z}\right)^2\right]}.$$

If we change the variable in the line integral to $\Gamma'=i(z-\omega)$, then the dominant contribution comes from the branch point $\Gamma'=0$. Therefore, placing $\Gamma'=0$ in those terms of the denominator which give finite contributions, we obtain

$$\int_L=-\frac{g^2N}{2\omega}e^{-i\omega t}\int_0^\infty d\Gamma'\frac{e^{-\Gamma' t}}{[\omega-ig^2N\pi/4\omega+(g^2N/2\omega)\ln(2\omega/\Gamma')]^2+(\pi g^2N/2\omega)^2}.$$

If we place $y=\Gamma' t$ and neglect all but the singular behavior as $t\to\infty$, we obtain

$$\int_L=-\frac{g^2N}{2\omega t}\frac{1}{[(g^2N/2\omega)\ln t]^2}\int_0^\infty dye^{-y}.$$

Thus, the resulting expression is

$$G(\epsilon,t)=-i\frac{\exp[-iE_{\rm I}(\epsilon)t]}{1+g^2N/[\omega^2-E_{\rm I}^2(\epsilon)]}$$
$$-i\frac{\exp[-iE_{\rm II}(\epsilon)+\Gamma_{\rm II}t]}{1+g^2N\omega^2/[\omega^2-(E_{\rm II}+i\Gamma_{\rm II})]^2}$$
$$-\frac{2\omega e^{-i\omega t}}{g^2Nt(\ln t)^2}. \quad (2.2)$$

Of course, for t increasingly large the damped term will be negligible not only compared with the undamped term but also with respect to the $1/t(\ln t)^2$ term. In fact, the technique used in the evaluation of the line integral supposed t much greater than all the energies which entered. Thus, when this technique applies, the damped term may be mathematically neglected. However, we include it since it represents a physically important state of the system.

When ϵ is less than ω we use the same integration technique but change the contour so that both poles are included. The result of the line integration, depending as it does only on the behavior at the point $z=\omega$, remains unchanged.

III. MULTIPLE-PHONON PRODUCTION

In Sec. I we saw that our approximation for $\Sigma(p_0)$ did not reflect multiple-phonon processes in that Σ was a smooth function of p_0 near the multiphonon emission thresholds 2ω, 3ω, $\cdots$. We show below that this result, while approximately correct, is strictly valid only if the ϵ integral is extended symmetrically to infinity. We break particle-hole symmetry to investigate the approximations of Sec. I. Results identical with this section,

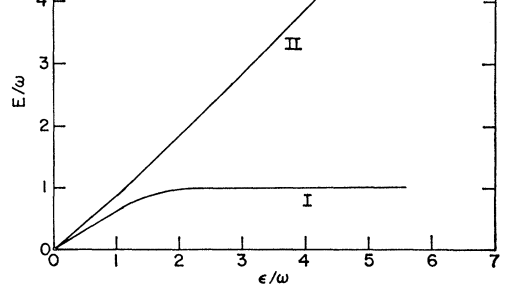

FIG. 6. Poles of the electron Green's function on the first and second branches. For a given kinetic energy ϵ_p, the poles are labeled by E.

except for numerical factors, are obtained if a large symmetric cutoff is chosen. Thus, we will again use the expression (1.3) for $\Sigma(p)$ but replace the lower limit $-\infty$ by $-\mu$ in the ϵ integration. When the imaginary part is taken and the spectral representation for G inserted we find

$$\mathrm{Im}G^{-1}(p_0)=-\mathrm{Im}ig^2\int\frac{d^4k}{(2\pi)^4}\frac{1}{(p_0-k_0)^2-\omega^2+i\delta}\left\{-\int_0^\infty\frac{dk_0'}{\pi}\frac{\mathrm{Im}G(\mathbf{k},k_0')}{k_0-k_0'+i\eta}+\int_{-\infty}^0\frac{dk_0'}{\pi}\frac{\mathrm{Im}G(\mathbf{k},k_0')}{k_0-k_0'-i\eta}\right\}\quad\delta,\eta\to 0^+. \tag{3.1}$$

We perform the k_0 integration by closing the contour so that only the poles of the phonon propagator contribute

$$\begin{aligned}\mathrm{Im}G^{-1}(p_0)&=\mathrm{Im}\frac{g^2}{\omega}\int\frac{d^3k}{(2\pi)^4}\left\{\int_0^\infty dk_0'\frac{\mathrm{Im}G(\mathbf{k},k_0')}{p_0-\omega-k_0'+i\eta}-\int_{-\infty}^0 dk_0'\frac{\mathrm{Im}G(\mathbf{k},k_0)}{p_0+\omega-k_0'-i\eta}\right\}\\&=-\frac{g^2}{2\omega}\int\frac{d^3k}{(2\pi)^3}\left\{\int_0^\infty dk_0'\,\mathrm{Im}G(\mathbf{k},k_0')\delta(p_0-\omega-k_0')+\int_{-\infty}^0 dk_0'\,\mathrm{Im}G(\mathbf{k},k_0')\delta(p_0+\omega-k_0')\right\}.\end{aligned} \tag{3.2}$$

Since $\mathrm{Im}G^{-1}(p_0)$ is an odd function of p_0 we need consider only positive values of p_0. Equation (3.2) leads to the result

$$\begin{aligned}\mathrm{Im}G^{-1}(p_0)&=-\frac{g^2}{2\omega}\int\frac{d^3k}{(2\pi)^3}\mathrm{Im}G(\mathbf{k},p_0-\omega)\quad\text{for}\quad p_0\geq\omega\\&=0\qquad\qquad\qquad\qquad\text{for}\quad 0\leq p_0<\omega.\end{aligned} \tag{3.3}$$

Thus, continuing the constant density of states approximation, we have for $p_0\geq\omega$

$$\begin{aligned}\mathrm{Im}G^{-1}(p_0)&=\frac{g^2N}{2\omega}\int_{-\mu}^\infty d\epsilon\frac{\mathrm{Im}G^{-1}(p_0-\omega)}{[p_0-\omega-\epsilon-\Sigma_R(p_0-\omega)]^2+[\mathrm{Im}G^{-1}(p_0-\omega)]^2}\\&=\frac{g^2N}{2\omega}\left\{\frac{\pi}{2}+\tan^{-1}\left[\frac{\mu+p_0-\omega-\mathrm{Re}\Sigma(p_0-\omega)}{\mathrm{Im}G^{-1}(p_0-\omega)}\right]\right\}.\end{aligned} \tag{3.4}$$

As required, this result agrees with (1.8) in the limit $\mu\to\infty$. We may make use of the fact that $\mu\gg|\mathrm{Im}G^{-1}(p_0-\omega)|$ and consider the energy region where $\mu\gg|p_0-\omega-\mathrm{Re}\Sigma|$ by expanding (3.4) to form a linear difference equation

$$\mathrm{Im}G^{-1}(p_0)=\frac{g^2N}{2\omega}\left\{\pi-\frac{\mathrm{Im}G^{-1}(p_0-\omega)}{\mu}\right\} \tag{3.5}$$

with the boundary condition $\mathrm{Im}G^{-1}(p_0=0)=0$. If we denote

$$\gamma_k=\mathrm{Im}G^{-1}(p_0),$$

where k gives the integer part of p_0/ω, the difference equation (3.5) may be written

$$\gamma_k+\frac{g^2N}{2\omega\mu}\gamma_{k-1}=\frac{g^2N\pi}{2\omega}. \tag{3.6}$$

The solution to (3.6) is

$$\begin{aligned}\gamma_0&=0\\\gamma_m&=\frac{g^2N\pi}{2\omega}\sum_{n=0}^{m-1}(-x)^n=\frac{g^2N\pi}{2\omega}\left(\frac{1-(-x)^m}{1+x}\right),\end{aligned} \tag{3.7}$$

where

$$x=\frac{g^2N}{2\omega\mu}\ll 1.$$

Thus, as the energy goes through multiples of the Einstein frequency, $\mathrm{Im}G^{-1}$ goes through oscillations of the order of magnitude 1/800 times $\mathrm{Im}G^{-1}(\omega)$. We have considered only the no lines crossing diagrams in

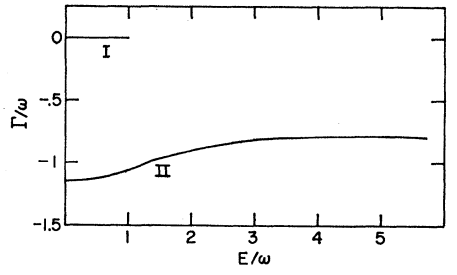

FIG. 7. Imaginary part of the energy, Γ, as a function of E for the poles of the electron Green's function corresponding to the curves drawn in Fig. 6.

our approximation for the self-energy. We cannot trust the accuracy of these small fluctuations since the contribution of the crossed line diagrams which arise by including the full vertex may be of the same order of magnitude.

