Calculation of the Superconducting State Parameters with Retarded Electron-Phonon Interaction

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The energy gap and other parameters of the superconducting state are calculated from the Bardeen-Cooper-Schrieffer theory in Gor'kov-Eliashberg form, using a realistic retarded electron-electron interaction via phonons and including the Coulomb repulsion. The solution is facilitated by observing that only the local phonon interaction, mediated entirely by short-wavelength phonons, is important, and that a good approximation for the phonon spectrum is therefore an Einstein model rather than Debye model. The resulting equation is solved by an approximate iteration procedure. The results are similar to earlier gap equations but the derivation gives a precise meaning to the interaction and cutoff parameters of earlier theories. The numerical results are in good order-of-magnitude agreement with the observed transition temperatures but lead to an isotope effect at least 15% less than the accepted $-\frac{1}{2}$ exponent (T_c proportional to $M^{-\frac{1}{2}}$). Also, the present theory predicts that all metals should be superconductors, although those not observed to do so would have remarkably low transition temperatures.

INTRODUCTION

ALTHOUGH the original Bardeen, Cooper, and Schrieffer (BCS) theory of superconductivity[1] has gone far in explaining the basic processes which account for the condensation of fermion systems, it must still be considered as a phenomenological theory with respect to the use which is made of a rather nonphysical "effective potential" to describe the complex Coulomb and phonon-induced interactions between the electrons in a metal. We may recall that the BCS effective potential is instantaneous and displays a strongly oscillating behavior in coordinate space (since its Fourier transform is sharply cut off in momentum space). Since the strength V of this effective interaction appears only as an adjustable parameter, the BCS model is still adequate to describe most properties of superconductors; it is difficult, however, to see how this parameter V could be related to the retarded, time-dependent electron-phonon interaction and the essentially instantaneous Coulomb repulsion or a combination thereof.

On the contrary, several physical reasons lead us to the conclusion that the coordinate space dependence of the interaction potential plays a very subsidiary role whereas its retardation in time is indeed of major importance in determining the various cutoff phenomena. Firstly, it appears that the quite long range part (in space) of the phonon-induced interaction results primarily from the emission and absorption of very long wavelength phonons. These phonons can enter either through "direct" processes, in which the dielectric screening of the metal is nearly complete, or through "umklapp" processes. These latter processes have been supposed in the past[2,3] to play a major role, but this appears very much in doubt in view of the deformation potential theorem which requires that the effective potential acting to cause scattering by any phonon be, to first order, proportional to the strain produced by the phonon and not to the displacement. In this perspective, an Umklapp process may be viewed as the excitation of a true phonon corresponding to an actual deformation of the lattice plus a stationary wave corresponding to a translation of the lattice as a whole. Since the electron wave functions follow adiabatically a translation of the lattice, only the actual deformation causes any scattering. Consequently, Umklapp processes are no more effective than direct ones. The net result, then, is that the phonon-induced interaction is mediated primarily through short-wavelength phonons. It is well known experimentally and theoretically that the short-wavelength part of the phonon spectrum is rather sharply peaked about a few definite frequencies, so that it is a quite good approximation to think in terms of an Einstein model of a few groups of single-frequency, nonpropagating phonons. And of course, phonons which do not propagate in space lead directly to a localized interaction.

A second line of reasoning leading to the same conclusion stems from the particular form of the Gor'kov-Eliashberg energy gap equation.[4,5] In these works, the energy gap function in coordinate space

[1] J. Bardeen, L. N. Cooper, and J. R. Schrieffer, Phys. Rev. **108**, 1175 (1957); hereafter referred to as BCS.

[2] D. Pines, Phys. Rev. **109**, 280 (1958).

[3] P. Morel, J. Phys. Chem. Solids **10**, 277 (1959).

[4] L. P. Gor'kov, J. Exptl. Theoret. Phys. (U.S.S.R.) **34**, 735 (1958). [Translation: Soviet Phys.—JETP **7**, 505 (1958).] G. M. Eliashberg J. Exptl. Theoret. Phys. (U.S.S.R.) **38**, 966 (1960). [Translation: Soviet Phys.—JETP **11**, 696 (1960).]

[5] P. W. Anderson, *Proceedings of the Seventh International Conference on Low-Temperature Physics* (University of Toronto Press, Toronto, 1960).

and time is

$$\Sigma(\mathbf{r}-\mathbf{r}', t-t')=F(\mathbf{r}-\mathbf{r}', t-t')V(\mathbf{r}-\mathbf{r}', t-t'),$$

where V is the retarded potential caused by phonons and F is the Gor'kov pair Green's function. F has a long range in space and oscillates with a wavelength of the order of $2k_0^{-1}$ (k_0 is the Fermi momentum), while the spatial dependence of V is only related to the particular features of the phonon spectrum and may display an oscillating behavior with wavelength of the order of the inverse of the Debye momentum. Destructive interference makes the product of F and V small for all but quite small spatial distances ($\mathbf{r}-\mathbf{r}'$). Thus, we find once more that only the short-range part of the interaction potential is important.

It is therefore desirable that a treatment actually taking into account the time dependence of the electron-phonon interaction be developed, with the hope that the main features of the BCS model, and particularly the isotope effect, may be retrieved by this approach. Fortunately, a new and powerful analysis of the condensation phenomenon in terms of particle propagators has been derived by several authors,[4] thereby providing us with a suitable formalism for our purpose. In the first section, we shall briefly set up our notation and write the Dyson equation for the problem. In Sec. II, we reduce this equation to a single integral equation after integrating over all spatial variables; we then solve this equation approximately by a suitable iteration process in the case of electron-phonon interaction only and within the frame of the Einstein model; we find that the corresponding gap equation is identical to the BCS equation. It has been known since the work of Bogoliubov[6] that the screened Coulomb interaction acts to a degree like a hard core, at least in the instantaneous interaction model previously used, and so is quite ineffective in weakening the phonon-induced attraction. In Sec. III, we find that this result does indeed hold in our time-dependent treatment; adding an essentially instantaneous repulsive potential to the retarded phonon-induced potential, we solve the integral gap equation to find identically Bogoliubov's result. All the above results are derived in the case where the phonon spectrum reduces to a single frequency. We investigate in Sec. IV the effect of the spreading of this spectrum about one central frequency and we find closely similar results (identical in the weak-coupling limit) thereby justifying *a posteriori* our use of the Einstein model. Finally (Sec. V), we derive the expression for the isotope effect and we compute the transition temperatures for nontransition metals. Unfortunately, as in the calculation of Swihart,[7] the exponent in the isotope effect is found to differ appreciably (10 to 20%) from the ideal value $\frac{1}{2}$, more in fact than the quoted errors of the present experimental data. On the other hand, we find a general order-of-magnitude agreement between the computed and measured transition temperatures better than that of Morel.[3]

