Anisotropy of the electron-phonon interaction in niobium

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We calculate the anisotropy in the electron-phonon contribution to the many-body enhancement factor λ for niobium, using the nonorthogonal tight-binding method.

In recent years there has been a great deal of interest in calculating the properties of superconductors from first-principles calculations. Much of this interest has focused on the transition metals and their compounds because of their high superconducting transition temperatures. Several calculations have appeared for determining the Fermi-surface average of the electron-phonon coupling constant, $\langle I^2\rangle$, where

$$\langle I^2\rangle = N(0)^{-2}\sum_{\mu\mu'}\int_{\mathrm{FS}}\frac{d\sigma_{\vec{k}}}{|v_{\vec{k}\mu}|}\int_{\mathrm{FS}}\frac{d\sigma_{\vec{k}'}}{|v_{\vec{k}'\mu'}|}\sum_{\alpha}|g^{\alpha}_{\vec{k}\mu,\vec{k}'\mu'}|^2 \tag{1}$$

and $N(0)$ is the Fermi-surface density of states, μ is the band index, $v_{\vec{k}\mu}$ is the electronic velocity in the state $\vec{k}\mu$, $\sigma_{\vec{k}}$ is an element of the Fermi surface over which the integrals are taken, and $g^{\alpha}_{\vec{k}\mu,\vec{k}'\mu'}$ is the fully renormalized electron-phonon matrix element for scattering from the states $\vec{k}\mu$ to $\vec{k}'\mu'$ by mode α. One of these calculations[1] uses the nonorthogonal tight-binding method to express the electron-phonon matrix elements and gives good results compared to experiment. Another calculation uses orthogonal tight binding[2] and yields rather poor agreement with experiment because it ignores the important overlaps of atomic d functions.

Other calculations[3–6] decompose $\langle I^2\rangle$ into phase shifts of various angular momentum components and use the rigid-ion or rigidly moving muffin-tin approximation to express the electron-phonon matrix elements. This method yields roughly the same agreement with experiment as nonorthogonal tight binding for $\langle I^2\rangle$.

A quantity which is closely related to $\langle I^2\rangle$ and can provide another valuable measure of electron-phonon coupling is the electron-phonon many-body enhancement factor, λ_{ep}. McMillan[7] derived the approximate relationship that

$$\langle\lambda_{\mathrm{ep}}\rangle = \frac{N(0)\langle I^2\rangle}{M\langle\omega^2\rangle}\ , \tag{2}$$

where M is the ion mass and $\langle\omega^2\rangle$ is an average of the square of the phonon frequencies defined below. More rigorously, $\langle\lambda_{\mathrm{ep}}\rangle$ is most conveniently defined in terms of the electron-phonon spectral distribution function, $\alpha^2(\omega)F(\omega)$, as

$$\langle\lambda_{\mathrm{ep}}\rangle = 2\int\omega^{-1}\alpha^2(\omega)F(\omega)\,d\omega\ , \tag{3}$$

where

$$\alpha^2(\omega)F(\omega) = N(0)^{-1}\sum_{\mu\mu'}\int\frac{d\sigma_{\vec{k}}}{|dv_{\vec{k}\mu}|}\int\frac{d\sigma_{\vec{k}}}{|dv_{\vec{k}'\mu'}|}\sum_{\alpha}\frac{|g^{\alpha}_{\vec{k}\mu,\vec{k}'\mu'}|^2}{2M\omega_{\vec{k}-\vec{k}',\alpha}}\delta(\omega-\omega_{\vec{k}-\vec{k}',\alpha}) \tag{4}$$

and $\omega_{\vec{k}-\vec{k}',\alpha}$ is the phonon frequency of mode α at wave vector $\vec{k}-\vec{k}'$. We also have in Eq. (2) that

$$\langle\omega^2\rangle = \frac{\int\omega\alpha^2(\omega)F(\omega)\,d\omega}{\int\omega^{-1}\alpha^2(\omega)F(\omega)\,d\omega}\ .$$