To summarize, although by taking a finite cutoff, the effects of multiple-phonon processes may be seen, their effect is too small to be considered reliable in our approximation.

IV. ELECTRONIC POLARIZABILITY

To investigate the effect the modified electron spectrum has on the response of the system to external fields, we consider the irreducible polarizability $P(q)$ defined by[5]

$$P(q)=-2i\int\frac{d^4p}{(2\pi)^4}G(p+q)G(p)\Gamma(p,q), \quad (4.1)$$

and illustrated in Fig. 10. At first sight one might be tempted to replace Γ by unity as in the expression for the electron self-energy part $\Sigma(p)$. That such an approximation is inconsistent is most readily seen from the Ward identity[6]

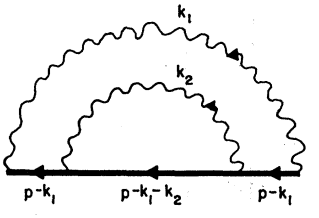

FIG. 8. A multiple-phonon process (4th order in g) included in the approximation for the electron self-energy.

$$\Gamma(p,0)=\frac{\partial G^{-1}(p)}{\partial p_0}=1-\frac{\partial\Sigma(p)}{\partial p_0}. \quad (4.2)$$

This relation and a "generalized" Ward identity of the form

$$q_0\Gamma(p,q)=G^{-1}(p+q)-G^{-1}(p) \quad (4.3)$$

is valid in the limit $\mathbf{q}\to 0$. These relations are a consequence of charge and current conservation. The proof of these relations is given in Appendix B. If Σ is approximated by (1.1) it is straightforward to show that (4.2) and (4.3) are satisfied if Γ is evaluated within the ladder approximation,[7] illustrated in Fig. 11. That is, the scalar vertex, Γ is approximated by the solution of the integral equation

$$\Gamma(p,q)=1+ig^2\int\frac{d^4k}{(2\pi)^4}G(k+q)G(k)\times D(p-k)\Gamma(k,q). \quad (4.4)$$

[5] See D. Pines, *The Many-Body Problem* (W. A. Benjamin, Inc., New York, 1962).
[6] J. C. Ward, Phys. Rev. **78**, 182 (1950).
[7] Y. Nambu, Phys. Rev. **117**, 648 (1960).

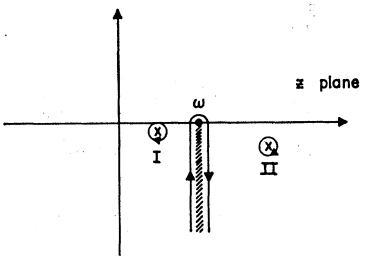

FIG. 9. Integration contour used in evaluating $G(\epsilon,t)$ for large t.

We introduce a vector vertex, Γ, as the solution to the equation

$$\mathbf{\Gamma}(p,q)=\frac{2\mathbf{p}+\mathbf{q}}{2m}+ig^2\int\frac{d^4k}{(2\pi)^4}G(k+q)\times G(k)D(p-k)\mathbf{\Gamma}(k,q). \quad (4.5)$$

The fact that solutions of these equations satisfy

$$q_0\Gamma(p,q)-\mathbf{q}\cdot\mathbf{\Gamma}(p,q)=G^{-1}(p+q)-G^{-1}(p) \quad (4.6)$$

follows by taking a linear combination of Eqs. (4.4) and (4.5) to form an equation for $(q_0\Gamma-\mathbf{q}\cdot\mathbf{\Gamma})$. By direct substitution of the assumed relation (4.6) into this equation one finds

$$\begin{aligned}q_0\Gamma(p,q)-\mathbf{q}\cdot\mathbf{\Gamma}(p,q)&=q_0-\epsilon_{p+q}+\epsilon_p-\Sigma(p+q)+\Sigma(p)\\&=G^{-1}(p+q)-G^{-1}(p),\end{aligned} \quad (4.6)$$

as required, since in our approximation

$$\Sigma(p)=-ig^2\int\frac{d^4k}{(2\pi)^4}G(k)D(p-k). \quad (4.7)$$

The Ward identity (4.2) follows if we first take the limit $q\to 0$ and then let $q_0\to 0$:

$$\Gamma(p,0)=\lim_{q_0\to 0}\frac{G^{-1}(p+q_0)-G^{-1}(p)}{q_0}=\frac{\partial G^{-1}(p)}{\partial p_0}.$$

Therefore, in the limit $q_0\to 0$ and $\mathbf{q}v_F/q_0\to 0$, we have

$$\Gamma(p,0)=1-\frac{\partial\Sigma}{\partial p_0}=1+\frac{g^2N}{\omega^2-p_0^2}. \quad (4.8)$$

Since g^2N/ω^2 is typically $\sim\frac{1}{2}$, the corrections to the free vertex are at least of order unity in this limit rather than $\sim\omega/E_F\ll 1$ which Migdal has found for $|\mathbf{q}|\gg(\omega/E_F)p_F$.

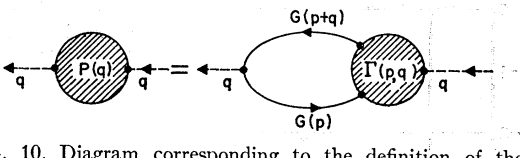

FIG. 10. Diagram corresponding to the definition of the irreducible polarizability, $P(q)$.

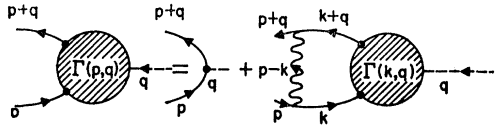

FIG. 11. Ladder approximation for the vertex function.

Long-Wavelength Polarizability

We now turn to the problem of determining the polarizability in the long-wavelength limit subject to the condition that the phase velocity $q_0/|\mathbf{q}|$ of the wave being considered is large compared to the Fermi velocity v_F.

It is convenient to rewrite $P(q)$ as

$$P(q)=-2i\int\frac{d^4p}{(2\pi)^4}\mathcal{G}(p,q)X(p,q)\,, \tag{4.9}$$

where $\mathcal{G}$ is defined as

$$\mathcal{G}(p,q)\equiv G(p+q/2)G(p-q/2)\,. \tag{4.10}$$

The vertex function $X(p,q)\equiv\Gamma(p-q/2,q)$ satisfies the equation

$$X(p,q)=1+ig^2\int\frac{d^4k}{(2\pi)^4}G(k+q/2)\times G(k-q/2)D(p-k)X(k,q)\,. \tag{4.11}$$

Since the right-hand side of (4.11) is independent of p, we assume X can be expanded for small $|\mathbf{q}|$ as a power series in $\mathbf{q}^2$:

$$X(p,q)=\sum_{\nu=0\ (\text{even})}^{\infty}|\mathbf{q}|^\nu X_\nu(p,q_0)\,. \tag{4.12}$$

If P and G are also expanded as a power series in $|\mathbf{q}|$, it is clear that only terms even in $|\mathbf{q}|$ enter and that only the spherical average of $\mathcal{G}$ need be considered; thus

$$P(q)\equiv\sum_{\nu=0\ (\text{even})}^{\infty}|\mathbf{q}|^\nu P_\nu(q_0) \tag{4.13}$$

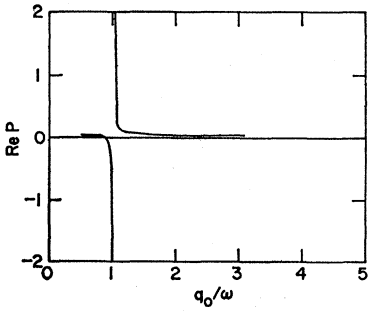

FIG. 12. Re$P(q)$ plotted as a function of q_0 in the limit $q_0/|\mathbf{q}|\gg v_F$.

and the angular average of $\mathcal{G}$ is defined to be

$$\frac{1}{4\pi}\int\mathcal{G}(p,q)d\Omega_p=\sum_{\nu=0\ (\text{even})}^{\infty}|\mathbf{q}|^\nu\mathcal{G}_\nu(p,q_0)\,. \tag{4.14}$$

Thus, Eq. (4.9) becomes

$$P_\nu(q_0)=-2i\int\frac{d^4p}{(2\pi)^4}[\mathcal{G}_0(p,q_0)X_\nu(p,q_0)+\mathcal{G}_2(p,q_0)X_{\nu-2}(p,q_0)+\cdots\mathcal{G}_\nu(p,q_0)X_0(p,q_0)]\,. \tag{4.15}$$

While all the $\mathcal{G}$'s are known explicitly, we know X_ν explicitly only for $\nu=0$. Nevertheless, an exact solution can be given for $P_0(q_0)$ and $P_2(q_0)$.

