

(1972); M. A. Smithard and R. Dupree (unpublished).

⁴For a general discussion of the application of linear-response techniques to the many-electron system see,

for example, C. Kittel, *Quantum Theory of Solids*

(Wiley, New York, 1963), Chap. 6; S. Strässler, *Physik Kondensierten Materie* **10**, 219 (1969).

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Neutron Spectroscopy of Superconductors

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A complete understanding of the mechanism for superconductivity requires knowledge of the details of electrons, phonons, and their interactions, and can be summarized by the function $\alpha^2 F(\omega)$. This function is often very similar to the phonon density of states $F(\omega) = \sum \delta(\omega - \omega_Q)$, which can be derived from an analysis of neutron-scattering data. In this paper it is pointed out that the complete function $\alpha^2 F(\omega)$ is also (in principle) contained in neutron-scattering data if the intrinsic linewidth γ_Q is measured as well as the dispersion relation ω_Q . It is shown that $\alpha^2 F$ differs from F by having a weighting factor $2\gamma_Q/\pi N(0)\omega$ inside the summation, where $N(0)$ is the electronic density of states at the Fermi surface for both spin orientations. The dimensionless coupling constant λ can also be expressed in terms of $N(0)$, ω_Q , and γ_Q . In practice, for most superconductors, the average widths γ_Q are smaller than presently available resolution. However, for materials with a high density of states like β -W superconductors, the widths γ_Q may be measurable. Also, the question of whether superconductivity arises predominantly from coupling to certain groups of phonons can be answered experimentally by searching for anomalously large widths. Estimates of average phonon widths are given for a variety of metals.

Recently, there have been several investigations of the phonon modes of high-transition-temperature superconductors by inelastic neutron scattering.¹⁻³ In the A15-structure materials^{1,2} Nb₃Sn and V₃Si these studies have revealed that the soft transverse-acoustic (TA) modes (known from ultrasonic work) extend out to fairly large wave vectors. In the rocksalt-structure materials³ like TaC, these studies have revealed anomalous regions of the LA and LO modes at large wave vector. It would be very interesting to know whether the large observed values of T_c arise in good part from electrons coupling to these anomalous phonons. This paper proposes a direct method for answering this question.

The equilibrium superconducting properties of any material can be derived from a knowledge of the spectral function $\alpha^2 F(\omega)$.⁴ In the special case of strong-coupling s - p metals like lead, $\alpha^2 F$ can be deduced from tunneling data.⁵ For the great majority of superconductors, however, there is no presently feasible method of determining $\alpha^2 F$. The main result of this paper is a relation between $\alpha^2 F(\omega)$ and the electron-phonon-induced width γ_Q of a phonon mode of frequency ω_Q . (The symbol Q incorporates the wave vector $\vec{Q}$ and a mode index.)

The spectral function is closely related to the density of phonon states $F(\omega)$:

$$F(\omega) = \sum_Q \delta(\omega - \omega_Q). \quad (1)$$

However, the connection is obscured somewhat in the usual definition,

$$\alpha^2 F(\omega) \equiv \sum_{kk'} |M_{kk'}|^2 \delta(\omega - \omega_{k-k'}) \delta(\epsilon_k) \delta(\epsilon_{k'}) / N(0). \quad (2)$$

In this formula $M_{kk'}$ is the matrix element for scattering from an electron state k of energy ϵ_k to a state k' of energy $\epsilon_{k'}$ via a phonon $k - k'$. The summations are restricted by the δ functions to run over states at the Fermi energy (which is taken as the zero of energy). The symbol k incorporates the wave number $\vec{k}$, band index, and spin index. The symbol $N(0)$ is the electronic density of states at the Fermi surface of states at the Fermi surface for both spin orientations,

$$N(0) = \sum_k \delta(\epsilon_k). \quad (3)$$

The matrix element M includes a host of many-body corrections such as screening, vertex corrections, and the measured rather than the bare-phonon frequency, as explained, for example, in Ref. 5. From a knowledge of $\alpha^2 F$ we may determine the transition temperature T_c by solving a complicated integral equation. For qualitative understanding, however, it is preferable to bypass that step and use instead the approximate equation of McMillan^{6,7}

$$T_c = (\langle \omega \rangle / 1.20) \times \exp[-1.04 (1 + \lambda) / (\lambda - \mu^* - 0.62\lambda\mu^*)] . \quad (4)$$

In this equation μ^* is the Coulomb pseudopotential and λ is the dimensionless electron-phonon coupling parameter and mass-enhancement parameter given by

$$\lambda = 2 \int \frac{d\omega \alpha^2 F(\omega)}{\omega} , \quad (5)$$

and $\langle \omega \rangle$ is an average phonon frequency given by $\langle \omega^n \rangle$ with n equal to unity and

$$\langle \omega^n \rangle = (2/\lambda) \int d\omega \omega^{n-1} \alpha^2 F(\omega) . \quad (6)$$

The parameter λ plays the role of the BCS parameter $N(0) V_{ph}$ and is the most important single number characterizing electron-phonon coupling.

