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Pressure dependence of the electron-phonon interaction and Fermi-surface properties of Al, Au, bcc Li, Pb, and Pd

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The electrical resistance of Li, Pd, Au, and Pb is measured as a function of temperature and pressure in the region $-20\,^{\circ}\mathrm{C}$ to $+30\,^{\circ}\mathrm{C}$ and 0—1.3 GPa. Self-consistent linear muffin-tin orbital band-structure calculations of these elements and of Al are performed at normal and reduced volumes. Results are obtained for the density of states $N(E_F)$, the average Fermi velocity, the optical mass, the plasma frequency ω, and the volume dependence of these parameters. The pressure dependence of the electron-phonon interaction $\lambda(p)$ is obtained from these measurements and the calculated $\omega(p)$. For the superconducting elements there is good agreement with the measured superconducting $T_c(p)$. Results from our previous measurements and calculations on Al, V, Nb, and La and published results for $\omega(p)$ are included in this comparison. $\lambda(p)$ increases with pressure for bcc Li and decreases for Pd and Au. Pressure is expected to suppress spin fluctuations much faster than $\lambda(p)$ in Pd. The possibility of inducing superconductivity by pressure in Pd and bcc Li is discussed. The electronic Grüneisen parameter γ_e is obtained from $\lambda(p)$ and the volume dependence of $N(E_F)$. Comparison with other results for γ_e generally shows good agreement.

I. INTRODUCTION

It was shown recently[1,2] that the pressure dependence of the electron-phonon—interaction parameter $\lambda(p)$ can be obtained from a combination of the calculated electron plasma frequency $\omega(p)$ and the measured pressure dependence of the temperature derivative of the electrical resistivity, $d\rho/dT$. By this method the electron-phonon—coupling matrix elements are essentially measured by the resistance, which gives most of the pressure variation of $\lambda(p)$ for the nontransition metals. $\omega(p)$ represents a correction factor which, however, is particularly important for the transition metals. $\omega(p)$ is essentially a Fermi-surface average of the magnitude of the Fermi velocity v. Therefore, to obtain $\lambda(p)$, we do not need the density of states or the electron-phonon—coupling matrix elements, both of which are more difficult to calculate than $\omega(p)$.

This method to determine $\lambda(p)$ is also independent of measurements in the superconducting state, such as the superconducting critical temperature $T_c(p)$, the critical field, the volume change at T_c, or tunneling spectroscopy. Our results for $\lambda(p)$ can conveniently be checked by comparison with such results, particularly with $T_c(p)$, using McMillan's formula and reasonable assumptions for the Coulomb pseudopotential and average phonon properties. This comparison was made previously for Al and La with encouraging results.[1] In these cases, however, available band-structure calculations were performed at large volume reductions, well outside the range of pressures in our hydrostatic experiment. Therefore, for Nb we calculated $\omega(p)$ for a series of small volume reductions in steps of 1% to make comparison with experiments more meaningful.[2] The result for $\lambda(p)$ was in favorable agreement with that deduced from $T_c(p)$.

We now extend this method to include also nonsuperconducting elements and report results for $\lambda(p)$ of bcc Li, Pd, Au, and Pb. Our previous measurements of Al are supplemented with a new band-structure calculation to obtain comparable results for this metal. These elements were chosen with the aim to cover, together with our previous results, representative superconducting and nonsuperconducting elements from different parts of the Periodic Table. However, we have restricted ourselves to cubic metals to facilitate the calculations.

In Sec. II the method used to obtain $\lambda(p)$ is briefly outlined and some useful formulas are recalled. In Sec. III the measurements are described and the results are presented and analyzed. The band-structure calculation is described in Sec. IV. We obtain results for the volume dependence of the plasma frequency and some other average Fermi-surface properties, i.e., the Fermi velocity, the optical mass, and the density of states $N(E_F)$. The results for $\lambda(p)$ are presented and discussed in Sec. V. Having obtained the volume dependence of $N(E_F)$ as well as λ, it is useful to compare them with the electronic Grüneisen parameter γ_e. This is briefly discussed in Sec. VI. The main conclusions are summarized in Sec. VII.

II. SUMMARY OF THEORETICAL DESCRIPTION

We follow the same procedures as employed previously[1,2] to analyze the experimental data, calculate band-structure properties, and obtain $\lambda(p)$. Therefore only a brief description is given here.

The measured resistance $R(p,T)$ at pressure p(GPa) and temperature T(°C) around room temperature is fitted to the form

$$R(p,T)=R(0,0)(1+AT)[1+Bp+(Cp^2)] . \tag{1}$$

The term Cp^2 can only be determined occasionally in the available pressure range. In principle, only the pressure dependence of R at a few different temperatures is needed. This is difficult to achieve in the practice, however, since even small temperature changes are important. For the resistance of many metals a temperature change of 1 K corresponds to a pressure change on the order of kilobars.

The volume dependence of the electron-gas plasma frequency, $\omega(V)$, is conveniently described by a parameter q defined by

$$\omega^2(V)=\omega^2(V_0)/(1+q\,\Delta V/V_0) , \tag{2}$$

where $\Delta V=V-V_0$. With these definitions of B and q, one obtains the following expression for $\lambda(p)$:

$$\lambda(p)=\lambda(0)\frac{1+\Delta V/3V_0}{1+q\,\Delta V/V_0}(1+Bp) . \tag{3}$$

In the derivation of this formula, it is assumed that $d\lambda_{\text{tr}}/dp=d\lambda/dp$. Here, λ_{tr} is the transport electron-phonon interaction, which differs from λ by a factor containing an average of the scattering angle, and which is of order unity.

In the calculation of ω^2, the following form is suitable for programming:

$$\omega^2=(e^2/12\pi^2\epsilon_0\hbar)\int v\,dS , \tag{4}$$

where the magnitude of the Fermi velocity, v, is integrated over the Fermi surface. A number of other Fermi-surface properties can then be calculated simultaneously as other averages of v:

$$N(E_F)=(V/8\pi^3N)\int v^{-1}dS , \tag{5}$$

$$\langle v^2\rangle=\left[\int v\,dS\right]\Big/\left[\int v^{-1}dS\right] , \tag{6}$$

$$m_{\text{op}}/m_0=v_0S_0\Big/\left[\int v\,dS\right] . \tag{7}$$

Here, $N(E_F)$ is the density of states at the Fermi level per atom and spin for N atoms in the crystal volume V, $\langle v^2\rangle$ is the expectation value of the Fermi velocity squared, and m_{op} is the optical effective mass. m_0, v_0, and S_0 refer to the free-electron values.

