Anisotropic Many-Body Effects in the Quasiparticle Velocity of Nb

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Fermi radii and velocities are determined by deconvoluting de Haas–van Alphen data. Comparison of these data with accurate augmented-plane-wave band-structure results establishes the reliability of the augmented-plane-wave calculations and allows a determination of the anisotropic many-body enhancement factor $\lambda(\vec{k})$. The Fermi-surface average $\langle\lambda\rangle$ of 1.33 suggests a large electron-electron contribution. Our anisotropic $\lambda(k)$ provide a detailed test and guide for model calculations of many-body enhancement.

Experimental data on the anisotropy of the electron-phonon coupling in transition metals would allow a detailed test of theories of the electron-phonon interaction and superconductivity in strongly coupled systems. This information has not been available from single-crystal tunneling as such experiments in transition metals have proven very difficult. In this paper we present the first detailed results for the anisotropy of the Fermi radius vector k_F, the quasiparticle veloc-

TABLE I. The band-structure density of states for each sheet of the surface and derived values of $\lambda(\vec{k})$ averaged over each sheet ($\langle\lambda\rangle_{\text{sheet}}$).

	s	p	d(e_g)	d(t_{2g})	f
η	-0.89602	2.7634	-2.1881	-2.0519	0.0043267
η'	4.2002	-0.17666	18.130	16.391	-0.17139

E_F = 0.695 ($2\pi/a$ units) lattice constant = 6.2286 (bohr radii)

		Ellipsoids (total of six)	Octahedron	Jungle Gym	Total
Number of carriers per atom (KKR fit)		-0.4118	-0.06919	-0.5224	-1.003
Enhanced density of states (KKR fit) states/eV-atom		1.249	0.547	1.573	3.360[a]
Band density of states (APW calculation) states/eV-atom		0.596	0.202	0.648	1.446
$\langle\lambda\rangle$sheet		1.10	1.71	1.43	1.33
$\langle\lambda_{ep}\rangle$ theory	Ref. 5	1.85	1.28	1.37	1.58
	Ref. 6	1.17	1.09	1.08	1.12
	Ref. 7	1.35	1.92	1.90	1.69

[a]Heat-capacity value of Ref. 8 is 3.320.

ity $v_{qp}(k)$, and the many-body renormalization $\lambda(k)$ due to the electron-phonon and electron-electron interactions in Nb. These anisotropic data provide a much deeper test of theory than can be made with the average values $\langle\lambda\rangle$ available from McMillan-like equations and polycrystalline tunneling. The available theoretical anisotropies based on the rigid-muffin-tin or rigid-ion approximation are not consistent with our results.

The anisotropy of k_F and the renormalized V_{qp} were derived from accurate, complete, de Haas-van Alphen (dHvA) data[1] in Nb utilizing a Koringa-Kohn-Rostoker (KKR) parametrization scheme.[2,3] The areas of[4] symmetry-direction orbits were fitted with five phase-shift parameters η in a nonrelativistic, non-muffin-tin parametrization to an rms error of 0.6%. (See Table I for details.) As a check on the quality of fit, the areas of many off-symmetry and noncentral orbits were calculated and found to agree with experiment to within 1.5% in the worst case.[9] The anisotropy of k_F in the (100) and (110) planes for the three sheets of the Fermi surface is shown in Fig. 1. The numbers of carriers contained in each sheet were found by numerical integration and are shown in Table I. The requirement of charge neutrality is satisfied to 0.3%, indicating the fit is highly accurate in the average sense since this requirement was not imposed during the fitting procedure.

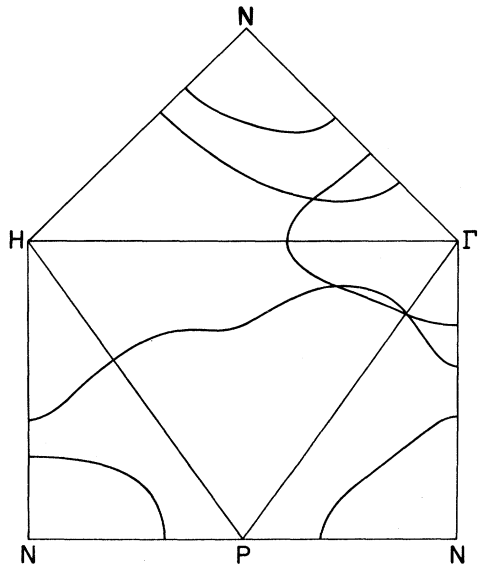

FIG. 1. The intersection of the Fermi surface of Nb with the (100) and (110) planes. The surface contains three sheets: the N-centered ellipsoids, the Γ-centered octahedron, and the multiply connected jungle gym.