I. THE DYSON EQUATION

Following closely the notation of Gor'kov and Eliashberg,[4] we define the Green's function $G(x-x')$ describing the propagation of an ordinary single particle:

$$G(x-x')=i\langle T\psi_+(x)\psi_+^*(x')\rangle=i\langle T\psi_-(x)\psi_-^*(x')\rangle, \quad (1)$$

as well as the Green's function $F(x-x')$ describing the merging of two particles into the condensed phase or the inverse process (i.e., the creation or the destruction of a "ground pair"):

$$\begin{aligned} F(x-x')&=ie^{i\mu(t+t')}\langle T\psi_+(x)\psi_-(x')\rangle \\ &=ie^{-i\mu(t+t')}\langle T\psi_-^*(x)\psi_+^*(x')\rangle, \end{aligned} \quad (2)$$

where the last equality is obtained by time reversal (provided we use a representation in which the state vectors are invariant under this transformation). Here x stands for the four-vector $\mathbf{x}$, t and T is the usual time ordering operator (see reference 4). The average in (1) is taken in the ground state $|\varphi_0(N)\rangle$ corresponding to a total number N of particles; the averages in (2) are taken between the ground states $|\varphi_0(N)\rangle$ and $|\varphi_0(N\pm2)\rangle$. Lumping together in ϵ_k the kinetic energy of a single particle and the mass correction due to the self-energy in the normal fluid, we may write the Dyson equations in momentum space:

$$\begin{aligned} G(\mathbf{k},\omega)&=-\frac{\omega+\epsilon_k}{\omega^2-\epsilon_k^2-\Sigma^2(\mathbf{k},\omega)+i\delta}, \\ F(\mathbf{k},\omega)&=\frac{\Sigma(\mathbf{k},\omega)}{\omega^2-\epsilon_k^2-\Sigma^2(\mathbf{k},\omega)+i\delta}, \end{aligned} \quad (3)$$

where $\Sigma(\mathbf{k},\omega)$ is the self-energy corresponding to the processes in which two particles either merge into the condensed phase or emerge from it. This self-energy plays the part of the "energy gap" of BCS theory since the energy spectrum of the individual excitations of the condensed fluid is now given, in the low-energy limit, by

$$E_k=[\epsilon_k^2+\Sigma^2(\mathbf{k},0)]^{\frac{1}{2}}. \quad (4)$$

$\Sigma(\mathbf{k},\omega)$ is related to the propagator $F(\mathbf{k},\omega)$ by

$$\Sigma(\mathbf{k},\omega)=\frac{i}{(2\pi)^4}\int\Gamma(\mathbf{k}-\mathbf{k}', \omega-\omega')F(\mathbf{k}',\omega')d^3\mathbf{k}'d\omega', \quad (5)$$

where Γ is the exact vertex part, i.e., the sum of the contributions of all possible interaction processes or combinations of elementary electron-phonon inter-

[6] N. N. Bogoliubov, V. V. Tolmachev, and D. V. Shirkov, *A New Method in the Theory of Superconductivity* (1958) (translation: Consultants Bureau, Inc., New York, 1959).

[7] J. C. Swihart, Phys. Rev. **116**, 45 (1959).

action:

$$H_{\text{el-ph}}=-i\sum_{\mathbf{k}\mathbf{k}'}\left(\frac{N}{M}\right)^{\frac{1}{2}}\frac{ZqV(q)}{[2\omega_{\mathbf{q}}]^{\frac{1}{2}}}(b_{\mathbf{q}}+b_{-\mathbf{q}}^*)c_{\mathbf{k}'}^*c_{\mathbf{k}}$$
$$=i\sum_{\mathbf{k}\mathbf{k}'}\alpha_{\mathbf{q}}(b_{\mathbf{q}}+b_{-\mathbf{q}}^*)c_{\mathbf{k}'}^*c_{\mathbf{k}}, \quad (6)$$

and direct Coulomb interaction:

$$H_{\text{Coul}}=\sum_{\mathbf{k},\mathbf{k}',\mathbf{K}}V(\mathbf{k}'-\mathbf{k})c_{\mathbf{k}'}^*c_{\mathbf{K}-\mathbf{k}'}^*c_{\mathbf{K}-\mathbf{k}}c_{\mathbf{k}}. \quad (7)$$

In the above expressions, N, M, and Z are, respectively, the number of ions per unit volume, the mass, and the valency of the ions; $b_{\mathbf{q}}$ ($b_{\mathbf{q}}^*$) and $c_{\mathbf{k}}$ ($c_{\mathbf{k}}^*$) are the usual annihilation (creation) operators of the phonon and electron fields, respectively; $V(q)$ is the Fourier transform of the screened electrostatic potential:

$$V(q)=\frac{4\pi e^2}{q^2+k_s^2}=\frac{4\pi e^2}{q^2+4\pi e^2N_0}, \quad (8)$$

where k_s^{-1} is the screening radius (for the Fermi-Thomas model, k_s^2 is proportional to the density of states N_0 on the Fermi surface). Finally, let us remark that the phonon momentum $\mathbf{q}$ appearing in Eq. (6) is equal to $(\mathbf{k}'-\mathbf{k})$ only if this vector happens to be in the first Brillouin zone (normal process). In general, $\mathbf{q}$ is a function of the vector $(\mathbf{k}'-\mathbf{k})$ given by the momentum conservation relation:

$$\mathbf{q}=\mathbf{k}'-\mathbf{k}+\mathbf{K}_N, \quad (9)$$

where $\mathbf{K}_N$ is a suitable vector of the reciprocal lattice. It must be clearly stated that the summation in (6) extends over all $\mathbf{k}$ and $\mathbf{k}'$ near the Fermi surface, since, because of the periodicity of the crystal, the deformation potential caused by the phonon of momentum $\mathbf{q}$ has nonvanishing matrix elements not only for scattering from the electron state $\mathbf{k}$ to the state $\mathbf{k}'$ such that:

$$\mathbf{k}'-\mathbf{k}=\mathbf{q},$$

but also to the states $\mathbf{k}'$ satisfying the more general condition (9). Because of the deformation potential theorem, the matrix element is approximately the same whether the scattering is a normal or an "umklapp" process, for a given $\mathbf{q}$.