To see this consider the $\mathbf{q}^2$ expansion of the vertex equation (4.11):

$$X_\nu(p,q_0)=\delta_{\nu,0}+ig^2\int\frac{d^4k}{(2\pi)^4}[\mathcal{G}_0(k,q_0)X_\nu(k,q_0)+\cdots\mathcal{G}_\nu(k,q_0)X_0(k,q_0)]D(p-k)\,. \tag{4.16}$$

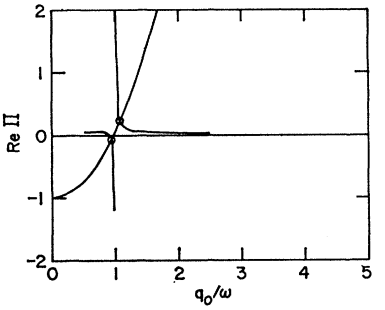

FIG. 13. Intersection of Re$\Pi(q)$ and $q_0^2-\omega^2$ giving the phonon frequencies for fixed q in the limit $q_0|\mathbf{q}|\gg v_F$.

For $\nu\neq0$ multiply by $\mathcal{G}_0(p,q_0)X_0(p,q_0)$ and integrate over p:

$$\int\frac{d^4p}{(2\pi)^4}\mathcal{G}_0(p,q_0)X_0(p,q_0)X_\nu(p,q_0)=\int\frac{d^4p}{(2\pi)^4}[\mathcal{G}_0(p,q_0)X_\nu(p,q_0)+\cdots\mathcal{G}_\nu(p,q_0)X_0(p,q_0)]\times[X_0(p,q_0)-1]\,. \tag{4.17}$$

In Eq. (4.17) we have used Eq. (4.16) for $\nu=0$ to simplify the right-hand side. By rearranging Eq. (4.17) we find the integral required to obtain $P_\nu(q_0)$ can be expressed as

$$\int\frac{d^4p}{(2\pi)^4}[\mathcal{G}_0(p,q_0)X_\nu(p,q_0)+\cdots\mathcal{G}_\nu(p,q_0)X_0(p,q_0)]=\int\frac{d^4p}{(2\pi)^4}[\mathcal{G}_2(p,q_0)X_{\nu-2}(p,q_0)+\cdots\mathcal{G}_\nu(p,q_0)X_0(p,q_0)]X_0(p,q_0)\,. \tag{4.18}$$

Thus for $\nu=2$ we find

$$P_2(q_0)=-2i\int\frac{d^4p}{(2\pi)^4}\mathcal{G}_2(p,q_0)X_0^2(p,q_0), \quad (4.19)$$

which can be evaluated directly since $\mathcal{G}_2$ and X_0 are known functions. We note that as in the exact expression for the polarizability, in our approximation, $P_0(q_0)$ vanishes since for $q=(0,q_0)$:

$$P_0(q_0)=-2i\int\frac{d^4p}{(2\pi)^4}G(p+q/2)G(p-q/2)X_0(p,q_0)$$

$$=2i\int\frac{d^4p}{(2\pi)^4}[G(p+q/2)-G(p-q/2)]=0. \quad (4.20)$$

Thus, to order $\mathbf{q}^2$ the real part of $P(q)$ for $q_0/|\mathbf{q}|\gg v_F$ is

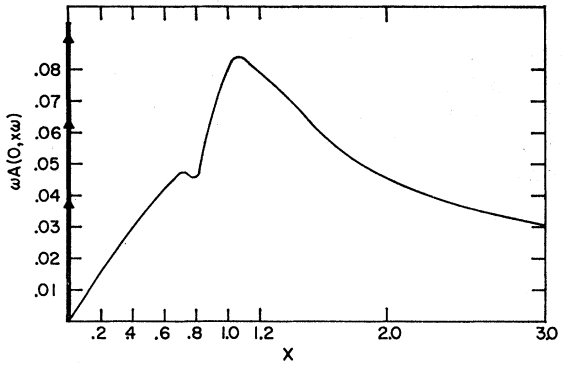

FIG. 14. Spectral weight function $A(\epsilon_p,x\omega)$ for the electron Green's function in the Debye model for $\epsilon_p=0$ and the coupling strength $\alpha=\frac{1}{4}$. There is a delta-function contribution at $x=0$.

given by

$$\mathrm{Re}P(q)=\frac{N}{3}\left(\frac{v_F}{q_0}\right)^2\frac{1}{(1+g^2N/\omega^2)^2}$$

$$\times\left\{2+\frac{3g^2N}{\omega^2}-\frac{g^2N}{\omega^2-q_0^2}\right\}. \quad (4.21)$$

A plot of $\mathrm{Re}P(q)$ as a function of q_0 is shown in Fig. 12 for $q_0/|\mathbf{q}|\gg v_F$.

We initially chose a phonon propagator corresponding to an undamped Einstein spectrum. Experimentally this is a valid assumption for large momentum transfers. One question we may answer at this stage is whether it is possible to arrive at this spectrum for the interacting phonon field starting from a Hamiltonian formulation. That is, our interacting phonon propagator is chosen to be

$$D^{-1}(q)=q_0^2-\omega^2.$$

We have implicitly calculated the phonon self-energy

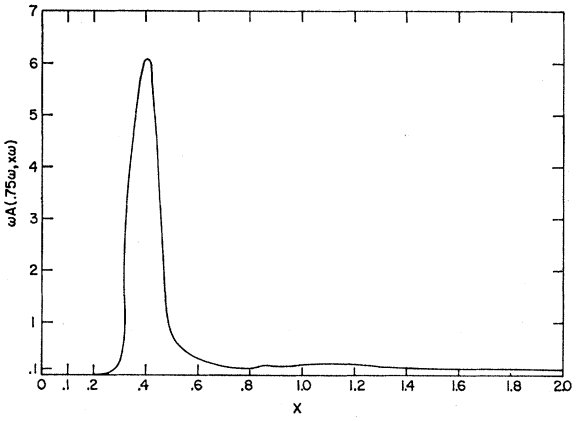

FIG. 15. Spectral weight function in the Debye model for $\epsilon_p=0.75\omega$ and $\alpha=\frac{1}{4}$.

$\Pi(q)$, since

$$\Pi(q)=g^2P(q).$$

But Dyson's equation gives

$$D(q)=D_0(q)+D_0(q)\Pi(q)D(q)$$

or

$$D_0^{-1}(q)=q_0^2-\omega^2-\Pi(q).$$

Since we are willing to accept a spatially nonlocal interaction, Π may be a function of $\mathbf{q}$. However, our result (4.21), is also a function of q_0 not linear in q_0^2. Thus, we could not start with a Hamiltonian formulation and arrive at an interacting phonon spectra with a single frequency for small wavelengths.

Another question we may put forward is the following. Suppose the initial Hamiltonian had an Einstein spectrum; using the perturbation approach of the previous sections, what is the interacting phonon spectrum? The condition $q_0/|\mathbf{q}|\gg v_F$ used in the calculation for the polarizability is appropriate for the long-wavelength Einstein phonons.

The dressed phonon frequencies are given by the poles of the dressed phonon propagator.

$$D^{-1}(q)=q_0^2-\omega^2-\Pi(\mathbf{q},q_0)=0, \quad (4.22)$$

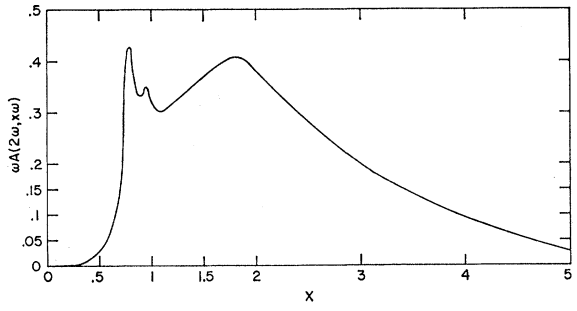

FIG. 16. Spectral weight function in the Debye model for $\epsilon_p=2\omega$ and $\alpha=\frac{1}{4}$.