III. EXPERIMENTAL METHODS AND RESULTS

A. Sample characterization and experimental details

The source and nominal purity of the elements used are given in Table I. The Pb sample was identical to that used previously in an investigation of the high-temperature resistivity.[3] The sample was in the form of a 0.4-mm-diam wire. The residual resistance ratio was above 6300 prior to the present measurements. The Au sample was cold-drawn to a wire of 0.40 mm diameter, annealed at 600 °C for 3 h, and water-quenched. Care was taken to minimize further cold-work, to which the temperature dependence of the resistivity is very sensitive for this element.[4] For Pd, care was taken to handle the sample without contact with contaminating tools. Therefore, a piece suitable for the measurements of dimensions $\sim 0.5\times 0.5\times 9$ mm^3 was spark-cut from a 10-mm-diam rod supplied by the manufacturer. The Li sample was in the form of a 3.2-mm-diam wire. Since this was too large for us to use directly, the wire was extruded in a small hand-operated hydraulic press to 1 mm in diameter.

TABLE I. Elements used.

Element	Nominal purity (wt. %)	Source
Li	99.9	Alfa/Ventron (FRG)
Pd	99.993	Materials Research Corp. (NY)
Au	99.9999	Cominco (Washington, D.C.)
Pb	99.9999	Materials Research, Ltd. (UK)

The Pb, Au, and Pd samples were provided with spot-welded current and potential leads. In our first experiment on Li, contacts were formed by simply pushing thin Ni wires directly through the sample, and applying a slight pressure on each contact afterward to press the two materials into close contact. Although these contacts were not stable for more than a few hours even under oil at normal pressure, they worked fairly well at high pressure. This is probably due to the large compressibility of Li, which caused the sample to shrink around the Ni contacts at elevated pressures, thus improving the contact. However, the sample is probably mainly plastically deformed in this process, and there was therefore a tendency for the contacts to break as soon as pressure was decreased. In the second run we tried to obtain better contacts by implementing small spring clips from piano wire. These were mounted in pairs, as current and potential clips, on miniature Perspex bases and soldered to the connecting leads in the usual way. To avoid cutting the soft Li wire, it was placed in a shallow groove in the Perspex base. Immediately after the spring clips were applied, the contact area was covered with a thin coat of nail varnish to protect it from oxidation. These contacts were quite stable at atmospheric pressure, even in air. However, we found that even these contacts had a tendency to break when pressure was released from above 1 GPa. A third resistance measurement was made using the contactless high-pressure method developed by Sundqvist and Lundberg.[5] However, since the resolution of this method necessarily is an order of magnitude smaller than that of the standard four-probe method, this experiment only confirmed the general trend of the results of the two previous experiments. Apart from the contactless measurements just mentioned, the experimental equipment and methods used were identical to those used before, and we refer to our previous papers[1,2,6] for details.

B. Results and analysis

The resistance was measured as a function of temperature and pressure in the range −25 °C to +35 °C and 0—1.4 GPa, respectively. The data are given in Table II in chronological order for each element. The analyses are summarized in Table III.

It was straightforward to fit these data to Eq. (1). We checked that the fitting errors were uniformly distributed, which led to the removal of only a few data points. These have been given within parentheses in Table II. Exclusion of these data had little influence on the parameters R_0, A, and B, but improved the rms value significantly. A term Cp^2 in the pressure-dependent term of Eq. (1) was required to adequately fit the data for Pb. For Pd and Au the magnitude of such a term could not be determined within the limited pressure range employed.

1. Lithium

For Li our value for the pressure coefficient of resistance, B, is slightly lower than Bridgman's results of[7] 0.077 or[8] 0.074 GPa^{-1}, and is also in agreement with the result of Dugdale and Gugan[9] for the pressure coefficient of the ideal resistivity. When our data for Li around 21 °C were corrected for small differences from a mean temperature and plotted versus pressure, it was found that the first correction to a linear term is a term Cp^2 with $C>0$. This observation is in agreement with that of Bridgman.[8] However, repeating this analysis around the lower measuring temperature of −22 °C gave a value of C which was much smaller. Therefore, presently we can only conclude that there are indications of a positive term Cp^2 in the resistance of Li at constant temperature. Further work is required to determine the magnitude of this term and its possible temperature dependence, which is not accounted for by Eq. (1).

The temperature coefficient of resistance, A, is somewhat smaller than that obtained by Bridgman[7] and by Dugdale and Gugan,[9] 0.0045 K^{-1}. In our experiment, however, temperature and pressure were varied simultaneously. For instance, when pressure is decreased in a pressure cycle, various internal strain conditions may remain which affect the temperature dependence.

The Li results discussed so far refer to our second and best experiment. For the first experiment the data (not shown) were more scattered and the parameters A and B

TABLE II. Resistance as a function of temperature and pressure for samples of the elements investigated.

T (°C)	p (GPa)	R (mΩ)	T (°C)	p (GPa)	R (mΩ)
		Li			
(20.63	0.0001	3.601)	21.16	0.937	3.849
21.26	0.093	3.630	21.24	1.083	3.893
21.29	0.196	3.653	(21.08	1.245	3.936)
21.29	0.356	3.694	−23.02	1.211	3.254
21.31	0.499	3.731	−23.22	1.074	3.220
21.21	0.662	3.777	−22.79	0.948	3.199
21.21	0.808	3.814	−22.47	0.797	3.172
22.18	0.939	3.862	−22.9	0.653	3.134
		Pd			
(20.79	0.0001	4.164)	−16.59	0.795	3.587
21.02	0.107	4.156	−15.31	1.013	3.590
20.95	0.260	4.143	21.18	1.021	4.083
21.08	0.503	4.124	35.34	1.030	4.266
21.00	0.757	4.103	35.77	0.802	4.292
21.18	1.003	4.085	35.39	0.607	4.302
21.08	1.266	4.063	34.95	0.399	4.312
21.58	1.242	4.072	35.11	0.218	4.329
0.85	1.205	3.799	35.62	0.106	4.345
−0.19	0.991	3.798	36.03	0.103	4.352
−0.76	0.811	3.805	22.26	0.072	4.171
−0.16	0.607	3.827	22.57	0.489	4.142
−0.05	0.399	3.845	22.84	1.002	4.104
(0	0.229	3.859)	22.97	1.365	4.076
0.76	0.123	3.878	22.89	1.160	4.091
−19.09	0.071	3.606	22.86	0.747	4.123
−18.95	0.185	3.599	22.71	0.254	4.160
−18.46	0.382	3.592	22.73	0.0001	4.183
−17.64	0.598	3.586			

TABLE II. (*Continued*).