Now, we shall restrict the vertex part Γ to its lowest order terms only, i.e., the sum of

$$D_0(\mathbf{q},\omega)=\alpha_{\mathbf{q}}^2\left[\frac{1}{\omega_{\mathbf{q}}-\omega-\eta_{\mathbf{q}}}+\frac{1}{\omega_{\mathbf{q}}+\omega-\eta_{\mathbf{q}}}\right]=\frac{2\alpha_{\mathbf{q}}^2}{\omega_{\mathbf{q}}}u_{\mathbf{q}}(\omega), \quad (10)$$

and $-V(q)$ for the phonon induced and Coulomb interactions respectively. Here $\omega_{\mathbf{q}}$ and $\eta_{\mathbf{q}}$ are the real and imaginary parts of the frequency of the phonon of momentum $\mathbf{q}$. Since the phonon damping is rather small ($\eta_{\mathbf{q}}$ is usually of the order of $10^{-2}\omega_{\mathbf{q}}$), the frequency dependent factor $u_{\mathbf{q}}(\omega)$ may be written:

$$u_{\mathbf{q}}(\omega)=P\left[\frac{\omega_{\mathbf{q}}^2}{\omega_{\mathbf{q}}^2-\omega^2}\right]+\frac{i\pi}{2}\omega_{\mathbf{q}}[\delta(\omega+\omega_{\mathbf{q}})-\delta(\omega-\omega_{\mathbf{q}})]. \quad (11)$$

It has been shown by Migdal[8] that this simplification is acceptable for the phonon-electron interaction since higher-order terms are of the order of $(M)^{-\frac{1}{2}}$ or smaller. We have approximated the exact Coulomb interaction by an instantaneous potential, neglecting high-order retarded polarization terms: This is perfectly acceptable since dispersion occurs only at rather high frequencies of the order of the plasma frequency and is completely negligible in the small energy range we are considering here. We are also neglecting mixed terms corresponding to a combination of phonon exchange and Coulomb interactions: These terms are certainly smaller than $(M)^{-\frac{1}{2}}$. The gap equation (5) together with (3) and (10) constitutes therefore the mathematical formulation of the problem. We shall now be concerned with simplifying and solving this equation in the perspective outlined in the introduction.

II. SOLUTION OF THE GAP EQUATION FOR ELECTRON PHONON COUPLING ONLY

We shall first neglect the Coulomb repulsion altogether and consider only the contribution $D_0(q,\omega)$ to the vertex part Γ. The gap equation then becomes

$$\Sigma(\mathbf{k},\omega)=\frac{i}{(2\pi)^4}\int\frac{2\alpha_{\mathbf{q}}^2}{\omega_{\mathbf{q}}}u_{\mathbf{q}}(\omega-\omega')F(\mathbf{k}',\omega')k'^2\times\sin\theta'd\theta'd\varphi'dk'd\omega', \quad (12)$$

where $F(\mathbf{k},\omega)$ depends only upon the kinetic energy:

$$\epsilon_k=v_0(k-k_0). \quad (13)$$

(v_0 is the velocity of the electrons on the Fermi level) and $\mathbf{q}$ is given by (9). Since F vanishes rapidly[9] when $\mathbf{k}'$ is allowed to depart from the Fermi surface, we may replace the integration over $\mathbf{k}'$ by integration over the energy and the angular variables. Moreover, we see from (6) that

$$\frac{2\alpha_{\mathbf{q}}^2}{\omega_{\mathbf{q}}}=\frac{NZ^2}{Mc^2}\left[\frac{4\pi e^2}{k_s^2+q^2}\right]^2=\frac{1}{N_0}\left[\frac{k_s^2}{k_s^2+q^2}\right]^2. \quad (14)$$

We have made use of the standard expression for the velocity of sound (see reference 3). Note that this factor is almost independent of q, so that we may replace q^2 by a mean value of the order of the square or the Debye momentum (more precisely $\frac{3}{5}q_D^2$). The factor

[8] A. B. Migdal, J. Exptl. Theoret. Phys. (U.S.S.R) **34**, 1438 (1958). [Translation: Soviet Phys.—JETP **7**, 996 (1958).]

[9] The q^{-2} dependence of $\Gamma(q,\omega)$ insures the convergence of the original equation (5). Replacing the integration over k' by integration over ϵ' may, however, introduce an artificial divergence in the case of an instantaneous interaction. We shall in this case cut off the energy integration at the Fermi energy.

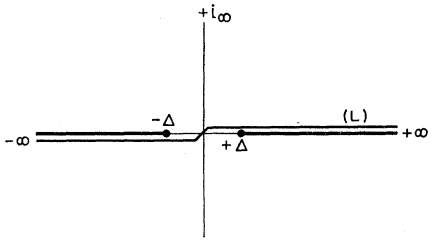

FIG. 1. Contour of integration (L) in the complex (z) plane for Eq. (18). Note that (L) does not cross the branch line of the function $D(z)$ on the real axis (heavy line).

$u_{\mathbf{q}}(\omega-\omega')$ is strongly dependent upon the phonon frequency $\omega_{\mathbf{q}}$. For polyvalent metals, however, the relation between $\omega_{\mathbf{q}}$ and the vector $(\mathbf{k}'-\mathbf{k})$ is quite complicated, so that the angular average of (12) requires a complicated procedure taking into account the structure of the crystal (see Morel, reference 3). On the other hand, since we expect $\Sigma(\mathbf{k},\omega)$ to be essentially independent of $\mathbf{k}$, we may average (12) over all $\mathbf{k}$ in the energy shell. This is equivalent to averaging $u_{\mathbf{q}}(\omega-\omega')$ over the phonon spectrum (all phonon momenta are roughly equiprobable). This approximation, which is akin to the spirit of BCS theory, is of course self-consistent since it removes all $\mathbf{k}$ dependence in the right-hand side of (12); it amounts simply to assuming that the gap is isotropic, which has been shown to be approximately correct from an experimental point of view.[10] We obtain then

$$\Sigma(\omega)=\frac{i\lambda}{2\pi}\int d\epsilon'\int d\omega'\,F(\epsilon',\omega')U(\omega-\omega'), \tag{15}$$

where λ is a parameter which plays the role of the "N_0V" of BCS:

$$\lambda=\tfrac{1}{2}\left[\frac{k_s^2}{k_s^2+\frac{3}{5}q_D^2}\right]^2, \tag{16}$$

and $U(\omega)$ is the average of the phonon propagator $u_q(\omega)$ over the phonon spectrum, represented by the distribution function $g(\omega_q)$:

$$U(\omega)=\int_0^{\omega_{\max}} u_q(\omega)g(\omega_q)d\omega_q. \tag{17}$$

It is worthwhile to pause at this point and remark that λ is not directly proportional to the density of states on the Fermi surface N_0 as the analogy with BCS's expression N_0V tends to suggest. The dependence of λ upon N_0 enters only through k_s^2 and we find particularly that however large N_0 may be or however complicated the structure of the crystal may be $[\langle q^2\rangle_{\text{av}}\ll q_D^2]$, the value of this parameter cannot exceed $\frac{1}{2}$.