The renormalized quasiparticle velocities $v_{qp}(k)$ (shown as the circles in Fig. 2) were derived by fitting eight symmetry-orbit effective masses (rms error 3.1%) using the energy derivatives of the phase shifts η' shown in Table I.[10] The enhanced densities of states for each sheet as calculated from this fit are shown in Table I. The total enhanced density of states agrees with heat-capacity results[11] to within 1.5%.

We define the many-body renormalization of the velocity by $\lambda(\vec{k}) = |v_{b.s.}(\vec{k})|/|v_{qp}(\vec{k})| - 1$, where $v_{b.s.}(\vec{k})$ is the Fermi velocity derived from a one-electron band-structure calculation. $\lambda(\vec{k})$ is the sum of two parts: $\lambda_{eph}(\vec{k})$ describing the effect of the electron-phonon interaction and $\lambda_{ee}(\vec{k})$ describing the electron-electron interaction. The band-structure results were obtained using the fully non-muffin-tin (nonspherical, nonflat) self-consistent, relativistic augmented-plane-wave programs of Elyashar and Koelling,[8] where $\alpha = \frac{2}{3}$ was used for the exchange-correlation contribution to the potential. To improve the agreement with the measured dHvA areas, the p-wave logarithmic derivatives were empirically shifted downward by[12] 0.05 Ry and the Fermi energy was redetermined. This reduced the rms error of ten symmetry-direction areas from 7% to 0.7%. The resulting Fermi-surface contours in the (100) and (110) planes are indistinguishable from those shown in Fig. 1. For other values of α or other exchange-correlation potentials, such empirical shifts did not produce such good agreement with experiment. The remarkably close agreement with the measured anisotropy of the Fermi surface gives confidence in the quality of the band-structure calculation.

The band-structure velocities and derived values of $\lambda(\vec{k})$ are shown as the squares and triangles in Fig. 2. The band-structure density of states for each sheet of the surface and derived values of $\lambda(\vec{k})$ averaged over each sheet ($\langle\lambda\rangle_{sheet}$) are shown in Table I. The average value for the entire surface is $\langle\lambda\rangle = 1.33$. Figure 2 shows that most of the anisotropy in $\lambda(\vec{k})$ occurs from sheet to sheet while within any given sheet $\lambda(\vec{k})$ is fairly uniform. Thus the anisotropy is well characterized by the three values of $\langle\lambda\rangle_{sheet}$ shown in Table I. These are the most reliable results we report, since local inaccuracies will contribute negligibly to the sheet average. Our fits further show that the ellipsoids are dominated by both p and d character while the jungle gym and octa-