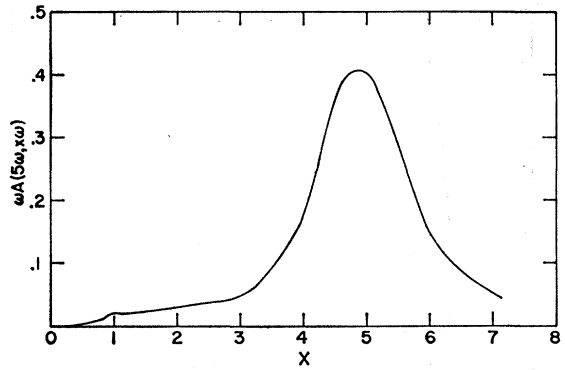

FIG. 17. Spectral weight function in the Debye model for $\epsilon_p=5\omega$ and $\alpha=\frac{1}{4}$.

where $\Pi(q)=g^2P(q)$. Thus, the dressed frequencies are given by the intersection of the curves $\Pi(q)$ and $q_0^2-\omega^2$ in Fig. 13. It is interesting to note that two roots exist for each value of $\mathbf{q}$, one above and one below the bare phonon frequency. As $\mathbf{q}\rightarrow 0$, the roots approach ω. So that if an Einstein spectrum is a reasonable choice for the noninteracting phonons, we would expect to observe experimentally the two branches splitting as we increase the momentum transferred to the lattice.

V. ELECTRON SPECTRUM IN THE DEBYE MODEL

We now consider a model of the lattice in which the phonons are described by a Debye spectrum,[4] that is, there exists a linear relation between the energy and momentum carried by a phonon, $\omega_q=c|\mathbf{q}|$, where c denotes the velocity of sound and q ranges from zero to q_D, the Debye wave number. The corresponding maximum phonon energy is denoted by ω. Zero phonon damping is again assumed. We begin immediately with the approximation for the self-energy used previously in which $\Gamma(p,q)=1$,

$$\Sigma(p)=i\int\frac{d^4k}{(2\pi)^4}\frac{g^2}{(p_0-k_0)^2-\omega_{\mathbf{p}-\mathbf{k}}^2+i\delta}\frac{1}{k_0Z(k)-\epsilon}. \quad (5.1)$$

To obtain an estimate of the coupling constant we use the deformation potential model without corrections for umklapp processes[8]:

$$g^2_{\mathbf{p}-\mathbf{k}}=|v_q{}^i/\kappa|^2=\left|\frac{4\pi Ze^2}{|\mathbf{q}|}\left(\frac{N}{M}\right)^{1/2}\frac{\mathbf{q}^2}{\mathbf{q}^2+k_s^2}\right|^2, \quad (5.2)$$

where we choose the static approximation to the dielectric function κ and k_s is the Fermi-Thomas screening length

$$k_s^2=4e^2mk_F/\pi,$$

where Z is the atomic number, N the ion density, M the ionic mass. In the long-wavelength limit, (2) becomes

$$g_q{}^2=\frac{\pi^2c^2q^2}{mk_F}=\frac{\pi^2\omega_q{}^2}{mk_F},$$

where

$$c^2=mv_F{}^2/3M.$$

The variables of integration are changed by introducing

$$\mathbf{q}^2=(\mathbf{p}-\mathbf{k})^2,\quad 2|\mathbf{q}|d|\mathbf{q}|=2|\mathbf{p}||\mathbf{k}|dx.$$

Equation (5.1) may then be written

$$\Sigma(p)=-\frac{i\pi^2mc^2}{|\mathbf{p}|p_F}\int\frac{dk_0d\epsilon}{(2\pi)^3}qdq\frac{q^2}{(p_0-k_0)^2-c^2q^2+i\delta}\times\frac{k_0Z+\epsilon}{\epsilon^2-(k_0Z)^2}. \quad (5.3)$$

The only dependence of Σ on $\mathbf{p}$ is in the factor $1/|\mathbf{p}|$. If we put $|\mathbf{p}|=k_F$ then Σ and Z are independent of ϵ, and the techniques used in the treatment of the Einstein spectrum are applicable. Since the dominant contribution to Σ comes from states of energy $\lesssim\omega$ about the Fermi surface, this replacement is justified. If particle-hole symmetry is maintained and the cutoff extended to infinity the self-energy is

$$\Sigma(p_0)=\frac{\pi^2c^2}{2p_F{}^2}\left\{\int_{k_0>0}dk_0-\int_{k_0<0}dk_0\right\}\times\left\{\int_0^{q_0}\frac{dq\,q^3}{(2\pi)^2}\frac{1}{(p_0-k_0)^2-c^2q^2\delta+i}\right\}. \quad (5.4)$$

As in the Einstein case, the boundary value of ImZ from above for $p_0>0$ is obtained from the delta-

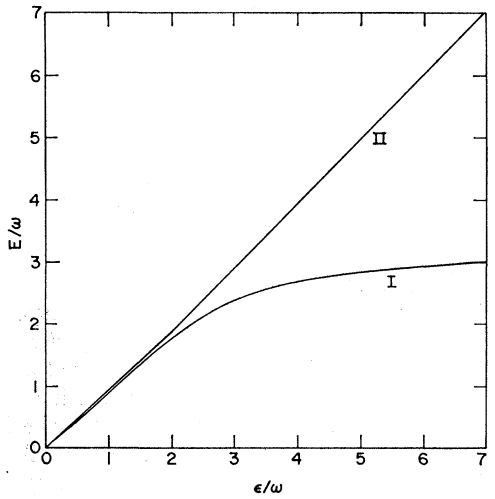

FIG. 18. Poles of the electron Green's function on the first and second branches in the Debye model. The real part of the energy, E, is plotted as a function of the kinetic energy ϵ_p measured relative to the Fermi surface. The parameter α was chosen to be 1/24 for this calculation.

[8] J. Bardeen and D. Pines, Phys. Rev. **99**, 1140 (1955).

function contribution and is given by

$$\frac{-i\pi p_0^3}{3p_F^2c^2} \quad \text{for} \quad p_0<\omega$$

$$\frac{-i\pi\omega^3}{3p_F^2c^2} \quad \text{for} \quad p_0>\omega.$$

The results of the integration are

$$\mathrm{Re}\Sigma(E+i\Gamma)=\frac{-1}{16c^2p_F^2}\left\{\tfrac{2}{3}E\omega^2+\tfrac{1}{3}(E^3-E\Gamma^2)\ln\frac{[(E+\omega)^2+\Gamma^2][(E-\omega)^2+\Gamma^2]}{(E^2+\Gamma^2)^2}+\frac{\omega^3}{3}\ln\frac{(E+\omega)^2+\Gamma^2}{(E-\omega)^2+\Gamma^2}\right.$$
$$\left.+(\tfrac{2}{3}\Gamma^3-2\Gamma E^2)\tan^{-1}\frac{2E\Gamma\omega^2}{(E^2+\Gamma^2)^2+(\Gamma^2-E^2)\omega^2}\right\},$$

$$\mathrm{Im}\Sigma(E+i\Gamma)=-\frac{1}{8c^2p_F^2}\left\{\frac{\omega^2\Gamma}{3}-\left(\frac{\Gamma^3}{6}-\frac{E^2\Gamma}{2}\right)\ln\frac{[(E+\omega)^2+\Gamma^2][(E-\omega)^2+\Gamma^2]}{(E^2+\Gamma^2)^2}\right.$$
$$\left.+\left(\frac{E^3}{3}-E\Gamma^2\right)\tan^{-1}\frac{2E\Gamma\omega^2}{(E^2+\Gamma^2)^2+(\Gamma^2-E^2)\omega^2}+\frac{\omega^3}{3}\tan^{-1}\frac{2\Gamma\omega}{E^2+\Gamma^2+\omega^2}\right\}. \quad (5.5)$$

The spectral weight function $A(\epsilon_p,p_0)$ which is defined by (1.7) can be calculated from (5.5) with $\Gamma\to 0$. One finds

$$\omega A(\epsilon_p,x\omega)=\frac{\alpha\varphi(x)}{\{x-\epsilon_p+\alpha[x+x^3\ln|1-1/x^2|+\ln|(x+1)/(x-1)|]\}^2+(\alpha\pi)^2\varphi^2(x)}, \quad (5.6)$$

where

$$\varphi(x)=\begin{cases}|x|^3; & 0\le|x|\le 1\\ 1; & |x|>1\end{cases} \quad (5.7)$$

and

$$\alpha\equiv\frac{\omega^2}{24p_F^2c^2}. \quad (5.8)$$

Plots of A for $\alpha=\frac{1}{4}$ are shown for $\epsilon_p=0$, 0.75ω, 2ω, and 5ω in Figs. 14, 15, 16, and 17, respectively. This value of α was chosen to make the damping rate for the Debye model agree with the calculation presented above for the Einstein model when $x>1$. It should be noted that in Fig. 14 the delta function at $x=0$ (for $\epsilon_p=0$) is the dominant part of the weight function. It is clear from the plots that as in the Einstein model, the quasiparticle description breaks down unless $\epsilon\ll\omega$ or $\epsilon\gg\omega$.