T (°C)	p (GPa)	R (mΩ)	T (°C)	p (GPa)	R (mΩ)
			Au		
(20.66	0.0001	14.053)	0.55	0.221	12.947
(20.63	0.084	14.015)	1.85	0.093	13.058
20.58	0.258	13.94	34.80	0.094	14.717
20.63	0.498	13.845	34.82	0.259	14.648
20.63	0.752	13.746	35.47	0.521	14.567
20.60	0.995	13.642	35.36	0.719	14.48
20.63	1.264	13.542	35.23	0.995	14.357
8.67	1.249	12.97	35.00	1.257	14.241
20.47	1.242	13.549	22.00	1.234	13.625
0.11	1.229	12.565	21.89	1.006	13.706
−0.03	1.229	12.556	21.89	0.755	13.801
−0.79	1.002	12.597	21.84	0.503	13.9
0.33	0.810	12.72	21.79	0.255	13.994
−0.08	0.611	12.77	21.66	0.096	14.05
−0.38	0.400	12.833	(21.81	0.0001	14.077)
			Pb		
20.76	0.0001	36.443	21.29	0.112	35.94
(20.87	0.102	35.935)	−0.33	0.103	33.12
21.05	0.269	35.15	−0.25	0.263	32.43
21.02	0.500	34.067	(−0.22	0.406	31.822)
20.89	0.765	32.907	(−0.49	0.610	30.945)
21.08	1.006	31.944	−0.55	0.821	30.10
21.16	1.263	30.977	−0.11	1.020	29.40
34.70	1.270	32.513	−19.81	0.991	27.185
35.82	0.981	33.80	−20.42	0.793	27.77
35.93	0.742	34.833	−19.63	0.607	28.545
35.47	0.493	35.93	−20.12	0.383	29.342
35.47	0.238	37.20	−19.83	0.270	29.827
35.72	0.231	37.265	(−19.43	0.130	30.445)
35.70	0.159	37.632			

were therefore more difficult to determine. The best fit to Eq. (1) for these data gave values for A and B which were, respectively, 20% and 2% higher than those in Table III, and a rms value of the scatter which was about 5 times larger. Besides the increased scatter of the data, this may again reflect that Eq. (1) be inadequate for Li. For instance, including the possibility that the pressure coefficient of resistance, B, depends on temperature within our measuring range improves the fit somewhat and would suggest that B increases with temperature by about 0.3%/K. This result is in qualitative agreement with the results by Dugdale and Gugan,[9] who found significant temperature dependence of the pressure coefficient of resistivity at lower temperatures. In Bridgman's report,[7] however, the pressure coefficient is temperature independent between 0 and 100 °C.

It is more informative to compare the temperature derivatives of $d\rho/dp$ since there is also a strong temperature dependence in the pressure coefficients from the factor $1/R$. We take[9] $\rho_0=8.5\ \mu\Omega\,\mathrm{cm}$ at 0 °C and $\rho^{-1}\,d\rho/dT=0.0045\ \mathrm{K}^{-1}$, and the compressibility[10] $\kappa=0.080\ \mathrm{GPa}^{-1}$. From Bridgman's measurements[8] at 30 and 75 °C, we then obtain $d^2\rho/dT\,dp=1.8\ \mathrm{n\Omega\,cm/K\,GPa}$. From Eq. (1) one has $d^2\rho/dT\,dp=\rho_0 A(B-\kappa/3)$, which yields 1.7 nΩ cm/K GPa from Table III and 2.0 nΩ cm/K GPa for our first Li experiment. From the work of Dugdale and Gugan, the corresponding result is 3.8 nΩ cm/K GPa, which may not be directly comparable since it involves lower temperatures down to 220 K.

In conclusion of our discussion of our experimental results for Li, we find that there may be a number of interesting questions concerning the detailed temperature and pressure dependence of the resistance that remain to be resolved. The main features, however, are in agreement with previous work. In particular, the quantities required for the present work have been determined and we find $d^2\rho/dT\,dp=1.8\pm0.2\ \mathrm{n\Omega\,cm/K\,GPa}$ for two different experiments.

TABLE III. Analysis of resistance data.

Element	A (10^{-3} K)	B (10^{-2} GPa^{-1})	C (10^{-2} GPa^{-2})	No. of data points	rms (10^{-4})
Li	4.19	+7.36		14	7
Pd	3.52	−1.88		35	8
Au	3.85	−2.79		27	3
Pb	4.01	−13.86	1.51	23	3

2. Palladium, gold, and lead

The rms error of the Pd fit was larger than for Au and Pb. This is due, in part, to the low resistance of this sample, which increased the measurement error somewhat, and, in part, to the following observation. The resistance of the first eight data points for Pd was about 0.15% larger than expected from the rest of the data. This may have been caused by a contact displacement. We did not correct for this error in our final analysis since this implies some arbitrariness. The effects on the parameters A and B from such a constant error were small and can be disregarded.

For Pd, Au, and Pb the temperature coefficients of resistance at 0 °C are also somewhat lower than those obtained from experiments where the temperature was varied at $p=0$. For Pd, a handbook value[11] for A is $3.9\times10^{-3}\ \mathrm{K}^{-1}$. For Au, $A=4.06\times10^{-3}\ \mathrm{K}^{-1}$ was previously obtained[4] for a similarly treated sample from the same ingot, while for Pb we calculate $A=4.11\times10^{-3}\ \mathrm{K}^{-1}$ from previous measurements[3] on the same sample. As mentioned, these differences are presumably due to the sensitivity of A to various states of strain in the sample. Despite the form of Eq. (1), we do not completely separate the effects of pressure and temperature, but rather measure an average temperature coefficient under the conditions of the experiment.

The pressure coefficients of resistance B for Pd and Au given in Table III are somewhat smaller than those reported by Bridgman. For Pd at 26 °C his average value of B up to 1.5 GPa was[12] $-2.03\times10^{-2}\ \mathrm{GPa}^{-1}$, while for Au at 30 °C the corresponding result was[8] $-2.89\times10^{-2}\ \mathrm{GPa}^{-1}$. For Pb Bridgman reported[8] $B=-0.1278\ \mathrm{GPa}^{-1}$ up to 1 GPa at 30 °C and, later,[13] $-0.1298\ \mathrm{GPa}^{-1}$ to 0.7 GPa at 0 °C. These values are not directly comparable to B in Table III since we have also used a term Cp^2 for lead. If this term is excluded, the rms value is significantly larger, about a factor of 7, and B is $-0.1203\ \mathrm{GPa}^{-1}$, which again deviates from Bridgman's results in the same direction. Recently, Eiling and Schilling reported on the resistance of Pb up to 10 GPa under hydrostatic conditions.[14] From their Fig. 2 the results for $R(p)$ versus p at large p smoothly join the Bridgman data at lower p.

IV. BAND-STRUCTURE CALCULATION

A. Zero-pressure results

A series of self-consistent linear muffin-tin orbital (LMTO) band-structure calculations were performed for each of the elements investigated experimentally, and for Al, to supplement our previous measurements.[6] The procedures used in these calculations were identical to those employed previously[2] and details were given there. The results for $N(E_F)$, v_F, m_{op}, and $\hbar\omega$ at zero pressure are given in Table IV.

There have been a number of band-structure calculations for Pd which report $N(E_F)$. In units of $(\mathrm{Ry\,spin\,atom})^{-1}$, several results are 14.8,[15] 15.3,[16] 15.5,[17–20] 16.0,[21] 16.3,[22] 16.8,[23] 17.0,[24] and 17.3.[25] The scatter of these data reflect the difficulty of obtaining reliable results for $N(E_F)$ in a high-density-of-states material. Our result may be somewhat too low.

TABLE IV. Band-structure results at zero pressure.