Restricting ourselves for the time being to the Einstein model, i.e., to the case where the phonon spectral distribution function g reduces to a single δ function centered at $\omega_q=\omega_1$, we shall proceed to integrate (15) over the energy. Before doing so, however, we write this equation in the equivalent form:

$$\Sigma(\omega)=\frac{i\lambda}{2\pi}\int_{(L)}dz\int_{-\infty}^{+\infty}d\epsilon'\frac{\Sigma(z)}{D^2(z)-\epsilon^2}U(\omega-z), \tag{18}$$

$$D(z)=[z^2-\Sigma^2(z)]^{\frac{1}{2}}. \tag{19}$$

Note that $D(z)$ retains the same determination when z follows the contour (L) represented in Fig. 1. If we choose the determination in the upper half of the complex plane, we obtain in a straightforward fashion:

$$\Sigma(\omega)=\lambda\int_{(L)}\frac{\omega_1}{2}\left[\frac{1}{\omega_1-z+\omega-i\eta}+\frac{1}{\omega_1+z-\omega-i\eta}\right]\frac{\Sigma(z)}{2D(z)}dz. \tag{20}$$

As we expect from the time-reversal invariance of F and V, this equation is compatible with an even solution on the real axis. On the other hand, the detailed features of the solution do not appear clearly. It is, therefore, illuminating to go back temporarily to the time representation of relations (3) and (18):

$$F(\mathbf{k},t)\simeq[\Sigma(E_{\mathbf{k}})/2E_{\mathbf{k}}]e^{iE_{\mathbf{k}}t},$$
$$\Sigma(t)=\lambda U(t)C(t)=\lambda U(t)\int_{-\infty}^{+\infty}F(\mathbf{k}',t)d\epsilon'. \tag{21}$$

The oscillating time dependence of the integrand is smeared out by the integration and $C(t)$ is a rather slowly varying function of time (see Sec. IV) so that the resulting $\Sigma(t)$ behaves essentially like $U(t)$. Consequently, we expect that the solution of the integral equation (20), may be approximately proportional to $U(\omega)$. In order to test this possibility, we shall try to solve it by iteration, starting from the trial function:

$$\Sigma_1(\omega)=\Delta U(\omega),$$
$$\Sigma_2(\omega)=\lambda\Delta\int_0^{\Delta}\frac{U(z)U(\omega-z)dz}{i[\Delta^2-z^2]^{\frac{1}{2}}}+\int_{\Delta}^{\infty}\frac{U(z)U(\omega-z)dz}{[z^2-\Delta^2]^{\frac{1}{2}}}, \tag{22}$$

where we have taken advantage of the smallness of $\Sigma(\omega)$ to replace it by the constant $\Sigma(0)=\Delta$ in the expression for $D(z)$. These integrals cannot be computed with any accuracy near the singularity $\omega\simeq\omega_1$; however, in the regions both above and below this singularity, the integration can be carried out approximately and

[10] P. W. Anderson, Ph. D. thesis, unpublished.

one finds:

$$\Sigma_2(\omega)=\lambda\Delta[\ln(2\omega_1/\Delta)U(\omega)+\tfrac{3}{4}(1-i\pi/2)\omega/\omega_1+O(\omega^3)], \quad \omega\ll\omega_1,$$
$$\Sigma_2(\omega)=\lambda\Delta[\ln(2\omega_1/\Delta)U(\omega)-i\pi(\omega_1^3/\omega^3)+O(1/\omega^4)], \quad \omega\gg\omega_1. \tag{23}$$

This expression is reasonably similar to the trial function $\Sigma_1(\omega)$ and, indeed, converges toward Σ_1 in the weak coupling limit ($\lambda\ll1$) if the value of the gap $\Sigma(0)=\Delta$ satisfies the following condition:

$$1/\lambda=\ln(2\omega_1/\Delta), \tag{24}$$

identical to the BCS gap equation. Finally, let us note, for further reference, that $\Sigma_2(0)$ is real and also that $\Sigma_2(\omega)$ has no singularity at $\omega=2\omega_1$ although its complete analytical expression includes the term:

$$\frac{\lambda\Delta\omega_1^3}{2\omega(\omega-2\omega_1+2i\eta)}\left[i\pi\left(\frac{1}{\omega-\omega_1}-\frac{1}{\omega_1}\right)+\frac{1}{\omega-\omega_1}\ln\left|\frac{\omega-\omega_1}{\Delta}\right|-\frac{1}{\omega_1}\ln\left(\frac{\omega_1}{\Delta}\right)\right],$$

which corresponds to a pole with a vanishing residue.

III. SOLUTION OF THE GAP EQUATION INCLUDING THE COULOMB INTERACTION

On account of the reasonable success of the above scheme, we wish to extend it to solve the gap equation including the Coulomb repulsion $-V(q)$. Since Eq. (5) is linear with respect to the vertex part Γ, the introduction of the essentially instantaneous Coulomb interaction is equivalent to adding a constant to the frequency-dependent potential, i.e., replace $\lambda U(\omega)$ by

$$U'(\omega)=\lambda U(\omega)-\mu, \tag{25}$$

where μ is the angular average of $V(q)$:

$$\mu=\frac{1}{4\pi^2v_0}\int_0^{2k_0}\frac{4\pi e^2}{k_s^2+q^2}qdq=\frac{k_s^2}{8k_0^2}\ln\left[\frac{k_s^2+4k_0^2}{k_s^2}\right]. \tag{26}$$