The poles of $G(p)$ on the first and second sheets are given for the Debye model in Fig. 18 for $\alpha=1/24$. There is a strong similarity between this plot and the corresponding curves for the Einstein model shown in Fig. 6. The imaginary part of the electron self-energy $\Sigma_I(E)$ is plotted in Fig. 19 for the two branches of Fig. 18, showing the well-known cubic damping rate for small E on branch I.

CONCLUSION

While the above calculations are for highly idealized models of the coupled electron-phonon system, we believe the qualitative features of the results are characteristic of physical systems. Specifically, we expect in general multiple peaks in the electron spectral weight function which describe various decay modes of an injected electron. Although one peak may have a majority of the total weight in limiting cases (i.e., $\epsilon\to 0$ and $\epsilon\to\infty$), a quasiparticle picture is expected to be insufficient for calculating system properties involving finite wavelength and frequency excitations. This does not preclude the use of Green's function methods since the approximations used above may well give an adequate description of these properties even though the quasiparticle scheme is inappropriate.

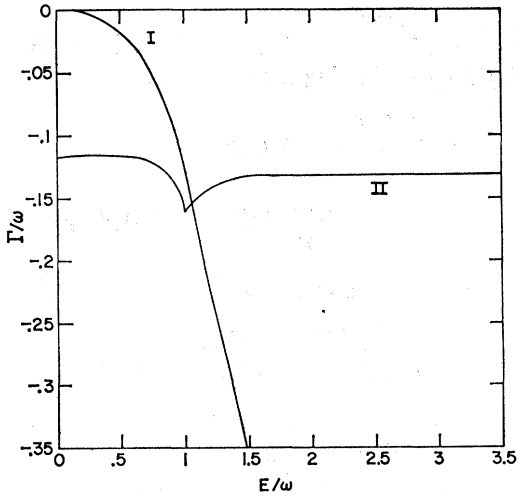

FIG. 19. The imaginary part of the energy Γ, plotted as a function of E corresponding to the curves given in Fig. 18.

ACKNOWLEDGMENTS

We would like to thank Dr. T. T. Wu for indicating the integration technique used in Sec. II. We are also grateful to Dr. Kenneth Johnson and Dr. E. P. Wigner for several helpful discussions.

APPENDIX A. FORMAL DEVELOPMENT OF EQUATIONS

The Hamiltonian we start with is[1,8] ($\hbar=1$)

$$H=\sum_{\mathbf{k},\sigma}\epsilon(\mathbf{k})c_\sigma^\dagger(\mathbf{k})c_\sigma(\mathbf{k}) +\tfrac{1}{2}\sum_{\mathbf{k}}[\Pi^\dagger(\mathbf{k})\Pi(\mathbf{k})+\omega^2(\mathbf{k})\varphi^\dagger(\mathbf{k})\varphi(\mathbf{k})] +\sum_{\mathbf{k},\mathbf{k}',\sigma}g(\mathbf{k}')c_\sigma^\dagger(\mathbf{k})c_\sigma(\mathbf{k}-\mathbf{k}')\varphi(\mathbf{k}') +\sum_{\mathbf{k}}J(-\mathbf{k})\varphi(\mathbf{k}), \quad \text{(A1)}$$

where $\epsilon(\mathbf{k})\equiv\epsilon(|k|)$ is the electron's kinetic energy as a function of momentum, minus the chemical potential μ; $g(\mathbf{k})\equiv g(|k|)$ is the electron-phonon coupling function and $\omega(|k|)$ is the phonon frequency. $J(\mathbf{k})$ is an external source of phonons which we will use in generating the

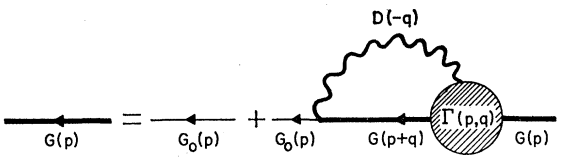

FIG. 20. Diagram representing Dyson's equation for the electron Green's function.

Green's function equations and then set equal to zero. We work with a box of unit volume and use periodic boundary conditions.

The equation of motion for the electron field is obtained by considering the commutator

$$[c(\mathbf{k},t),H]=i\frac{\partial c(\mathbf{k},t)}{\partial t}=\epsilon(\mathbf{k})c(\mathbf{k},t) +\sum_{\mathbf{k}'}g(\mathbf{k}')c(\mathbf{k}-\mathbf{k}',t)\varphi(\mathbf{k}',t), \quad \text{(A2)}$$

where we have used the anticommutation relations

$$\{c_\sigma(\mathbf{k},t),c_{\sigma'}^\dagger(\mathbf{k}',t)\}=\delta_{\sigma,\sigma'}\delta_{\mathbf{k},\mathbf{k}'}$$
$$\{c_\sigma(\mathbf{k},t),c_{\sigma'}(\mathbf{k}',t)\}=\{c_\sigma^\dagger(\mathbf{k},t),c_{\sigma'}^\dagger(\mathbf{k}',t)\}=0.$$

Since the interaction is spin-independent, the spin variables, σ, are suppressed.

The equation of motion for the phonon field is generated by considering the commutator of the Hamiltonian with $\Pi(\mathbf{k})$, and then with $\varphi(\mathbf{k})$, making use of the commutation relations

$$[\varphi(\mathbf{k},t),\Pi^\dagger(\mathbf{k}',t)]=i\delta_{\mathbf{k},\mathbf{k}'}$$
$$[\varphi(\mathbf{k},t),\varphi^\dagger(\mathbf{k}',t)]=[\Pi(\mathbf{k},t),\Pi^\dagger(\mathbf{k}',t)]=0.$$

Since we choose the phonon field Hermitian in coordinate space, we have

$$\varphi^\dagger(\mathbf{k})=\varphi(-\mathbf{k}), \quad \Pi^\dagger(\mathbf{k})=\Pi(-\mathbf{k}).$$

The equation of motion obtained is

$$\frac{\partial^2}{\partial t^2}\varphi(\mathbf{k},t)=-\omega(\mathbf{k})^2\varphi(\mathbf{k},t) -2g(\mathbf{k})\sum_{\mathbf{k}'}c^\dagger(\mathbf{k}',t)c(\mathbf{k}'+\mathbf{k},t)-J(\mathbf{k},t), \quad \text{(A3)}$$

where the spin sum has been accounted for by the factor of 2. The electron and phonon time-ordered Green's functions are defined by the equations[1]

$$G(\mathbf{k},t;\mathbf{k}'t')=-i\frac{\langle\Phi,+\infty\,|\,T(c(\mathbf{k},t)c^\dagger(\mathbf{k}',t'))\,|\Phi,-\infty\rangle}{\langle\Phi,\infty\,|\Phi,-\infty\rangle} \equiv-i\langle T\{c(\mathbf{k},t)c^\dagger(\mathbf{k}',t')\}\rangle$$

$$D(\mathbf{k},t;\mathbf{k}',t')=\frac{\delta\langle\varphi(\mathbf{k},t)\rangle}{\delta J(\mathbf{k}',t')}=\frac{\delta\langle\varphi(-\mathbf{k}',t)\rangle}{\delta J(-\mathbf{k},t)} =-i\{\langle T(\varphi(\mathbf{k},t)\varphi^\dagger(\mathbf{k}',t'))\rangle -\langle\varphi(\mathbf{k},t)\rangle\langle\varphi^\dagger(\mathbf{k}',t')\rangle\}. \quad \text{(A4)}$$

The Heisenberg state vector $|\Phi,-\infty\rangle$ represents the ground state of the electron-phonon system, specified by a complete set of observables whose eigenvalues are given at the time minus infinity. The definition of the electron Green's function and the field equation (A2) are sufficient to obtain

$$\left[i\frac{\partial}{\partial t}-\epsilon(\mathbf{k})\right]G(\mathbf{k},t;\mathbf{k}'t') =\delta_{\mathbf{k},\mathbf{k}'}\delta(t-t')-i\sum_{\mathbf{k}''}g(\mathbf{k}'') \times\langle T(\varphi(\mathbf{k}'',t)c(\mathbf{k}-\mathbf{k}'',t)c^\dagger(\mathbf{k}',t'))\rangle. \quad \text{(A5)}$$