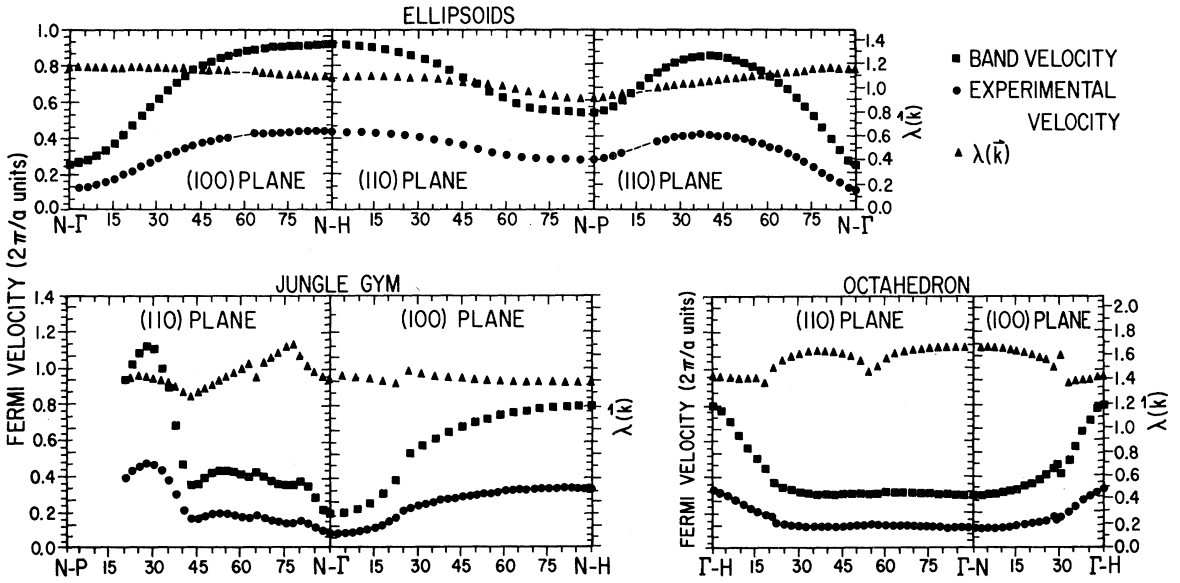

FIG. 2. The absolute value of the band-structure velocity $|\vec{v}_{b.s.}|$, the quasiparticle velocity $|\vec{v}_{qp}|$, and the many-body enhancement factor $\lambda(\vec{k})$. The scale for the velocity is on the left-hand side and that for $\lambda(\vec{k})$ is on the right-hand side. The dashed lines on the ellipsoid curves are smooth interpolations through regions of free-electron singularities where the KKR fit experiences difficulty. The sharp bumps on the $\lambda(\vec{k})$ curves for the octahedron and jungle gym are artifacts of the fitting procedure which occur where these two sheets touch and the velocities are allowed to be discontinuous in the nonrelativistic fit.

hedron are dominated by t_{2g} character.

Tunneling data can in principle be deconvoluted to obtain the electron-phonon spectral function $\alpha^2F(\omega)$ whose ω^{-1} moment gives $\langle\lambda_{eph}\rangle$. Unfortunately, agreement is not good among the tunneling experiments; some reported values of $\langle\lambda_{eph}\rangle$ are 0.58,[13] 0.81,[4,14] and 0.98.[15] Empirical values of $\langle\lambda_{eph}\rangle$ can be deduced from the experimental T_c if an approximate solution to the Eliashberg equation is assumed. McMillan,[16] and more recently Allen and Dynes,[17] have used this approach; from Fig. 9 of Ref. 17 and $T_c/\langle\omega\rangle = 0.66$ from tunneling,[4] a value $\langle\lambda_{eph}\rangle = 0.95$ would be expected. Our average value $\langle\lambda\rangle$ of 1.33 is considerably larger than these experimentally derived values. As the band-structure results agree so well with the measured areas, it seems unlikely that this difference could be due to uncertainties in the band structure.[18] This would imply a large electron-electron enhancement which like Cu exceeds the limits of the simple local theory.[19] Nonetheless the enhancement implied by our results is smaller than that deduced from optical mass data.[20]

Of the recent calculations of the electron-phonon coupling[5-7,21] in Nb three have considered the anisotropy (see Table I). Comparing the p-d admixed ellipsoid to the other two mostly d-like sheets (and assuming that electron-electron effects are reasonably constant), one sees that the rigid-muffin-tin results[5,6] give the wrong anisotropy while the tight-binding method[7] gives a more nearly correct trend. This has been attributed[5] to the omission of neighboring site interactions in the rigid-muffin-tin approximation which would provide a channel for d-d coupling. In none of the cases is reasonable quantitative agreement obtained.

Here we have presented data characterizing the dependence of the quasiparticle excitation spectrum. Further analysis to characterize the electronic interactions beyond a local-density-functional approach and better treatments of the electron-phonon interaction incldiuing screening are both needed. Because our understanding of the quasiparticle interactions is at a rudimentary level we believe that future work should eliminate the complication of global averages and study the k-dependent properties directly.

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[10]Our method of deducing the quasiparticle velocities absorbs the many-body effects into η_l', which are intended to describe only the one-electron behavior. From an empirical point of view the method appears to work in that the rms error of the fit to the enhanced effective masses is consistent with the experimental errors, and the calculated enhanced density of states agrees very well with the specific heat. A uniform enhancement of all masses can be handled exactly by multiplying all η_l' by the same factor, if the structure constant mass term, $\pi^{-1}(\partial A/\partial E)\eta_l$, is suppressed. This is permissible (we thank O. K. Andersen for pointing this out) because of the weak dependence of the fits on the Fermi-energy parameter. Compared to the very large anisotropy in the bare band-structure velocity, the additional anisotropy due to enhancement is rather mild. It is reasonable that the variation of the enhancement about its average can be accounted for with a small adjustment of the η_l'.

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