We are looking for a solution displaying the general behavior of $U'(\omega)$ and more precisely, we shall start the iteration process with the trial function:

$$\Sigma_1'(\omega)=\Delta[(1+\xi)U(\omega)-\xi], \tag{27}$$

with two adjustable parameters Δ and ξ. We have then

$$\Sigma_2'(\omega)=\Delta\int_0^{\Delta}\frac{[(1+\xi)U(z)-\xi][\lambda U(\omega-z)-\mu]}{i[\Delta^2-z^2]^{\frac{1}{2}}}dz+\int_{\Delta}^{\epsilon_F}\frac{[(1+\xi)U(z)-\xi][\lambda U(\omega-z)-\mu]}{[z^2-\Delta^2]^{\frac{1}{2}}}dz. \tag{28}$$

Note that we have introduced a cutoff of the order of the Fermi energy in the last integral in order to prevent the logarithmic divergence due to the constant term $\xi\mu$ in the numerator of the integrand (see footnote 9). As before, these integrals cannot be computed near the singularity $\omega\approx\omega_1$ but we obtain the following expressions for $\Sigma_2'(\omega)$ in the low- and high-frequency limits, respectively:

$$\Sigma_2'=\Delta[\lambda\ln(2\omega_1/\Delta)-(1+\xi)\mu\ln(2\omega_1/\Delta)+\xi\mu\{\ln(2\epsilon_F/\Delta)-i\pi/2\}+(\omega/\omega_1)\{\tfrac{3}{4}\lambda(1+\xi)(1-i\pi/2)+(i\pi/2)\xi\lambda\}+O(\omega^2)], \quad \omega\ll\omega_1,$$
$$\Sigma_2'=-\Delta[\mu(1+\xi)\ln(2\omega_1/\Delta)-\xi\mu\{\ln(2\epsilon_F/\Delta)-i\pi/2\}+i\pi\lambda\xi\omega_1/\omega+O(1/\omega^2)], \quad \omega\gg\omega_1. \tag{29}$$

Although (27) and (29) are not as accurately self-consistent as (22) and (23) in the previous section,[11] Σ_2' does indeed converge towards Σ_1' in the weak-coupling limit ($\lambda,\mu\ll1$). In this limit, the adjustable parameters Δ and ξ must satisfy

$$(\lambda-\mu)\ln(2\omega_1/\Delta)+\mu\xi\ln(\epsilon_F/\omega_1)=1,$$
$$\mu\ln(2\omega_1/\Delta)-\mu\xi\ln(\epsilon_F/\omega_1)=\xi. \tag{30}$$

Hence,

$$\ln\left(\frac{2\omega_1}{\Delta}\right)=\left[\lambda-\frac{\mu}{1+\mu\ln(\epsilon_F/\omega_1)}\right]^{-1}. \tag{31}$$

This relation is identical to the equation found by Bogoliubov and coworkers[6] using a similar model, with the difference that the cutoff ω_1 of the phonon-induced interaction and the cutoff ϵ_F of the instantaneous Coulomb repulsion appear now as the consequence of the frequency dependence of these interactions rather than as arbitrary cutoffs in momentum space of an effective instantaneous interaction. The effect of the Coulomb repulsion is indeed a reduction of the parameter "N_0V" as expected but we find also that the Coulomb repulsion is somewhat less effective than the phonon-induced attraction on account of its instantaneous character {μ appears in reference 6, Eq. (3.7) reduced by the factor $[1+\mu\ln(\epsilon_F/\omega_1)]^{-1}$ of the order of 0.4}.

IV. EFFECT OF THE FINITE RANGE OF THE PHONON SPECTRUM

The actual phonon spectrum of a solid extends over a finite range, the width $2\omega_2$ of which may be a significant fraction of the Debye frequency (of the order of 20% for example). Accordingly, we see from (17) that the singularities of the average phonon induced interaction $U(\omega)$ are spread over the same range and therefore, $U(\omega)$ is much smoother than its components $u_q(\omega)$. Equivalently, $U(t)$ has only a rather short range in time, of the order of ω_2^{-1}, since the components $u_q(t)$ interfere destructively if the time interval t is of the

[11] The most striking deficiency is the appearance of an imaginary term $-i(\pi/2)\xi\mu$ in the zero-order term of the expansion (29). It is likely that this imaginary term (negligible in the weak-coupling limit) is spurious and due to our introducing an artificially sharp cutoff of the term proportional to $\xi\mu$ at the Fermi energy.

order of ω_2^{-1} or larger. This may be best demonstrated by taking a simple model for the phonon spectrum, namely a Lorentz distribution:

$$g(\omega_q)=\frac{1}{\pi}\frac{\omega_2}{(\omega_q-\omega_1)^2+\omega_2^2}. \tag{32}$$

Note that this mathematically simple model is still a reasonably accurate approximation of the "well-behaved" phonon spectra found for a rather large class of metals. It would not be a satisfactory approximation for multi-peaked spectra observed in some instances. The corresponding phonon-induced interaction is found immediately to be

$$U(t)=\tfrac{1}{2}(\omega_1-i\omega_2)e^{-i\omega_1|t|}e^{-\omega_2|t|},$$
$$U(\omega)=\tfrac{1}{2}(\omega_1-i\omega_2)\left[\frac{1}{\omega_1+\omega-i\omega_2}+\frac{1}{\omega_1-\omega-i\omega_2}\right]. \tag{33}$$

Note the rapid damping due to the large imaginary part of the pseudo-phonon frequency $(\omega_1-i\omega_2)$. Because $U(\omega)$ is actually smoother than $u_q(\omega)$, one sees physically that the actual solution of (20) should be smoother than (27). However, the computation scheme used in the previous sections is not suited for this generalization because it relies upon the sharpness of the singularity of $u_q(\omega)$. We shall, therefore, take a different approach to the problem, involving the transformation of Eq. (20) to the time representation (21).

Our iteration procedure now consists in the following steps. Firstly, we choose a trial function

$$\Sigma_1(\omega)=\Delta[(1+\xi-\zeta)U(\omega)+\zeta A(\omega)-\xi], \tag{34}$$

where Δ, ξ, and ζ are adjustable parameters and $A(\omega)$ an even function of the frequency, smoothly decreasing from 1 at $\omega=0$ to zero at $\omega=\pm\omega_1$. Secondly, we carry (34) into the expression for $C(t)$:

$$C(t)=C(-t)=\int_{(L)}\frac{\Sigma_1(z)}{2D(z)}e^{-izt}dz. \tag{35}$$

Thirdly, we compute $\Sigma_2(t)$ according to relation (21):

$$\Sigma_2(t)=[\lambda U(t)-\mu\delta(t)]C(t), \tag{36}$$

and finally, we shall Fourier-transform the resulting expression for Σ_2 in order to compare it to the initial Σ_1. In the course of this program, however, we shall need to make some approximations, the most important of which is described below.