Recently, detailed experimental results[8] were reported for the anisotropy in the total many-body enhancement factor, $\lambda(\vec{k})$, in niobium where $\lambda(\vec{k})$ relates the electron quasiparticle velocity to the band-structure velocity by $\vec{v}_{\mathrm{qp}} = \vec{v}_{\mathrm{bs}}/[1+\lambda(\vec{k})]$. $\lambda(\vec{k})$ includes λ_{ep} plus an enhancement due to electron-electron interactions. These results were derived by deconvoluting de Haas–van Alphen data and comparing it to accurate augmented plane wave (APW) band-structure results. They can be used to provide a rigorous test for theories of electron-phonon coupling.

The Fermi surface of niobium consists of three "sheets"; namely, an ellipsoid centered at the N

TABLE I. Comparison of sheet averages of λ with experimental and other theoretical results.

	λ experimental	λ_{ep} theoretical			
	Crabtree *et al.* Ref. 8	Simons *et al.* Results of this paper	Peter *et al.* Ref. 2	Butler *et al.* Ref. 9	Harmon *et al.* Ref. 10
Ellipse	1.10	0.80	1.35	1.17	1.85
Jungle-gym	1.43	1.14	1.90	1.08	1.37
Octahedron	1.71	1.10	1.92	1.09	1.28
Total	1.33	0.99	1.69	1.12	1.58

point, a Γ-centered octahedron, and an open jungle-gym surface with arms along the [100] direction. The de Haas–van Alphen experiments found that there was little anisotropy of $\lambda(\vec{k})$ within a given sheet. The authors thus chose to report sheet averages of $\lambda(\vec{k})$ as a simple and fairly accurate means of describing the anisotropy as these sheet averages will tend to be insensitive to local inaccuracies. Their results are shown in Table I.

The corresponding sheet averages of λ_{ep} could be computed from theory by limiting the integrations in Eq. (4) to the relevant regions of the Fermi surface. Butler, Pinski, and Allen[9] and Harmon and Sinha[10] have computed these sheet averages using the rigid-muffin-tin approximation. The anisotropy in λ_{ep} that they found was inconsistent with the anisotropy found in $\lambda(\vec{k})$ from the de Haas–van Alphen experiment.

Peter, Ashkenazi, and Dacorogna[2] computed these same sheet averages of λ_{ep} using orthogonal tight binding. While their results were consistently larger than expected from the de Haas–van Alphen experiment, the anisotropy they showed matched the experimental trends better.

We calculate here the sheet averages of the electron-phonon many-body enhancement factor using the nonorthogonal tight-binding method. We have achieved this by decomposing the contributions to $\langle I^2 \rangle$ into separate sheet-sheet scattering contributions by extending the integrals in Eq. (1) only over the relevant portions of the Fermi surface. We have inferred an effective average value of ω^2 for each sheet-sheet scattering by using the separate sheet-sheet scattering results for λ_{ep} and η given by Butler *et al.*,[9] where

$$\eta = 2\int \omega\alpha^2(\omega)F(\omega)\,d\omega \ .$$

Butler *et al.* calculate their frequencies by fitting a Born–von Karman model to neutron scattering data.

In nonorthogonal tight binding the electron-phonon matrix is given by

$$g^{\alpha}_{\vec{k}\mu,\vec{k}'\mu'} = \sum A^{\dagger}_{\mu m}(\vec{k})[\gamma^{\alpha}_{mn}(\vec{k}) - \gamma^{\alpha}_{mn}(\vec{k}')]A_{n\mu'}(\vec{k}') \ ,$$

where the $A(\vec{k})$'s are expansion coefficients for the Bloch waves and the γ's are Fourier transforms of $\nabla_{\alpha}H_{im,jn} - E_{\vec{k}}\nabla_{\alpha}S_{im,jn}$ and H and S are the Hamiltonian and overlap matrices. Squaring $g^{\alpha}_{\vec{k}\mu,\vec{k}'\mu'}$ we get four terms. Two of them are cross terms with $\gamma(\vec{k})\gamma(\vec{k}')$. It has been shown in the past[1] that these two terms are about two orders of magnitude smaller than the other two, and are neglected in this calculation.