Element	$N(E_F)$ $[(\mathrm{Ry\,spin\,atom})^{-1}]$	$\langle v^2\rangle^{1/2}$ (10^8 cm/s)	m_{op}/m	$\hbar\omega$ (eV)
Li	3.25	0.83	1.62	6.33
Al	2.61	1.51	1.82	11.72
Pd	14.3	0.35	20.6	6.76
Au	1.76	1.43	11.1	8.99
Pb	3.55	1.44	0.49	9.65

For the nontransition elements, results for $N(E_F)$ are not so sensitive to details of the calculation. For Li our result is identical to that by Janak[19] and a few percent smaller than that by Papaconstantopoulus *et al.*,[15] and for Al our result is in between those in these two papers.[15,19] Our result for $N(E_F)$ of Pb is a few percent smaller than in Ref. 26 and a few percent larger than in Ref. 27. For Au, finally, recent results for $N(E_F)$ are[28] 1.65 or[29] 1.76 $(\mathrm{Ry\,spin\,atom})^{-1}$. This last result, which is in excellent agreement with ours, was obtained by a relativistic augmented-plane-wave (APW) method with the $X\alpha$ $(\alpha=0.8)$ potential. It was noted in Ref. 29 that this potential gave very good reproduction of both the optical transition energies as well as the Fermi-surface parameters, and less good agreement with the observed electronic specific-heat coefficient γ. However, this last conclusion was based on unrenormalized γ values. With observed γ values in units of $(\mathrm{Ry\,spin\,atom})^{-1}$ of[30] $N_\gamma(E_F)=2.158\pm0.027$ or[31] 2.103 ± 0.017, and our value of $N(E_F)=1.76$, we obtain $\lambda=N_\gamma(E_F)/N(E_F)-1=0.23\pm0.02$ (Ref. 30) or 0.20 ± 0.01 (Ref. 31). Recent resistivity measurements gave[32] $\lambda=0.24$.

Our results for $N(E_F)$ are thus in agreement with previous calculations. This supports our computational methods and further results for which there is little comparable information available in the literature. The following results provide some examples. The Fermi velocity of Li was found to be[33] 0.84×10^8 cm/s. m_{op}/m for Li was calculated by an APW method with results in the range 1.4—1.6 for different realistic values of a screening parameter.[34] A pseudopotential calculation for Al gave values for m_{op}/m of about[35] 1.35. For Pd the average Fermi velocity was found to be[20] 0.33×10^8 cm/s, while the plasma frequency calculated by us from the results of Ref. 20 is $\hbar\omega=6.65$ eV. All of these results are in agreement with ours, except perhaps m_{op}/m for Al, where the result of Ref. 35 is about 25% smaller than that in Table IV.

B. Volume dependence

The volume dependence of $N(E_F)$, $\langle v^2\rangle^{1/2}$, m_{op}/m, and ω was obtained by performing the band-structure calculation for a series of reduced volumes in steps of 1% down to $0.95V_0$. Repeated calculations with small volume steps facilitate the control of possible numerical errors and allow for more direct comparison with experiments in a pressure region where hydrostatic conditions

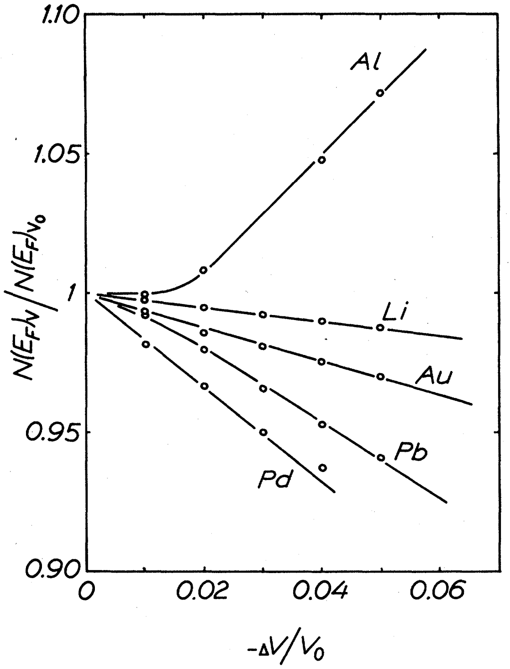

FIG. 1. Density of states normalized to its zero-pressure value as a function of volume reduction.

are feasible. The results are shown in Figs. 1–4 normalized to the values at $p=0$ which were given in Table IV. The plasma frequency is plotted as $\omega^2(V_0)/\omega^2(V)$ versus $\Delta V/V_0$ to permit an immediate evaluation of q from Eq. (2). The advantage of this form is that it reduces to the free-electron-like limit, $q=1$, at all pressures. For example, if the data for Pd are plotted as $\omega^2(V)/\omega^2(V_0)$ versus $\Delta V/V_0$, there is a clear (upward) curvature, in contrast to the straight line of Fig. 4. The results for q are given in Sec. V below.

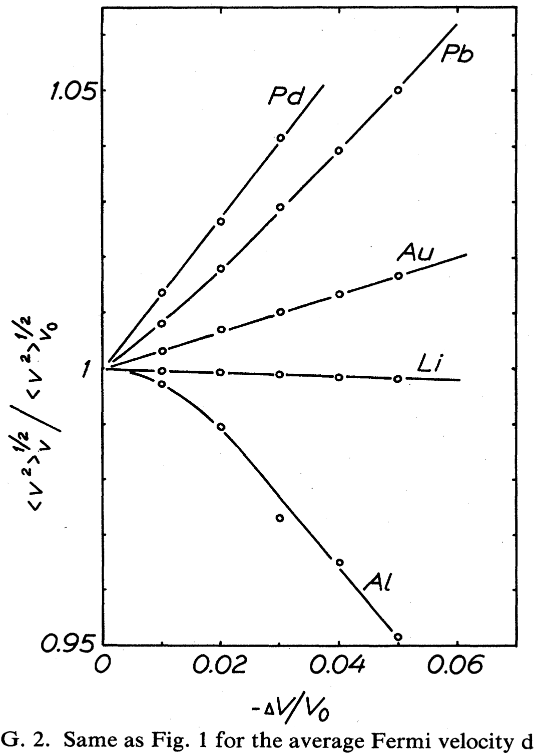

FIG. 2. Same as Fig. 1 for the average Fermi velocity defined in Eq. (6).