The phonon Green's function equation is generated by taking the functional derivative of the ground-state expectation of the phonon field equation with respect to $J(k',t')$

$$\frac{\partial^2}{\partial t^2}D(\mathbf{k},t,\mathbf{k}',t')+\omega^2(\mathbf{k})D(\mathbf{k},t;\mathbf{k}'t') =\delta_{\mathbf{k},\mathbf{k}'}\delta(t-t')-2g(\mathbf{k})\sum_{\mathbf{k}''}\frac{\delta\langle c^\dagger(\mathbf{k}'',t)c(\mathbf{k}''+\mathbf{k},t)\rangle}{\delta J(\mathbf{k}',t')}. \quad \text{(A6)}$$

We use the following identity to rewrite the equation for the electron Green's function

$$-i\langle T\{\varphi(\mathbf{k}'',t'')c(\mathbf{k},t)c^\dagger(\mathbf{k}',t')\}\rangle$$
$$=\frac{\delta}{\delta J(-\mathbf{k}'',t'')}\langle T\{c(\mathbf{k},t)c^\dagger(\mathbf{k}',t')\}\rangle$$
$$-i\langle\varphi(\mathbf{k}'',t'')\rangle\langle T\{c(\mathbf{k},t)c^\dagger(\mathbf{k}',t')\}\rangle.$$

Then (A5) becomes

$$\left[i\frac{\partial}{\partial t}-\epsilon(\mathbf{k})\right]G(\mathbf{k},t;\mathbf{k}'t')$$
$$+i\sum_{\mathbf{k}''}g(\mathbf{k}'')\left[-\frac{\delta}{\delta J(-\mathbf{k}'',t'')}+i\langle\varphi(\mathbf{k}'',t)\rangle\right]$$
$$\times G(\mathbf{k}-\mathbf{k}'',t;\mathbf{k}',t')=\delta_{\mathbf{k},\mathbf{k}'}\delta(t-t')$$

which may be rewritten as

$$\left[i\frac{\partial}{\partial t}-\epsilon(\mathbf{k})\right]G(\mathbf{k},t;\mathbf{k}'t')-\sum_{\mathbf{k}'''}g(\mathbf{k}-\mathbf{k}''')\langle\varphi(\mathbf{k}-\mathbf{k}''',t)\rangle G(\mathbf{k},t;\mathbf{k}',t')$$
$$+i\int dt_1dt_2\sum_{\mathbf{k}''',\mathbf{k}_1,\mathbf{k}_2}g(\mathbf{k}-\mathbf{k}''')G(\mathbf{k}''',t;\mathbf{k}_1,t_1)\frac{\delta G^{-1}(\mathbf{k}_1,t_1;\mathbf{k}_2,t_2)}{\delta J(\mathbf{k}'''-\mathbf{k},t)}G(\mathbf{k}_2,t_2;\mathbf{k}',t')=\delta_{\mathbf{k},\mathbf{k}'}\delta(t-t'),$$

where $\mathbf{k}'''=\mathbf{k}-\mathbf{k}''$. Thus,

$$\left[i\frac{\partial}{\partial t}-\epsilon(\mathbf{k})\right]G(\mathbf{k},t;\mathbf{k}',t')-\sum_{\mathbf{k}'''}g(\mathbf{k}-\mathbf{k}'')\langle\varphi(\mathbf{k}-\mathbf{k}''',t)\rangle G(\mathbf{k}''',t;\mathbf{k}',t')+i\int dt_1dt_2dt_3\sum_{\mathbf{k}''',\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3}g(\mathbf{k}-\mathbf{k}''')G(\mathbf{k}''',t;\mathbf{k}_1,t_1)$$
$$\times\frac{\delta G^{-1}(\mathbf{k}_1,t_1;\mathbf{k}_2,t_2)}{\delta\langle\varphi(\mathbf{k}_3,t_3)\rangle}G(\mathbf{k}_2,t_2;\mathbf{k}',t')D(\mathbf{k}_3,t_3;\mathbf{k}'''-\mathbf{k},t)=\delta_{\mathbf{k},\mathbf{k}'}\delta(t-t'). \quad \text{(A7)}$$

By defining the vertex function as

$$\Gamma(\mathbf{k}_1,t_1;\mathbf{k}_2,t_2;\mathbf{k}_3,t_3)=-\frac{1}{g(\mathbf{k}_3)}\frac{\delta G^{-1}(\mathbf{k}_1,t_1;\mathbf{k}_2,t_2)}{\delta\langle\varphi(\mathbf{k}_3,t_3)\rangle}, \quad \text{(A8)}$$

Dyson's equation for the electron Green's function may be written

$$\int dt''\sum_{\mathbf{k}''}[G_0^{-1}(\mathbf{k},t;\mathbf{k}'',t'')-\Sigma(\mathbf{k},t;\mathbf{k}'',t'')]G(\mathbf{k}'',t'';\mathbf{k}',t')=\delta_{\mathbf{k},\mathbf{k}'}\delta(t-t'). \quad \text{(A9)}$$

In (A9) we define the inverse of the free-electron Green's function by

$$G_0^{-1}(\mathbf{k},t;\mathbf{k}'',t'')=\left\{\left[i\frac{\partial}{\partial t}-\epsilon(k)\right]\delta_{\mathbf{k},\mathbf{k}''}-g(\mathbf{k}-\mathbf{k}'')\langle\varphi(\mathbf{k}-\mathbf{k}'',t)\rangle\right\}\delta(t-t'')$$

and the self-energy,

$$\Sigma(\mathbf{k},t;\mathbf{k}''t'')=i\int dt_1dt_2\sum_{\mathbf{k}''',\mathbf{k}_1,\mathbf{k}_2}g(\mathbf{k}-\mathbf{k}''')g(\mathbf{k}_2)G(\mathbf{k}''',t';\mathbf{k}_1,t_1)\Gamma(\mathbf{k}_1,t_1;\mathbf{k}'',t'';\mathbf{k}_2,t_2)D(\mathbf{k}_2,t_2;\mathbf{k}'''-\mathbf{k},t). \quad \text{(A10)}$$

We may take advantage of the translational invariance of the system for the source term set equal to zero, and define

$$G(\mathbf{k}''',t;\mathbf{k}_1,t_1)=\delta_{\mathbf{k}''',\mathbf{k}_1}G(\mathbf{k}_1;t,t_1)$$
$$=\delta_{\mathbf{k}''',\mathbf{k}_1}\int\frac{dk_1{}^0}{2\pi}e^{-ik_1{}^0(t-t_1)}G(k_1) \quad \text{(A11)}$$

and similarly for the other two-point functions. The three-point function, due to translational invariance depends only on two 4-momenta

$$\Gamma(\mathbf{k}_1,t_1;\mathbf{k}'',t'';\mathbf{k}_3,t_3)=\delta_{\mathbf{k}_1-\mathbf{k}'',\mathbf{k}_3}\Gamma(\mathbf{k}'',\mathbf{k}_3;t_1,t'',t_3)$$
$$=\delta_{\mathbf{k}_1-\mathbf{k}'',k_3}\int\frac{dk_0''}{2\pi}\frac{dk_3{}^0}{2\pi}e^{ik_0''(t_1-t'')}e^{-ik_3{}^0(t_1-t_3)}\Gamma(\mathbf{k}'',k_3). \quad \text{(A12)}$$

These properties when used in (A10), lead to the standard form (Fig. 18)

$$\Sigma(p)=+i\int\frac{d^4q}{(2\pi)^4}g^2(\mathbf{q})G(p+q)\Gamma(p,q)D(q)\,, \tag{A13}$$

when we take the limit of an infinite volume continuum. The phonon Green's function equation, (A6), may be written in a similar form:

$$\left(\frac{\partial^2}{\partial t^2}+\omega^2(\mathbf{k})\right)D(\mathbf{k},t;\mathbf{k}',t')=-\delta_{\mathbf{k},\mathbf{k}'}\delta(t-t')+2ig(\mathbf{k})\sum_{\mathbf{k}''}\frac{\delta G(\mathbf{k}''+\mathbf{k},\,t;\,\mathbf{k}''t^+)}{\delta J(\mathbf{k}',t')}$$

$$=-\delta_{\mathbf{k},\mathbf{k}'}\delta(t-t')+2ig(\mathbf{k})g(\mathbf{k}')\int dt_1dt_2dt_3\sum_{\mathbf{k}'',\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3}G(\mathbf{k}''+\mathbf{k},\,t;\,\mathbf{k}_1,t_1)\Gamma(\mathbf{k}_1,t_1;\,\mathbf{k}_2,t_2;\,\mathbf{k}_3,t_3)$$

$$\times G(\mathbf{k}_2,t_2;\,\mathbf{k}'',t^+)D(\mathbf{k}_3,t_3;\,\mathbf{k}',t')\,. \tag{A14}$$