The results for our calculation are also shown in Table I. The anisotropy we find obeys the same trend as the de Haas–van Alphen experiments show when comparing the *p-d* admixed ellipsoid to the other two sheets dominated by t_{2g} character. The anisotropy shown between the jungle-gym and the octahedron, however, is not in agreement with the de Haas–van Alphen results. It should be mentioned here that the anisotropy in the averages of ω^2 as derived from the results of Butler *et al.* was quite considerable and may indicate that using only sheet-to-sheet averages for ω^2 is not sufficient for a truly accurate calculation. Another possibility is that our Fermi surface may not be entirely accurate. This can be especially important in the region where the jungle-gym and octahedron come very close. A much less likely possibility is that the electron-electron renormalizations are highly anisotropic.

Our quantitative result for the total Fermi-surface average of λ_{ep} is much smaller than the result obtained for the total λ found by the de Haas–van Alphen experiments. Our result is, however, much more in line with the results of tunneling[11–15] experiments which give only the electron-phonon part of λ by measuring the electron-phonon spectral function and making use of Eq. (4). Our result is also in excellent agreement with experiments[7,12,16] which infer the value of only the electron-phonon contribution to λ by measuring the superconducting transition temperature and making use of an approximate solution to the Eliashberg equation. This seems to lead one to believe that electron-electron effects may indeed be quite significant. This is in accord with some other recent work.[17]

[1]C. M. Varma, E. I. Blount, P. Vashishta, and W. Weber, Phys. Rev. B 19, 6130 (1979); C. M. Varma, P. Vashishta, W. Weber, and E. I. Blount, Solid State Commun. 27, 919 (1978).
[2]M. Peter, W. Klose, G. Adam, P. Entel, and E. Kudla, Helv. Phys. Acta 47, 807 (1974); M. Peter, J. Ashkenazi, and M. Dacorogna, *ibid.* 50, 267 (1977).
[3]I. R. Gomersall and B. L. Gyorffy, J. Phys. F 4, 1204 (1974).
[4]B. M. Klein and D. A. Papaconstantopoulos, Phys. Rev. Lett. 32, 1193 (1974).
[5]W. H. Butler, Phys. Rev. B 15, 5267 (1977).
[6]B. N. Harmon and S. K. Sinha, in *Superconductivity in d- and f-Band Metals,* edited by D. H. Douglass (Plenum, New York, 1976), p. 391.
[7]W. L. McMillan, Phys. Rev. 167, 331 (1968).
[8]G. W. Crabtree, D. H. Dye, D. P. Karim, D. D. Koelling, and J. B. Ketterson, Phys. Rev. Lett. 42, 390 (1979).
[9]W. H. Butler, F. J. Pinski, and P. B. Allen, Phys. Rev. B 19, 3708 (1979).
[10]B. N. Harmon and S. K. Sinha, Phys. Rev. B 16, 3919 (1977).
[11]J. Bostock, K. H. Lo, W. N. Cheung, V. Diadiuk, and M. L. A. MacVicar, Ref. 6, p. 367; J. Bostock, V. Diadiuk, W. N. Cheung, K. H. Lo, R. M. Rose, and L. A. MacVicar, Phys. Rev. Lett. 36, 603 (1976).
[12]R. Robinson, T. H. Geballe, and J. M. Rowell, Ref. 6, p. 381.
[13]E. L. Wolf and J. Zasadzinski, in *Transition Metals 1977,* edited by M. J. G. Lee, J. M. Pertz, and F. Fawcett (Institute of Physics, Bristol and London, 1978), p. 666.
[14]B. Robinson and J. M. Rowell, Ref. 13, p. 666.
[15]K. Gärtner and A. Hahn, Z. Naturforsch. A 31, 861 (1976).
[16]P. B. Allen and R. C. Dynes, Phys. Rev. B 12, 905 (1975).
[17]H. Rietschel and H. Winter, Phys. Rev. Lett. 43, 1256 (1979).