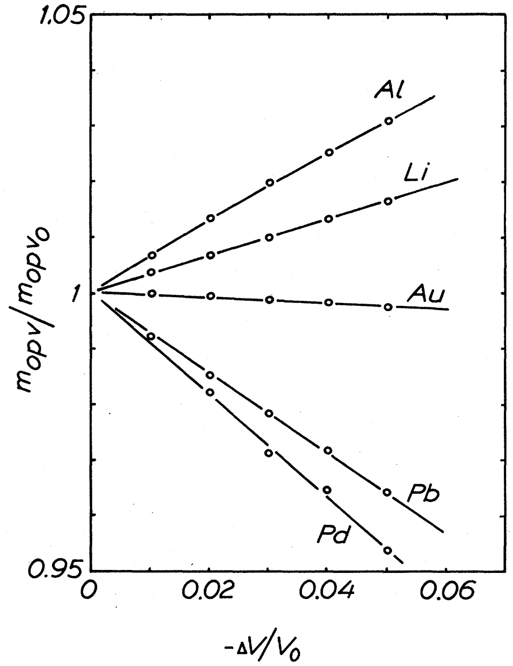

FIG. 3. Same as Fig. 1 for the optical mass defined in Eq. (7).

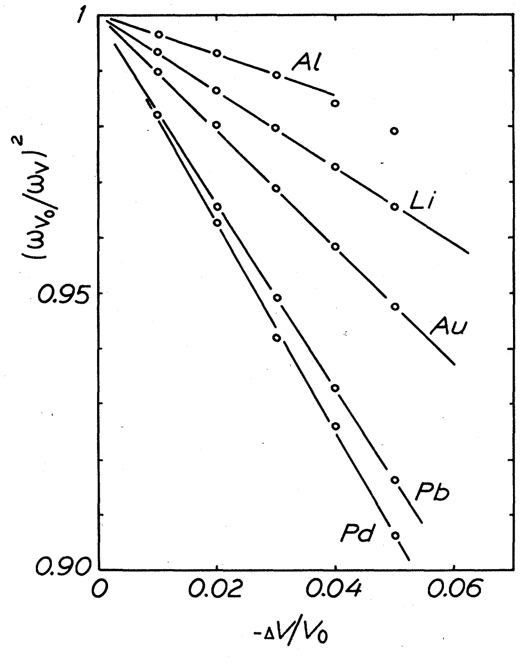

FIG. 4. Volume dependence of the plasma frequency plotted to evaluate q from Eq. (2).

It can be seen from Figs. 1–4 that ω increases with pressure for all five elements, while for the other quantities studied the pressure effect has different signs for different elements, with Al and usually Li deviating from the heavier elements. Different volume variations in the sequence Al, Li, Au, Pb, and Pd are observed for each of the four properties studied. In free-electron-like models, $d\ln[N(E_F)]/d\ln V=\frac{2}{3}$, $d\ln\langle v^2\rangle^{1/2}/d\ln V=-\frac{1}{3}$, m_{op} is independent of volume, and, as mentioned, $q=1$. Figures 1–4 show that only Au is close to free-electron-like behavior, while none of these properties scales with volume in such a simple way for the other elements studied.

There are few results in the literature for band-structure properties under pressure, and in these cases the volume reductions used are usually large. An exception is the calculation of the effect of pressure on the Fermi surface of Au by Ramchandani,[36] where reduced volumes of 98.5% and 97%, respectively, were used. Unfortunately $N(E_F)$ or other average Fermi-surface properties were not calculated. The Fermi energy was given in Ref. 36, however, and from two data points we calculate $d\ln E_F/d\ln V=-2.1\pm0.2$, which can be compared with our average value of -1.96 ± 0.1 from five reduced volumes. The Fermi velocity for Li was calculated at 10% volume reduction,[33] from which we deduce a small value for $d\ln\langle v^2\rangle^{1/2}/d\ln V$ of 0.12, in fair agreement with our result of 0.04 from Fig. 2, for smaller compressions.

The calculation of m_{op} for Al at large volume reductions[35] would suggest that m_{op} increases faster than linearly with larger reduced volume. From Fig. 3 we obtain $d\ln m_{\text{op}}/d\ln V=-0.6$, while, from Ref. 35, $\Delta m_{\text{op}}V_0/m_{\text{op}}\Delta V_0$ is -2, -2.6, and -3.5 at 10%, 20%, and 30% volume reduction, respectively. There is also a calculation of pressure-dependent properties of Al which confirms that q for Al is small.[37] From Fig. 2 in that paper the variation of ω^2 is nonmonotonic over a pressure range corresponding to $\Delta V=-5\%$, but an upper limit of q would be about 0.2. The pressure dependence of $N(E_F)$ will be discussed in Sec. VI in connection with the electronic Grüneisen parameter γ_e.

V. $\lambda(p)$

Some results have been collected in Table V, from which the pressure dependence of $\lambda(p)$ can be calculated from Eq. (3). q was evaluated from the slopes of the straight lines in Fig. 4. Our older measurements[6] of B for Al supplement the present calculation of q, and the results[2] for B and q of Nb are also given for comparison. Since there is some useful information available about q for V and La, our previous results[1] for B of these metals have also been included.

With the compressibility $\kappa=-\Delta V/(V_0 p)$, the low-pressure limit of Eq. (3) can conveniently be written as

$$\frac{d\ln\lambda}{dp}=B+\kappa(q-\tfrac{1}{3})\ . \tag{8}$$

The values calculated from Eq. (8) are listed in Table V.

For the superconducting elements these results can be compared with measured properties. We choose to compare them with the measured $T_c(p)$ and use the following simplified method. $T_c(p)$ for each element is calculated from McMillan's formula,[49]

$$T_c=\frac{\Theta}{1.45}\exp\left[-\frac{1.04(1+\lambda)}{\lambda-\mu^*(1+0.62\lambda)}\right]\ , \tag{9}$$

where Θ is the Debye temperature and μ^* the Coulomb pseudopotential. $\lambda(p)$ is taken from Table V and we assume that

$$\mu^*=\text{const} \tag{10}$$

and

$$\Theta(p)=\Theta(0)(1+\gamma_G\kappa p)\ . \tag{11}$$

γ_G is the Grüneisen parameter. For each element, γ_G is taken from Ref. 30 and κ according to Table V, and a combination of Θ, μ^*, and $\lambda(0)$ is chosen which is in agreement with accepted values and reproduces the observed zero-pressure T_c in Eq. (9). These values are shown in Table VI. The calculated change of T_c at 1 GPa, $\Delta T_c=T_c(1\text{ GPa})-T_c(0\text{ GPa})$, is compared to the

TABLE V. Results for $d\ln\lambda/dp$. Unfootnoted values are from the present work.

					$\Delta T_c=T_c$ (1 GPa) $-T_c$(0 GPa)	
Element	B (10^{-2} GPa^{-1})	κ (10^{-2} GPa^{-1})	q	$d\ln\lambda/dp$ (10^{-2} GPa^{-1})	Calculated (K)	Observed (K)
Li (bcc)	$+7.4$	8.00^{d}	0.70	$+10.3$		
Al	-4.25^{a}	1.26^{e}	0.35	-4.2	-0.26	-0.28^{k}
V	-1.61^{b}	0.70^{f}	1.6^{h}	-0.7	-0.07	$+0.06^{l}$
Nb	-1.56^{c}	0.68^{f}	1.95^{c}	-0.5	0^{j}	-0.02^{m}
Pd	-1.88	0.53^{g}	1.87	-1.1		
La (dhcp)	-0.81^{b}	4.06^{e}	2.6 ± 0.2^{i}	$+8.4\pm0.8$	$+1.1\pm0.1$	$+1.3^{n}$
Au	-2.79	0.67^{e}	1.03	-2.3		
Pb	-13.86	2.36^{e}	1.69	-10.7	-0.34	-0.36^{o}

[a] Reference 6.
[b] Reference 1.
[c] Reference 2.
[d] Reference 10.
[e] Reference 38.
[f] Reference 39.
[g] References 30 and 40.
[h] Reference 41.
[i] Reference 42.
[j] Reference 43.
[k] Reference 44.
[l] Reference 45.
[m] Reference 46.
[n] Reference 47.
[o] Reference 48.