Since expression (35) is practically linear with respect to Σ [we may replace $\Sigma(z)$ by $\Sigma(0)=\Delta$ in the expression for $D(z)$], the three terms of (34) contribute, respectively,

$$(1+\xi-\zeta)C_1(t),\quad \zeta C_2(t),\quad -\xi C_3(t),$$

to the final expesstion of $C(t)$. The most important term is the first one and is found to be (for positive t):

$$C_1(t)=\Delta[\ln 2-\mathrm{Ci}(\Delta t)]+\Delta[\cos(\omega_1 t)\,\mathrm{Ci}(\omega_1 t)+\sin(\omega_1 t)\{\mathrm{Si}(\omega_1 t)-\pi/2\}]-i(\pi/2)\Delta+i(\pi/2)\Delta e^{-i(\omega_1-i\omega_2)t}, \tag{37}$$

where $\mathrm{Si}(z)$ and $\mathrm{Ci}(z)$ are the sine and cosine integral functions. In spite of its appearance, the second bracket is a perfectly smooth function of t, increasing monotonically from $-\infty$ at $t=0$ [logarithmic divergence, of the order of $\ln(\omega_1 t)$] and approaching zero like $-(\omega_1 t)^{-2}$ for large t. Consequently, this function is very accurately approximated by

$$\ln(e^{\gamma}\omega_1 t)-\tfrac{1}{2}\ln(1+e^{2\gamma}\omega_1^2 t^2).$$

Both the third and the fourth terms are imaginary and we notice that the latter introduces a correction proportional to $\exp[-2i(\omega_1-i\omega_2)t]$ in the expression for $\Sigma_2(t)$ or equivalently a pole at $2(\omega_1-i\omega_2)$ in the corresponding expression for $\Sigma_2(\omega)$. Moreover, this extra term will in turn bring about corrections at $3\omega_1$, $4\omega_1$, etc., upon iteration. Our intent is, of course, to neglect these high-energy corrections (which are quite small in the weak-coupling limit) but we must not overlook the fact that the corrections at $2\omega_1$, $4\omega_1$, $6\omega_1$, $\cdots$ bring small imaginary contributions which ultimately cancel the imaginary contribution of the third term $-i(\pi/2)\Delta$ of (37) [for $\Sigma_2(\omega)$ is the average of (29) with respect to the phonon frequency and, therefore, $\Sigma_2(0)$ must be real]. In order to be consistent, we shall therefore neglect both imaginary terms of (37) and retain only

$$C_1(t)\simeq\Delta[\ln(2\omega_1/\Delta)-\tfrac{1}{2}\ln(1+e^{2\gamma}\omega_1^2 t^2)],\ 0<t<\Delta^{-1}. \tag{38}$$

Here γ is the Euler constant. Similarly, the second term of (34) is cut off at a frequency of the order of $\frac{1}{2}\omega_1$ and therefore

$$C_2(t)\simeq\Delta[\ln 2-\mathrm{Ci}(\Delta t)+\mathrm{Ci}(\tfrac{1}{2}\omega_1 t)]\simeq\Delta[\ln(\omega_1/\Delta)-\tfrac{1}{2}\ln(1+\tfrac{1}{4}e^{2\gamma}\omega_1^2 t^2)]. \tag{39}$$

Finally, the last term of (34) is cut off at a frequency of the order of the Fermi energy; thus:

$$C_3(t)\simeq\Delta[\ln 2-\mathrm{Ci}(\Delta t)+\mathrm{Ci}(\epsilon_F t)]\simeq\Delta[\ln(2\epsilon_F/\Delta)-\tfrac{1}{2}\ln(1+e^{2\gamma}\epsilon_F^2 t^2)]. \tag{40}$$

Collecting terms and performing the required Fourier transformation, we obtain the expression for $\Sigma_2(\omega)$ in the three regions: $\omega\simeq 0$, $\omega\simeq\omega_1$, and $\omega\gg\omega_1$, respectively:

$$\Sigma_2''(\omega)_{\omega\approx 0}=\lambda\Delta[\ln(2\omega_1/\Delta)+0.23(1+\xi)+0.14\zeta]-\mu\Delta[\ln(2\omega_1/\Delta)-\zeta\ln 2-\xi\ln(\epsilon_F/\omega_1)],$$
$$\Sigma_2''(\omega)_{\omega\approx\omega_1}=\lambda\Delta U(\omega)[\ln(2\omega_2/\Delta)+0.28+0.12\xi+0.12\zeta]-\mu\Delta[\ln(2\omega_1/\Delta)-\zeta\ln 2-\xi\ln(\epsilon_F/\omega_1)], \tag{41}$$
$$\Sigma_2''(\omega)_{\omega\to\infty}=-\mu\Delta[\ln(2\omega_1/\Delta)-\zeta\ln 2-\xi\ln(\epsilon_F/\omega_1)].$$

Adjusting Δ, ξ, and ζ to fit Σ_2 and Σ_1 in these regions, we find the following self-consistency condition:

$$\ln\left(\frac{2\omega_1}{\Delta}\right)=\left[\frac{\lambda}{1-0.23\lambda}-\frac{\mu}{1+\mu\ln(\epsilon_F/\omega_1)}\right]^{-1}, \quad (42)$$

almost identical to (31). Note that the phonon-induced interaction (attraction) is enhanced by the factor $(1-0.23\lambda)^{-1}$ typically of the order of 1.05 to 1.1. This close similarity with the results of Sec. III justifies *a posteriori* our use of the simplified Einstein model; this also encourages us to place actual numbers on the parameters λ and μ and compute the corresponding transition temperature. We have plotted the self-consistent "gap-function" $\Sigma_2(\omega)$ for the typical case $\lambda=0.3$, $\mu=0.25$, $\omega_2=\omega_1/5$ and $\ln(\epsilon_F/\omega_1)=6$ (Fig. 2). Note the striking similarity with the simple model of BCS and Bogoliubov, i.e., a constant gap, cutoff at $\omega=\omega_1$.