When translational invariance, the infinite volume limit and time Fourier transforms are used,

$$[D_0^{-1}(k)-\Pi(k)]D(k)=1\,, \tag{A15}$$

if the inverse of the free phonon Green's function and the phonon self-energy are defined by

$$D_0^{-1}(k)=k_0^2-\omega^2(\mathbf{k})$$

$$\Pi(k)=-2ig^2(k)\int\frac{d^4p}{(2\pi)^4}G(p+k)G(p)\Gamma(p,k)\,. \tag{A16}$$

To complete the formal development we consider the equation obeyed by the vertex function. Using (A8), (A9), and (A10), we obtain

$$\Gamma(\mathbf{k},t;\,\mathbf{k}'',t'';\,\mathbf{k}',t')=\delta_{\mathbf{k}-\mathbf{k}'',\mathbf{k}'}\delta(t-t'')\delta(t-t')+i\int dt_1dt_2dt_3dt_4\sum_{\mathbf{k}'',\mathbf{k}_1,\mathbf{k}_2}g(\mathbf{k}-\mathbf{k}''')g(\mathbf{k}_2)G(\mathbf{k}''',t;\,\mathbf{k}_3,t_3)\Gamma(\mathbf{k}_3,t_3;\,\mathbf{k}_4,t_4;\,\mathbf{k}',t')$$

$$\times G(\mathbf{k}_4,t_4;\,\mathbf{k}_1,t_1)\Gamma(\mathbf{k}_1,t_1;\,\mathbf{k}'',t'';\,\mathbf{k}_2,t_2)D(\mathbf{k}_2,t_2;\,\mathbf{k}'''-k,\,t)+i\int dt_1dt_2\sum_{\mathbf{k}''',\mathbf{k}_1,\mathbf{k}_2}g(\mathbf{k}-\mathbf{k}''')g(\mathbf{k}_2)$$

$$\times G(\mathbf{k}''',t;\,\mathbf{k}_1,t_1)\left(\frac{1}{g(\mathbf{k}')}\frac{\delta}{\delta\langle\varphi(\mathbf{k}',t')\rangle}\right)[\Gamma(\mathbf{k}_1,t_1;\,\mathbf{k}'',t'';\,\mathbf{k}_2,t_2)D(\mathbf{k}_2,t_2;\,\mathbf{k}'-\mathbf{k},\,t)]\,. \tag{A17}$$

The last term of (A17) represents the introduction of a new function since the functional derivative of ΓD with respect to $\langle\varphi(z)\rangle$ cannot be expressed in terms of the functions already introduced. As in the treatments using an infinite chain of coupled integral equations, the last term of (A17) is the introduction of a higher order correlation function.

A very useful approximation[4] is obtained when one uses an iterative approach and retains only the first term of (A17), approximating the vertex function by

$$\Gamma(p,q)=1\,. \tag{A18}$$

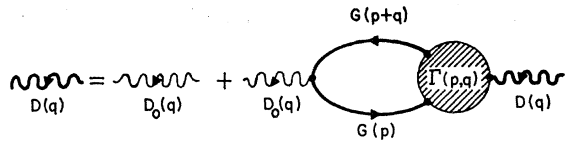

FIG. 21. Diagram representing Dyson's equation for the phonon Green's function.

The electron self-energy (A13) then becomes

$$\Sigma(p)=i\int\frac{d^4q}{(2\pi)^4}g^2(\mathbf{q})G(p+q)D(q)\,. \tag{A19}$$

The vertex equation, derived using (A8), (A9), and (A18) corresponds to the ladder approximation[7] shown in Fig. 11, when the variation of D with $\langle\varphi\rangle$ is neglected,

$$\Gamma(p,q)=1+i\int\frac{d^4k}{(2\pi)^4}g^2(\mathbf{p}-\mathbf{k})G(k+q)$$

$$\times\Gamma(k,q)G(k)D(p-k)\,. \tag{A20}$$

This approximation for Γ is used in Sec. IV to discuss the electronic polarizability.

APPENDIX B. WARD IDENTITIES

To derive the Ward identity[6] for Γ used in Sec. IV, we consider the related vertex function $\tilde{\Gamma}_\mu(x,y,z)$

($\mu=0, 1, 2, 3$), defined by

$$\Lambda_\mu(x,y,z)\equiv\langle T\{j_\mu(z)\psi(x)\psi^\dagger(y)\}\rangle$$
$$\equiv-\int\tilde{\Gamma}_\mu(x',y',z)G(x,x')G(y',y)dx'dy'. \quad \text{(B1)}$$

The current density 4-vector j_μ (for electrons of one spin orientation) is defined by

$$j_\mu(z)=\psi^\dagger(z)\psi(z), \quad \mu=0,$$
$$=\frac{1}{2mi}\{\psi^\dagger(z)\nabla_\mu\psi(z)-[\nabla_\mu\psi^\dagger(z)]\psi(z)\}, \quad \mu=1, 2, 3. \quad \text{(B2)}$$

In the absence of spin-dependent forces, j_μ satisfies the continuity equation

$$\sum_{\mu=0}^{3}\frac{\partial}{\partial z_\mu}j_\mu(z)=0, \quad z_\mu\equiv(t,\mathbf{z}). \quad \text{(B3)}$$

In the presence of spin-dependent forces, (B3) holds if j_μ includes electrons of both spin orientation. If we assume the system to be translationally invariant it follows that the Fourier transforms of G and $\tilde{\Gamma}$ can be represented by

$$G(x,x')\equiv G(x-x')=\int G(p)e^{ip(x-x')}\frac{d^4p}{(2\pi)^4}$$

$$\tilde{\Gamma}_\mu(x',y',z)=\int\tilde{\Gamma}_\mu(p,q)\exp[ip(x'-y')+iq(x'-z)]\frac{d^4pd^4q}{(2\pi)^8}. \quad \text{(B4)}$$

By taking the 4-divergence of (B1) and using the continuity equation (B3) one readily obtains the generalized Ward identity

$$q_0\tilde{\Gamma}_0(p,q)-\mathbf{q}\cdot\tilde{\Gamma}(p,q)=G^{-1}(p+q)-G^{-1}(p) \quad \text{(B5)}$$

for the vertex $\tilde{\Gamma}_\mu$.

To see this in detail, consider the 4-divergence of Λ_μ with respect to z_μ

$$\sum_{\mu=0}^{3}\frac{\partial\Lambda_\mu(x,y,z)}{\partial z_\mu}$$
$$=\langle T\{[j_0(z),\psi(x)]\psi^\dagger(y)\}\rangle\delta(z_0-x_0)+\langle T\{\psi(x)[j_0(z),\psi^\dagger(y)]\}\rangle\delta(z_0-y_0)+\langle T\left\{\sum_{\mu=0}^{3}\frac{\partial j_\mu(z)}{\partial z_\mu}\psi(x)\psi^\dagger(y)\right\}\rangle. \quad \text{(B6)}$$

The two commutator terms arise from differentiating the time ordering operator with respect to z_0, while the last term vanishes according to (B3). With the aid of the relations

$$[j_0(z),\psi(x)]=-\psi(z)\delta^3(\mathbf{z}-\mathbf{x}), \quad (z_0=x_0)$$
$$[j_0(z),\psi^\dagger(y)]=\psi^\dagger(z)\delta^3(\mathbf{z}-\mathbf{y}), \quad (z_0=y_0) \quad \text{(B7)}$$

(B6) can be reduced to

$$\sum_{\mu=0}^{3}\frac{\partial\Lambda_\mu(x,y,z)}{\partial z_\mu}=-iG(z-y)\delta(z-x)+iG(x-z)\delta(z-y). \quad \text{(B8)}$$

By inserting the Fourier representations of G and $\tilde{\Gamma}$ into (B1), it is easily seen that the 4-divergence of the right-hand side of (B1) is

$$\sum_{\mu=0}^{3}\frac{\partial\Lambda_\mu(x,y,z)}{\partial z_\mu}=i\int[\mathbf{q}\cdot\tilde{\mathbf{\Gamma}}(p,q)-q_0\tilde{\Gamma}_0(p,q)]G(p)G(p+q)\times\exp[ip(x-y)+iq(x-z)]\frac{d^4pd^4q}{(2\pi)^8}. \quad \text{(B9)}$$

Since the right-hand sides of (B8) and (B9) are equal, so are their Fourier transforms:

$$i[G(p+q)-G(p)]=i\{\mathbf{q}\cdot\tilde{\mathbf{\Gamma}}(p,q)-q_0\tilde{\Gamma}_0(p,q)\}G(p)G(p+q). \quad \text{(B10)}$$

This relation is equivalent to the Ward identity (B5) stated above.