TABLE VI. Zero-pressure parameters for the superconductors in Table V.

	γ_G[a]	$\Theta(0)$ (K)	μ^*	$\lambda(0)$
Al	2.1	430[b]	0.10[b]	0.384[b]
V	1.5	400[b]	0.13[b]	0.6[b]
Nb	1.74	280[b]	0.13[b]	0.815[b]
La	0.7	142[a]	0.13[b]	0.85[d]
Pb	2.8	75[c]	0.105[c]	1.55[c]

[a] Reference 30.
[b] Reference 49.
[c] Reference 50.
[d] Calculated from Eq. (9).

observed ΔT_c in the last two columns of Table V.

A correction to this model is the expected small decrease of μ^* with pressure which will lead to an increase of the calculated T_c at 1 GPa. One possibility of estimating this effect is based on a Thomas-Fermi model of μ^* by which Smith obtained[45]

$$d\ln\mu^*/d\ln V = 0.27\{d\ln[N(E_F)]/d\ln V\} .$$

A similar result is obtained by scaling a semiempirical fit of values of μ^* to a function of $N(E_F)$.[51] As an example, we recalculated ΔT_c in Table V with the Thomas-Fermi expression for μ^*, $d\ln[N(E_F)]/d\ln V$ for the superconductors of Table VII below, $d\ln[N(E_F)]/d\ln V = 1.1$ for fcc La,[52] and a rough value of 1.8 for V.[41] The following results are then found [element, ΔT_c(K)]: Al, -0.26; V, -0.06; Nb, $+0.02$; La, $+1.16$; Pb, -0.33.

The differences between these numbers and those in Table V are small, smaller, e.g., than those resulting from different reasonable choices of zero-pressure parameters and other element-specific considerations which are discussed below. By using one simple and common method to calculate ΔT_c, as in Table V, we emphasize the generality of our method to obtain $\lambda(p)$.

A. Aluminum, niobium, and lead

For these elements there is good agreement between the calculated and observed $T_c(p)$. For Nb and Pb the discrepancies between the observed and calculated T_c in Table V are both within the variation which may occur due to different choices of zero-pressure parameters. This was discussed previously[2] for Nb and is illustrated for Pb by the results of Clark and Smith.[48] They find $d\ln\lambda/d\ln V = 4.2$ from their observed $T_c(p)$ and McMillan-like zero-pressure parameters,[49] while we find a slightly smaller T_c depression than observed by them from $d\ln\lambda/d\ln V = 4.5$ in Table V and tunneling parameters in Table VI.

For Al it was previously found empirically that $q = 0$. The measured pressure dependence of dR/dT, including terms of order p^2, gave excellent agreement with observed $T_c(p)$ data up to about 4 GPa.[6] With the present calculation of q, this agreement is only slightly lessened. At higher pressures the values of ΔT_c^{calc} obtained with $q = 0.35$ and the previous resistivity results can be compared to the experimentally observed depression ΔT_c^{expt} from Ref. 44 or Ref. 53 by the following sequence of values [$-\Delta T_c^{\text{calc}}$(K) and $-\Delta T_c^{\text{expt}}$(K)]: at 2 GPa, 0.47 and 0.47; at 3 GPa, 0.64 and 0.64 ± 0.03; at 4 GPa, 0.78 and 0.82 ± 0.03, and larger differences at still higher pressures. Apparently, the result for $\lambda(p)$ is comparatively insensitive to the value of q for Al. The good result for this metal may instead be due to accurate higher-order terms in both the compressibility and the pressure dependence of dR/dT, C in Eq. (1).

Pb is the only other metal where we have succeeded in determining C. In this case, however, the calculated depression of T_c is significantly smaller than the observed[54] depression at higher pressures. This may be due to our value of C, since a reduction of C by 25% is sufficient to remove this discrepancy for pressures up to 4 GPa. Such a smaller value of C is not unreasonable since the corresponding value deduced by us[1] from Bridgman's data[8] was even smaller. In the p^2 term in the compressibility of Pb there is a difference of a factor of 4 between the results of Vaidya and Kennedy and those of Bridgman.[38]

B. Vanadium

The band-structure calculation[41] of q for V is not completely comparable to our later results since corrections to the atomic-sphere approximation were not applied and, furthermore, large volume reductions up to 25% were used. The reason for the discrepancy between the calculated and observed ΔT_c in Table V, however, is most likely not due to an inaccurate value of q but rather to spin fluctuations. Our result for q is confirmed by unpublished work.[55]

Spin fluctuations have long been expected to influence the properties of V. A range of different values of the paramagnon coupling constant λ_s has been suggested, such as 0.38,[56] 0.34,[57] 0.07,[58] or roughly 0.2 ± 0.1.[59] Apart from the magnitude of λ_s, it is also unclear how to account for the depression of T_c due to λ_s. One approach used frequently is based on rescaling of all parameters in McMillan's equation, yielding expressions of the type[60]

$$T_c = \frac{\Theta}{1.45}\exp\left[-\frac{1.04(1+\lambda+\lambda_s)}{\lambda-\lambda_s-\mu^*(1+0.62\lambda)}\right] . \tag{12}$$

The pressure dependence of λ_s can be estimated from[61]

$$\lambda_s = 4.5IN(E_F)\ln\left[1+\frac{\nu}{12}\frac{IN(E_F)}{1-IN(E_F)}\right] , \tag{13}$$

where I is the exchange-correlation integral and ν a cutoff parameter. It was argued[59] that Eq. (12) and similar expressions overestimated the effect on T_c due to λ_s, and that a third square-well potential, characterizing the paramagnon spectral function, had to be introduced in addition to the electron and phonon cutoff frequencies in conventional expressions for μ^*.

We have attempted to estimate $T_c(p)$ both from Eq. (12) and a simplified version of the formalism of Ref. 59. We chose $\lambda_s(0) = 0.2$ and took I and $N(E_F)$ from Ref. 19. By Eq. (13), this required $\nu \approx 0.73$, which is a reasonable value. I was assumed to be independent of pressure, while the rough value for $d\ln[N(E_F)]/d\ln V$ of[41] 1.8 was used. This gives the pressure dependence of λ_s by Eq. (13). $\lambda(0)=0.98$ yields the correct $T_c(0)$ in Eq. (12), and the pressure dependence was taken from Table V. Equations (10) and (11) were used for Θ and μ^*, with $\mu^*=0.13$. With these assumptions, ΔT_c at 1 GPa changed from -0.07 to $+0.27$ K. To compare Eq. (12) with the theory of Leavens and MacDonald, we use—as much as is possible—identical parameters and a number of additional assumptions.[62] The effect on ΔT_c is then smaller. We obtain $\Delta T_c=+0.13$ K.