Neutron scattering measures the imaginary part of the phonon Green's function $D(Q, \omega)$,

$$D(Q, \omega) = 2\Omega_Q / [(\omega^2 - \Omega_Q^2) - 2\Omega_Q \Pi(Q, \omega)] , \quad (7)$$

where Ω_Q represents the "bare" phonon spectrum in the absence of electron-phonon interaction and Π is the phonon self-energy. The actual frequency ω_Q and width γ_Q are determined from the real and imaginary parts of Π , respectively:

$$\omega_Q^2 = \Omega_Q^2 + 2\Omega_Q \Pi_1(Q, \omega_Q) , \quad (7a)$$

$$\gamma_Q = (\Omega_Q / \omega_Q) \Pi_2(Q, \omega_Q) . \quad (7b)$$

In terms of these quantities, the neutron-scattering line shape is approximately Lorentzian:

$$\text{Im } D(Q, \omega) = (\Omega_Q \gamma_Q / \omega_Q) [(\omega - \omega_Q)^2 + \gamma_Q^2]^{-1} . \quad (8)$$

Our main result is a new formula for $\alpha^2 F$ in terms of the width γ_Q measured at low temperatures,

$$\alpha^2 F(\omega) = 2/\pi N(0) \omega \sum_Q \gamma_Q \delta(\omega - \omega_Q) . \quad (9)$$

This formula has the advantage over Eq. (2) that it expresses $\alpha^2 F$ in a form parallel to the density of states $F(\omega)$, and entirely in terms of quantities accessible in principle to neutron measurement [except for the constant $N(0)$, which can be obtained by dividing the specific-heat electronic density of states by $1 + \lambda$].

The proof of Eq. (9) is quite simple. The Fermi "golden rule" gives a formula for γ_Q :

$$\gamma_Q = \pi \sum_k |M_{k, k+Q}|^2 [f(\epsilon_k) - f(\epsilon_k + \omega_Q)] \times \delta(\omega_Q - \epsilon_{k+Q} + \epsilon_k) . \quad (10)$$

Field-theoretic considerations^{4,5} strongly suggest⁸ that this equation is accurate to order $(m/M)^{1/2}$, where m and M are electron and ion masses. At temperatures low compared to the phonon frequency ω_Q , the Fermi factors restrict the $\vec{k}$ integration to a narrow region about the Fermi surface of width (in energy) ω_Q . Except for extremely pathological energy bands,⁹ it is an excellent approxi-

mation to replace the Fermi factors $f - f'$ in Eq. (10) by a factor $\omega_Q \delta(\epsilon_k)$ and to omit the energy ω_Q from the $\delta(\omega_Q - \epsilon_{k+Q} + \epsilon_k)$ in Eq. (10). Then we have an expression for γ_Q at low temperatures:

$$\gamma_Q = \pi \sum_k |M_{k, k+Q}|^2 \omega_Q \delta(\epsilon_k) \delta(\epsilon_{k+Q}) . \quad (11)$$

Substituting (11) into (9), we immediately recover definition (2). The extra factor of 2 arises because the sum over k includes a spin sum, whereas the sum over Q does not.

For purposes of actual measurement, the usefulness of Eq. (9) is limited because of the difficulty of measuring the width γ_Q of a typical phonon. However, some useful sum rules may be derived by substituting (9) into (5) and (6):

$$\sum_Q \gamma_Q / \omega_Q^2 = \frac{1}{4} \pi N(0) \lambda , \quad (12)$$

$$\sum_Q \gamma_Q = \frac{1}{4} \pi N(0) \lambda \langle \omega^2 \rangle \equiv 3N\bar{\gamma} . \quad (13)$$

In Eq. (13) we have introduced $\bar{\gamma}$, the average width of a phonon, where N is the number of atoms in the crystal. Let us also define an effective "bandwidth" W by the relation $N(0) = N/W$. Then we find that the average phonon width is

$$\bar{\gamma} / \bar{\omega} = (\frac{1}{12} \pi \lambda) (\bar{\omega} / W) , \quad (14)$$

where $\bar{\omega}$ is defined as $\langle \omega^2 \rangle^{1/2}$. Table I gives representative values of $\bar{\gamma} / \bar{\omega}$ calculated from Eq. (14). For *s-p*-band materials, the factor $\bar{\omega} / W$ is small (of order 0.003 for lead). This means that the average width $\bar{\gamma}$ is smaller than instrumental resolution ($\delta\omega / \omega \sim 0.01$ can be obtained in favorable cases for transverse phonons; 0.05 is the resolution available for longitudinal phonons). However, for narrow-band materials such as the A15 super-

TABLE I. Estimates of the average linewidth $\bar{\gamma}$ relative to the rms frequency $\bar{\omega}$ (approximated by $\Theta_D / 1.4$).