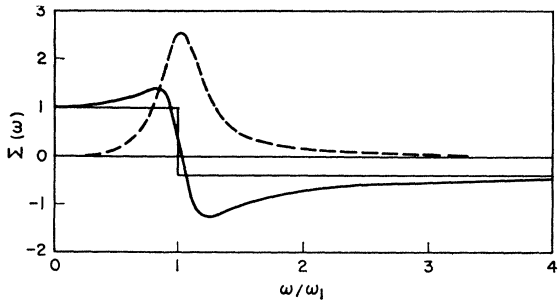

FIG. 2. Plot of the self-consistent energy-dependent "gap function" $\Sigma(\omega)$ for typical values of the parameter. The full line and the dashed line represent the real and imaginary part of $\Sigma(\omega)$, respectively. The step function represents the gap function used by Bogoliubov (equal to 1 from 0 to ω_1 and to $-\xi$ from ω_1 to the Fermi energy).

V. TRANSITION TEMPERATURE AND ISOTOPE EFFECT

It is interesting at this point to use our model to evaluate the critical temperature (or rather the corresponding "N_0V") for some well-behaved metals and compare our predictions with experimental data. Firstly, we notice that the two most important parameters characterizing the electronic behavior of metals, i.e., the electron density (or Fermi momentum) and the density of individual states on the Fermi level, enter the expressions for λ and μ only through the combination:

$$a^2=k_s^2/4k_0^2=4\pi e^2N_0/4k_0^2. \quad (43)$$

We may compute both k_0 and N_0 for the Fermi-Thomas model from the interelectron spacing (obtained from basic crystallographic data). Now, the actual density of states on the Fermi surface is the Fermi-Thomas value corrected for the effective mass (which in turn is estimated from specific-heat measurements). From (26), it is clear that

$$\mu=\tfrac{1}{2}\ln[(1+a^2)/a^2]. \quad (44)$$

On the other hand, we have not accurately computed the angular average of the strength of the phonon-induced interaction because of the complication brought by the existence of Umklapp processes; we have, rigorously,

$$\lambda=\int_0^1\left[\frac{a^2}{a^2+q^2/4k_0^2}\right]^2 x\,dx, \quad (45)$$

where $x=|\mathbf{k}-\mathbf{k}'|/2k_0$ is equal to $q/2k_0$ only for normal processes. For alkali metals, it is indeed a fair approximation to neglect the effect of umklapp processes and take

$$\lambda\simeq\int_0^1\left[\frac{a^2}{a^2+x^2}\right]^2 x\,dx=\frac{1}{2}\frac{a^2}{1+a^2}. \quad (46)$$

For polyvalent metals, however, the umklapp processes play an important role and it is preferable to replace $q^2/4k_0^2$ by the mean value over the first Brillouin zone. For metals with a simple structure (quasi-spherical zone), this mean value is of the order of $\frac{3}{5}(4Z)^{-\frac{2}{3}}$; then

$$\lambda\simeq\frac{1}{2}\left[\frac{a^2}{a^2+\frac{3}{5}(4Z)^{-\frac{2}{3}}}\right]^2. \quad (47)$$

Now, it must be emphasized that the above expression is no more than an order of magnitude estimate of λ; for, we have not taken into account any effect of the crystalline structure although it is clear that it determines the mean value of $q^2/4k_0^2$. Also, (47) is based on the assumption that the screening radius of the electron-ion interaction is the same as the screening radius of the direct Coulomb interaction between electrons and may be estimated on the basis of the Fermi-Thomas model. This assumption is very much open to doubt, particularly for the heaviest ions. In any case, it may be seen from Table I that this simple model leads to a fair order of magnitude agreement between the "N_0V" estimated from experimental data using the BCS expression for the critical temperature and our parameter:

$$\lambda-\mu^*=\lambda-\frac{\mu}{1+\mu\ln(\epsilon_F/\omega_1)}, \quad (48)$$

computed from basic crystallographic and thermal data.

We have also plotted both parameters λ and μ^* versus a^2 for monovalent, bivalent, and tetravalent metals [using a typical value $\ln(\epsilon_F/\omega_1)=6$]. Since a^2 is always of the order of 0.3 or larger (0.8 to 1 for alkali metals), this plot indicates that most if not all metals should be superconducting (see Fig. 3). On the other hand, the computed critical temperature is exceedingly low if $(\lambda-\mu^*)$ is smaller than 0.15, say. For example, the critical temperature of sodium would be of the order of 10^{-3} °K; it is then safe to assume that even if perfectly pure sodium were superconducting at such low temperatures in zero magnetic field,

TABLE I. In this table, a^2 is computed from crystallographic data and m^*/m is estimated from the electronic specific heat. These data, as well as the Debye temperature and the critical temperature (columns 3 and 4) are taken from the "*American Institute of Physics Handbook*," McGraw-Hill, 1957. N_0V (column 8) is estimated from the critical temperature with the help of BCS equation. The exponent of the isotope effect (last column) is derived from this experimental value of N_0V with the help of relation (50).

	a^2	m^*/m	Θ_D(°K)	T_c(°K)	λ	μ^*	$\lambda-\mu^*$	N_0V_{exp}	$-(d\Delta/\Delta)(M/dM)$
Na	0.67	1.6	160	···	0.25	0.12	0.13	···	···
K	0.83	···	100	···	0.25	0.12	0.13	···	···
Cu	0.45	1.15	343	···	0.20	0.10	0.10	···	···
Au	0.51	1.1	164	···	0.18	0.10	0.08	···	···
Mg	0.45	1.3	342	···	0.32	0.12	0.20	···	···
Ca	0.55	0.75	220	···	0.27	0.11	0.16	···	···
Zn	0.39	0.9	235	0.9	0.25	0.09	0.16	0.18	0.35
Cd	0.43	0.75	164	0.56	0.23	0.09	0.14	0.175	0.34
Hg	0.43	2	70	4.16	0.37	0.10	0.27	0.35	0.46
Al	0.35	1.5	375	1.2	0.33	0.10	0.23	0.175	0.34
In	0.40	1.35	109	3.4	0.34	0.10	0.24	0.29	0.44
Tl	0.415	1.15	100	2.4	0.32	0.09	0.23	0.27	0.43
Sn	0.37	1.2	195	3.75	0.34	0.10	0.24	0.25	0.42
Pb	0.38	2.1	96	7.22	0.40	0.10	0.30	0.39	0.47
Ti	0.32	≈3	430	0.4	0.41	0.11	0.30	0.14	0.25
Zr	0.51	1.1	265	0.55	0.37	0.11	0.26	0.16	0.30
V	0.28	≈9	338	4.9	0.47	0.12	0.35	0.24	0.41
Nb	0.29	≈8	320	8.8	0.47	0.12	0.35	0.32	0.45
Ta	0.29	≈5	230	4.4	0.45	0.11	0.34	0.25	0.42
Mo	0.27	1.9	360	···	0.38	0.10	0.28	···	···
U	0.30	8	200	1.1	0.47	0.12	0.35	0.19	0.36

the least residual field (magnetic impurities) would exceed the very small critical field and prevent superconductivity. This argument practically excludes all monovalent metals.