To connect Γ and $\tilde{\Gamma}_\mu$ we note that Γ satisfies the equation

$$\langle 0|T\{\varphi(\mathbf{q},t'')c(\mathbf{p}+\mathbf{q},t')c^\dagger(\mathbf{p},t)\}|0\rangle$$
$$=-\int g(\mathbf{q})\Gamma(\mathbf{p}+\mathbf{q},t_1;\mathbf{p},t_2;\mathbf{q},t_3)D(\mathbf{q},t_3-t'')\times G(\mathbf{p}+\mathbf{q},t-t_1)G(\mathbf{p},t_2-t')dt_1dt_2dt_3. \quad \text{(B11)}$$

[See (A5) and (A8)–(A10).] The phonon field, φ, satisfies the equation of motion

$$-\left(\frac{\partial^2}{\partial t''^2}+\omega_q{}^2\right)\varphi(\mathbf{q},t'')=D_0^{-1}(\mathbf{q},t'')\varphi(\mathbf{q},t'')=g_q\rho(\mathbf{q},t''), \quad \text{(B12)}$$

where

$$\rho(\mathbf{q},t'')=\int\psi^\dagger(z)\psi(z)e^{-i\mathbf{q}\cdot\mathbf{z}}d^3z \quad (z_0=t'').$$

Therefore, by applying the operator $D_0^{-1}(\mathbf{q},t'')$ to (B11) we obtain

$$\langle 0|T\{\rho(\mathbf{q},t'')c(\mathbf{p}+\mathbf{q},t')c^\dagger(\mathbf{p},t)\}|0\rangle$$
$$=-\int\Gamma(\mathbf{p}+\mathbf{q},t_1;\mathbf{p},t_2,\mathbf{q},t_3)D_0^{-1}(\mathbf{q},t'')D(\mathbf{q},t_3-t'')\times G(\mathbf{p}+\mathbf{q},t'-t_1)G(\mathbf{p},t_2-t)dt_1dt_2dt_3. \quad \text{(B13)}$$

We note, however, that aside from spatial coordinate

Fourier transforms, (B1) and (B13) differ for $\mu=0$ only by $\tilde{\Gamma}_0$ being replaced by $\Gamma D_0^{-1}D$. Hence, the relation

$$\tilde{\Gamma}_0(p,q)=D_0^{-1}(q)D(q)\Gamma(p,q) \qquad \text{(B14)}$$

is valid.

If we assume that $\tilde{\Gamma}_\mu(p,q)$ is analytic in q so that $\mathbf{q}\cdot\tilde{\boldsymbol{\Gamma}}(p,q)$ vanishes for $\mathbf{q}\to 0$, we need only show $D^{-1}(q)D_0(q)=1$ in the limit $\mathbf{q}\to 0$, in order to prove (4.3). The relation $q_0\Gamma(p,q)=G^{-1}(p+q)-G^{-1}(p)$ then follows from (B5), (B14) in the limit $\mathbf{q}\to 0$. To prove $D^{-1}(q_0)D_0(q_0)=1$ or equivalently $D_0^{-1}(q_0)D(q_0)=1$ we use Eq. (B12):

$$D_0^{-1}(\mathbf{q},t)D(\mathbf{q};t,t')=\delta(t-t')-ig(\mathbf{q})\langle T\rho(\mathbf{q},t)\varphi^\dagger(\mathbf{q},t')\rangle\,,$$

where $D(\mathbf{q};t,t')\equiv -i\langle T\{\varphi(\mathbf{q},t)\varphi^\dagger(\mathbf{q},t')\}\rangle$. Now for $\mathbf{q}=0$, $\rho(\mathbf{q},t)=N(t)=N$ is a constant of the motion, i.e., the total number of electrons. Thus,

$$q_0[D_0^{-1}(q_0)D(q_0)-1]=0$$

which completes our proof.

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Dynamical Motion and Gamma-Ray Cross Section of an Impurity Nucleus in a Crystal. I. Isolated Impurities in Germanium and Aluminum

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The general theory of the dynamical motion and gamma-ray cross section for a single impurity nucleus harmonically coupled to an arbitrary collection of N atoms is developed in supermatrix representation. The relevant properties of the system are expressed in terms of a functional matrix $f_0(\boldsymbol{\Omega})$ of order $3N\times 3N$, where $\boldsymbol{\Omega}$ is the mass-reduced force-constant matrix. Our approach is to use a Cauchy singular integral representation for $f_0(\boldsymbol{\Omega})$ involving an integration along the real frequency, ω, axis. Matrix partitioning techniques are used to reduce our problem to one of evaluating the 3×3 impurity atom dynamic response matrix, $\{\mathbf{G}\}_{11}=(1+\epsilon)[\mathbf{I}_3+\tau\epsilon\mathbf{A}_{11}]^{-1}\mathbf{A}_{11}$, where $\tau=\omega^2-i\delta$. Here, δ is an arbitrarily small number, and $\epsilon+1=$ ratio of impurity atom to host atom mass, (M_I/M_H). For an arbitrary physical arrangement of the atoms, $\mathbf{A}_{11}=\{[\mathbf{I}_{3(z+1)}-\mathbf{D}_{z+1}(\Delta\mathbf{F}/M_H)]^{-1}\mathbf{D}_{z+1}\}_{11}$, where the subscript, 1, refers to the impurity atom coordinates, $\Delta\mathbf{F}$ is the perturbation in force-constant matrix, and z is the number of sites over which the perturbation extends. The $\mathbf{D}_{z+1}$ matrix has matrix elements obtained from the elements of the pure host matrix $\mathbf{D}_H=[\tau\mathbf{I}_{3N}-\mathbf{F}_H M_H^{-1}]^{-1}$, $\mathbf{F}_H$ is the pure host force-constant matrix. $\mathbf{I}_k$ is a $k\times k$ unit matrix.

The general approach is used to study the dynamic response of an impurity atom substituted in the aluminum lattice with arbitrary ϵ and nearest neighbor $\Delta\mathbf{F}$. The $\mathbf{A}$ matrix is block diagonalized by introducing the molecular vibration symmetry coordinates and $\mathbf{A}_{11}$ is characterized by a 4×4 symmetry adapted Green's function matrix whose elements have been tabulated. A generalized tensor force-constant model is used with Walker's force constants characterizing $\mathbf{D}_H$, the pure aluminum lattice Green's function matrix. Similar studies are carried out for a Sn^{119} atom isotopically substituted in Ge, where the relevant Green's functions are derived from Phillip's frequency spectrum.

The dynamical motion and gamma-ray cross section of impurity nuclei are characterized by a dynamic response function, K, which is related to the imaginary part of $\{\mathbf{G}\}_{11}$. Typical K functions are presented for Fe^{57} in Al for various changes in $\Delta\mathbf{F}$ and for Sn^{119} in Ge with $\Delta\mathbf{F}=0$. Our results show that the dynamical behavior of impurity atoms in real lattices is quite sensitive to the vibrational properties of the host lattice. The resonant fraction of γ rays absorbed by the impurity nucleus, f, the Lamb-Mössbauer coefficient, $2W$, and mean-square velocity, $(v_I^2)_{\text{av}}$, of Fe^{57}-Al are tabulated for several $\Delta\mathbf{F}$ changes as a function of temperature. Our results are extrapolated to study the temperature dependence of $2W$ and f for Fe^{57}-Cu and Fe^{57}-Pt. From the results derived in this paper, it is possible to determine K, $2W$, and $(v_I^2)_{\text{av}}$ for any ϵ and $\Delta\mathbf{F}$ for Al as a host lattice.

I. INTRODUCTION

THE purpose of this paper is to present the results of detailed studies of the dynamical motion and γ-ray cross section of a Mössbauer impurity nucleus bound in a locally perturbed host crystal at an arbitrary temperature.[1] A completely general lattice dynamics model is assumed in which the impurity nucleus is harmonically coupled to the host lattice with force constants which differ from those of the pure host lattice.

A considerable amount of research has been carried out on vibrational as well as electronic impurity states in crystals. Green's function approaches to these problems appear to have been developed by Lifshitz,[2] Koster

[1] For a recent review article on the Mössbauer effect see H. Frauenfelder, *The Mössbauer Effect* (W. A. Benjamin, Inc., New York, 1962). Studies of a general nature involving impurity atom motion, resonant Mössbauer absorption by impurity nuclei, and optical absorption by impurity vibrational modes have been carried out by A. A. Maradudin, in Lecture Notes of Brandeis University 1962 Summer Institute of Theoretical Physics [W. A. Benjamin, Inc. (to be published)].

[2] Qualitative studies of the impurity vibrational problem have been carried out by I. M. Lifshitz and co-workers in Russia over the past twenty years. See I. M. Lifshitz, Suppl. Nuovo Cimento **3**, 733 (1956) for references to prior work.