Material	λ	$N(0) = W^{-1}$ (states of both spins per eV per atom)	$\bar{\omega}$ or $\Theta_D / 1.4$ (meV)	$\bar{\gamma} / \bar{\omega}$	Reference
Al	0.38	0.42	28	0.0012	a
Pb	1.5	0.47	6.5	0.0012	a
Nb	0.82	1.82	20	0.008	a
V	0.60	2.62	25	0.01	a
W	0.29	0.30	22	0.0004	a
Nb ₃ Sn	1.3	3.9	20	0.03	b
V ₃ Si	1.1	3.8	26	0.03	b
V ₃ Ge	0.68	2.5	24	0.01	b
V ₃ Ga	1.23	5.8	20	0.04	b
NbN	0.82	0.50	22	0.0024	c
TaC	0.62	0.37	30	0.0018	c

^aReference 6.

^bT. H. GeBalle, B. T. Matthias, J. P. Remeika, A. M. Clogston, V. B. Compton, J. P. Maita, and H. J. Williams, *Physics* **2**, 293 (1966).

^cJ. K. Hulm, M. S. Walker, and N. Pessall, in *Proceedings of the International Conference on the Science of Superconductivity, Stanford, 1969*, edited by F. Chilton (North-Holland, Amsterdam, 1971).

conductors, $\bar{\omega}/W$ may be as much as a factor of 20 larger (i.e., of order 0.04 for V_3Si and Nb_3Sn). In this type of material the *average* electron-phonon-induced width is comparable with experimental resolution. Certainly in these cases, and probably in many less favorable cases as well, the phonons most important for superconductivity should have easily measurable widths. In particular, the anomalous phonons observed in Refs. 1–3 should have widths much greater than the average

width, if they arise from strong electron-phonon coupling. Furthermore, if γ_Q can be measured, the sum rule (12) allows a determination of what proportion of the coupling λ arises from anomalous regions of the spectrum. Information of this type would greatly increase our understanding of the connection between unstable lattices and high- T_c superconductors.

I am grateful to G. Shirane and J. D. Axe for stimulating my interest in this subject.

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³H. G. Smith and W. Glaser, *Phys. Rev. Letters* **25**, 1611 (1970).

⁴D. J. Scalapino, in *Superconductivity*, edited by R. D. Parks (Marcel Dekker, New York, 1969).

⁵W. L. McMillan and J. M. Rowell, in Ref. 4.

⁶W. L. McMillan, *Phys. Rev.* **167**, 331 (1968).

⁷R. C. Dynes, *Solid State Commun.* **10**, 615 (1972).

⁸I have not succeeded in proving that the Coulomb

vertex corrections to the matrix elements in Eqs. (2) and (11) are completely identical. They are at least very similar, and the error in any case should be small and slowly varying with Q . I wish to thank P. J. Feibelman for a helpful discussion on this point.

⁹Such a pathological case would be for example, the Labbé-Friedel one-dimensional model for A15 compounds, with the Fermi level as close as ω_Q to a band edge. See, for example, J. Labbé, S. Barisic, and J. Friedel, *Phys. Rev. Letters* **19**, 1039 (1967). Even in this context, Eq. (10) remains valid for low-frequency phonons.

Magnetic Flux Penetration into Superconducting Thin Films*

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The absolute value of the penetration depth in Sn and Pb superconducting thin films was measured using a quantum-interference technique. The value of the penetration depth obtained for 1500-Å-thick films of Pb was 630 Å; the value for a 3000-Å-thick film of Sn was 770 Å, and for a 2000-Å-thick film was 730 Å. These results are probably consistent with the BCS microscopic theory within the experimental error, although a direct comparison between the theoretical and experimental values is made difficult by the uncertainty in the nonlocal correction for the film thickness. The temperature dependence of the penetration depth for Pb (measured for temperature less than 4.2 K) agrees with a previous measurement of Erbach *et al.* For Sn the temperature dependence deviates from the theoretically expected behavior near the transition temperature. Results are given to show that the critical current of a superconducting interferometer with two parallel junctions is not strictly periodic in the applied magnetic flux with a period equal to the flux quantum $hc/2e$ because of the magnetic field dependence of the critical currents of the junctions.

I. INTRODUCTION

Many years ago London and London¹ predicted the existence of the penetration depth λ , the characteristic distance that a magnetic field penetrates into a superconductor. A few years later Shoenberg² obtained a measured value of λ . Since then, there have

been many measurements of the penetration depth, but only recently has it been feasible to measure the absolute value of λ .

Summaries of early penetration-depth measurements are given by Shoenberg,³ London,⁴ and Serin⁵; more recent results are described by Jaggi and Sommerhalder,⁶ Waldram,⁷ and Meservey and