Unfortunately, the model parameters are not known accurately enough to calculate a reliable value of λ_s. These examples illustrate that such a calculation is possible in principle. The pressure-induced increase of the T_c of V may thus be due to the decrease of the destructive influence of spin fluctuations. This effect is apparently somewhat stronger than the weak decrease of λ with pressure obtained in Table V.

So far we have neglected the possibility that the observed $(d\rho/dT)_{\text{obs}}$ is modified by a spin-fluctuation contribution $(d\rho/dT)_s$. This problem is not resolved and different theories have suggested different forms and even different signs of $(d\rho/dT)_s$.[63–65] If an analogy can be made with the AlMn system, then the $(d\rho/dT)_s$ of V is negative and numerically much smaller, below about 2% of $d\rho/dT$.[56] Writing

$$(d\rho/dT)_{\text{obs}}=(d\rho/dT)_{\text{ph}}+(d\rho/dT)_s\ , \tag{14}$$

it is seen that the phonon contribution $(d\rho/dT)_{\text{ph}}$ would be somewhat larger than $(d\rho/dT)_{\text{obs}}$, and that this difference would decrease with pressure when spin fluctuations are suppressed. Hence, B of Table V would still be negative and of larger magnitude. In this case, therefore, the conclusion would be reinforced that the increase with pressure of T_c of V is due to suppression of spin fluctuations. If, instead, there is a small positive $(d\rho/dT)_s$ around 0 °C similar to what has been assumed for Pd,[20] then $|B|$ would be smaller and this would lead to a decreased value of the estimated paramagnon coupling constant λ_s.

C. Lanthanum

For La the measurements[1] were performed on dhcp La, while the band-structure calculations[42] were made on fcc La. Furthermore, the calculation of ω under pressure used highly compressed volumes far outside of the experimental range. We calculated q from the results of Ref. 42 at the two reduced volumes used there and found $q=2.8$ at $\Delta V/V_0=-16\%$ and $q=2.3$ at $\Delta V/V_0=-27\%$. The value for q in Table V is a rough average of these results.

There is, nevertheless, rather good agreement between the calculated and observed ΔT_c for La. In view of the poorer compatibility between theory and experiment for this metal, this agreement should not be overemphasized. The results suggest that our model for $\lambda(p)$ is valid for La and that different crystal structures do not appear to have a strong influence on the result for q of this element.

D. Lithium

It is well known that Li undergoes a martensitic transformation at a temperature T_1 of about 75 K. T_1 increases with pressure, although slowly,[66] and our experiments are completely within the bcc phase. Below T_1 the structure is complicated. Li transforms partially to a close-packed structure, hcp or fcc, by a fraction which depends on temperature and sample treatment.[67]

Such complexities are usually neglected in calculations of electronic properties. This may be justified from the often observed similarity between average electronic properties of elements and alloys in different crystal structures. There are notable exceptions to this similarity, however. Therefore our result for $\lambda(p)$ of bcc Li should be regarded as an indication only of the properties of real Li at low temperatures. In addition, we, of course, expect our result to be valid for the untransformed fraction of an experimental sample.

The result for $\lambda(p)$ of bcc Li in Table V shows that $\lambda(p)$ and hence also $T_c(p)$ are expected to increase with pressure. This conclusion is the opposite of that reached by Bose and Gupta,[68] who predict a large decrease of T_c with increasing p. Their result was based on the traditional relation $d\ln\lambda/d\ln V=2\gamma_G$, however. If $d\ln\lambda/d\ln V$ is calculated from Table V and compared to $2\gamma_G$ for the superconducting elements in Table VI, it is seen that this relation is clearly inadequate.

The absence of superconductivity in Li at zero pressure above[69] 6 mK is an unsolved problem. Various different results[70] suggest $\lambda\approx0.4$, which would correspond to a T_c of about 1 K with conventional parameters in the McMillan formula, Eq. (9). A possible reason for this failure is charge-density-wave—spin-density-wave mixing.[71] Pressure may inhibit such mixing and, furthermore, as we have shown, increase λ. It therefore seems that a low-temperature pressure experiment may promote superconductivity in Li.

E. Palladium

The result for $d\ln\lambda/d\ln p$ of Pd shows that λ decreases comparatively slowly with pressure. $N(E_F)$ decreases with pressure as in Fig. 1. Consequently, the spin-fluctuation contribution λ_s is expected to decrease significantly with pressure. To further investigate this question, we extended the band-structure calculation for Pd to higher volume reductions. The results are shown in Fig. 5.

$N(E_F)$ continues to decrease with decreasing volume, more rapidly in the region from 5% to 8% volume reduction and leveling off at smaller V/V_0. We do not know the reason for this steplike behavior of $N(E_F)$. Possibly, it is an artifact of the calculation, e.g., the slope of a flat part of an energy band may appear to increase too rapidly with pressure if the integration net were insufficiently dense. If so, the curves for $N(E_F)$ and $\langle v^2\rangle^{1/2}$ in Fig. 5 should be drawn more smoothly to average errors of about 5%. On the other hand, m_{op} and ω^2, which contain averages of v, are both linear in V to within 1%. Furthermore, from the results of Ref. 16 at reduced volume, there

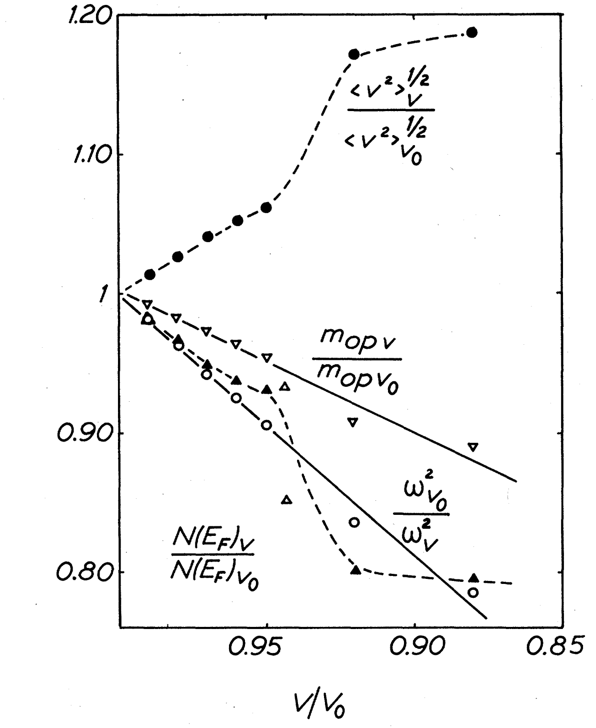

FIG. 5. Fermi-surface properties of Pd as functions of reduced volume normalized to their zero-pressure values. ▲, $N(E_F)$ from this work; △, $N(E_F)$ from Ref. 16 (also see Ref. 72); ●, $\langle v^2\rangle^{1/2}$ from this work; ▽, m_{op} from this work; ○, ω^{-2} from this work.

is some support for a strong reduction of $N(E_F)$.[72]

This strong decrease of the density of states under pressure should lead to suppression of spin fluctuations and possibly to superconductivity under pressure. A hypothetical phase diagram is illustrated in Fig. 6. The steep rise in T_c would reflect the vanishing spin fluctuations and the decrease at high pressures would correspond to the continued decrease of λ.