Finally, we notice that all experimental values of "N_0V" for metals appear to be smaller than 0.4 (see Table I) in good agreement with our prediction since μ^* is practically 0.10 in all cases and λ cannot exceed 0.5 (to the first order of the expansion in the electron-phonon interaction).

Isotope Effect

The isotope effect consists in the dependence of the energy gap Δ upon the phonon frequency ω_1 (the phonon frequency itself is proportional to $M^{-\frac{1}{2}}$, everything else being equal). Differentiating (31) with respect to the phonon frequency, we obtain in a straightforward fashion:

$$d\Delta/\Delta=-\tfrac{1}{2}(dM/M)\{1-[\lambda\ln(2\omega_1/\Delta)-1]^2\}. \quad (49)$$

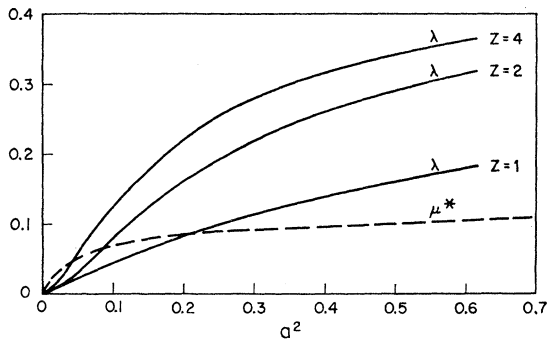

FIG. 3. Plot of the parameters λ and μ^* vs a^2 [see expressions (44) to (48)] for different valencies $Z=1$, 2, and 4.

Using the property $\mu^*=0.1$, we can derive from (49) a semiempirical relation:

$$d\Delta/\Delta=-\tfrac{1}{2}(dM/M)[1-0.01(N_0V)^{-2}], \quad (50)$$

indicating a significant discrepancy from the "ideal" value $-\frac{1}{2}(dM/M)$ postulated by BCS. Note that the discrepancy is larger for low temperature superconductors (see Table I).

VI. CONCLUSION

The positive aspect of our results is that they confirm the approximations to the effective potential made in the past, particularly Bogoliubov's approximation, and give a precise meaning to each parameter which can, therefore, in principle, be computed from the basic crystallographic data. Also, the orders of magnitude of the computed transition temperatures are generally satisfactory.

The negative features are, firstly, the isotope effect which is particularly in conflict with the results of Geballe and Matthias on zinc, secondly, the prediction that all metals should superconduct at sufficiently low temperatures, and thirdly, the fact that it is not obvious from the theory why no material with T_c higher than 18°K have yet been found. This last point is not really too disturbing since the drastic simplifications on which this theory is based could only be expected to be reasonable in the weak-coupling limit; in the strong-coupling case of high-transition-temperature superconductors, such effects as the phonon scattering lifetime and, in general, the complex diagrams which have been omitted from our Eq. (12), should be incorporated in the theory.

On the other hand, the first and second difficulties are of a more serious nature for they do occur in the weak-coupling limit. Because our results are essentially insensitive to the actual computation scheme [compare Eqs. (31) and (42), and also Eq. (6.21) of reference 6], we do not feel that our solution of the basic equation (5) could be in serious error, at least in the weak-coupling limit. Moreover, the predicted transition temperatures are not remarkably sensitive to the errors, or approximations, which do remain in our treatment, with the possible exception of the cases in which zone boundary perturbations are too extensive at the Fermi surface (such as Bi, Sb, $\cdots$), so that the free-electron Fermi sphere is a very poor approximation. This suggests strongly that the results derived here are exactly the logical conclusions of the original assumptions of the BCS theory. Consequently, what serious difficulties, such as the isotope effect, are to be found, seem to us to require either a new look at the basic assumptions of the theory, possibly using a different interaction taking into account more complex diagrams than the lowest order diagrams implicitly contained in the BCS's treatment, or re-examination of the experimental evidence.

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Effect of an Impurity Layer on Surface Waves*

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We study here the effects of a homogeneous impurity mass layer on the surface waves of a semi-infinite monatomic square lattice with nearest and next nearest neighbor central springs. In the long-wavelength limit the impurity layer does not alter the surface waves from those of a pure semi-infinite lattice. However, depending upon the ratio of the impurity mass to the host mass, and for wavelengths shorter than a critical wavelength, the long-wavelength surface wave may disappear and new surface waves with frequencies either higher or lower than the spectrum of the pure infinite lattice may appear. The relationship of this model to the analogous one- and three-dimensional problems is discussed. We expect this theory to be applicable to problems such as the effect of an oxide layer on the surface vibrations of a crystal.

I. INTRODUCTION

DURING the past several years a number of powerful experimental techniques for the study of the details of the vibration spectra of solids have become available. Specifically, analysis of the inelastic scattering of slow neutrons from crystals[1] has enabled plots of $\omega(\mathbf{k})$ (frequency as a function of wave number in a Brillouin zone) to be made in various directions in $\mathbf{k}$ space for many solids. Visscher[2] has discussed the application of the Mössbauer effect for similar determinations.

Along perhaps more conventional lines, Jacobsen[3] and Bömmel and Dransfeld[4] have produced strong microwave phonon beams in solids and plans exist for extending this technique to higher frequencies. One may therefore hope that an extension to infrared frequencies is not too far off. Changes in the velocities of propagation of elastic energy due to dispersion of both volume and surface waves could then be studied.

The existence of these high-frequency techniques makes it desirable to have a more detailed picture of the short-wavelength (dispersive) portion of the lattice vibration spectra of real crystals than was needed to interpret insensitive average properties such as the specific heat.

Various aspects of this problem have been studied by many authors: Montroll and Potts[5] and their collaborators and Lifshitz[6] and his collaborators have studied the nature of localized vibrational modes due to point impurities; Lax[7] and Cochran *et al.*[8] have clarified the nature of the dispersion of the volume

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