This suggestion was investigated recently in a brief report.[73] λ was extrapolated to higher pressures in two ways, viz., linearly in V and linearly in p using high-pressure compressibility results.[74] It seems likely that a linear extrapolation in p overestimates the depression of λ. Furthermore, λ_s was estimated from a simple one-parameter expression,[75]

$$\lambda_s = 4.5\ln\left[\frac{1}{3[1-IN(E_F)]}\right], \tag{15}$$

and T_c was calculated from Eqs. (9), (10), and (12). With these assumptions, the maximum in T_c in Fig. 6 would correspond to about 150 mK at 17 GPa.

Such an estimate is very uncertain. This can be illustrated by using the theory of Leavens and MacDonald[59] instead of Eq. (12). We take $\lambda(0)=0.41$,[76] $(1-IN)^{-1}=6$ at $p=0$, and I independent of pressure. The further assumptions are the same as those used above[62] for V. With

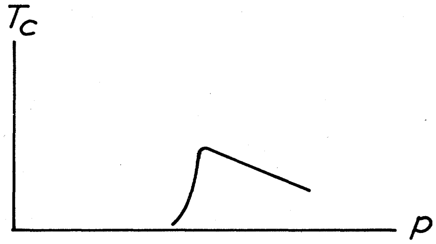

FIG. 6. Hypothetical phase diagram for Pd.

λ_s from Eq. (15), the maximum T_c would be about 200 mK. If Eq. (13) is used for λ_s, one can adjust v so that λ_s fits specific-heat data. This is roughly obeyed for $v=\frac{1}{4}$, with $\lambda_s(0)\sim 0.4$.[21] In this case, $T_c^{\max}$ is about 60 mK. The pressure at $T_c^{\max}$ would be about 17.5 ± 1.5 GPa, with some uncertainty mainly due to questions about the detailed volume dependence of $N(E_F)$.

If there is a contribution from spin fluctuations to the resistivity of Pd around 0 °C, this analysis will be modified as discussed above for V. From the treatment of Pinski *et al.*,[20] a small and positive $(d\rho/dT)_s$ of about 2% of $d\rho/dT$ in this temperature region would seem reasonable. If such a term is present the observation of superconductivity under pressure would be somewhat favored, with an increased estimate of $T_c^{\max}$ and a smaller required pressure.

From measurements of the magnetic susceptibility χ of Pd under pressure, it was inferred that the Stoner enhancement factor $S=[1-IN(E_F)]^{-1}$ should decrease only slightly with pressure.[77] Even when the volume dependence of λ is included in this analysis, the pressure dependence of S is much smaller than found presently. We do not understand the reason for this discrepancy. Our result, however, is in qualitative agreement with the observed strong enhancement of χ of Pd in Au-Pd-Au sandwiches,[78] and with the calculated finite magnetic moment of expanded Pd.[79] Furthermore, we find good quantitative agreement with the observed electronic Grüneisen γ_e as discussed in the next section.

One must also consider the possibility of breakdown in the assumption $d\lambda/dp=d\lambda_{\mathrm{tr}}/dp$, which was implied in Eqs. (3) and (8). Careful calculations support[20] the stronger statement that $\lambda\approx\lambda_{\mathrm{tr}}$. Recently, it has been argued that this agreement is accidental for Pd,[80] and that superconducting and transport properties are defined by different parts of the Fermi surface. The electron-phonon matrix elements between electron states on different sheets of the Fermi surface, which contribute to $d\rho/dT$, may change differently with pressure than the matrix elements of λ between predominantly d states. However, the dominant contribution to the pressure dependence of λ and λ_{tr} is due to the shift of the phonon frequencies. Although these frequencies are averaged in different ways in λ and λ_{tr}, the pressure dependence of these averages is similar unless there is a significant mode dependence in the Grüneisen parameter γ_G. Therefore it seems likely that the qualitative nature of the proposed hypothetical phase diagram, Fig. 6, will not be affected. The coordinates of the maximum T_c may shift, however, and further work is required to determine this shift.

F. Gold

For Au the result for $d\ln\lambda/dp$ gives a moderately strong decrease of λ with pressure. Au is a candidate for superconductivity at ultralow temperatures. The result for $\lambda(p)$ would therefore imply a strong relative decrease of the T_c of Au with pressure. If[32] $\lambda(0)\approx 0.24$ and $\mu^*=0.125$, then T_c is of order 0.1 mK at zero pressure and one would expect a 50% decrease of T_c already below 1 GPa.

VI. γ_e

The results for the volume dependence of $N(E_F)$ and λ permit the calculation of the electronic Grüneisen parameter γ_e. At a low temperature one has[70]

$$\frac{d\ln[N(E_F)]}{d\ln V}+\frac{\lambda}{1+\lambda}\left[\frac{d\ln\lambda}{d\ln V}\right]=\gamma_e\ , \tag{16}$$

where the right-hand member may be directly measured, e.g., in a thermal-expansion experiment. Such a comparison is thus a consistency check on three independent sources of information, viz., our band-structure calculation of $N(E_F)$ and q, the measurements of B, and the low-temperature thermal-expansion experiment.

This comparison is shown in Table VII. $d\ln[N(E_F)]/d\ln V$ is obtained from Fig. 1. When $N(E_F)$ varies linearly with volume, the slope of this line has been evaluated. For Al and Pb we have used the data at $V=0.99V_0$ and the accuracy is therefore lower. The factor $\lambda/(1+\lambda)$ is evaluated from Table VI and $\lambda(0)=0.4$ for[70] Li, 0.41 for[76] Pd, and 0.24 for[32] Au. The volume derivatives of λ are calculated from $\lambda(p)$ and κ in Table V.

For Li there are apparently no low-temperature thermal-expansion experiments,[81] nor have we found any results for $d\ln[N(E_F)]/d\ln V$. For Al the experimental $\gamma_e=1.60$ seems to be well established.[81] Results for γ_e from other experiments show considerable scatter,[82] but are generally larger than our calculated result. As mentioned, our result for $\lambda(p)$ agrees well with that expected from the observed $T_c(p)$. Therefore we must suspect that our result in the low-pressure region for $d\ln[N(E_F)]/d\ln V$ of Al is too small. For Nb and Pd there is excellent agreement between calculated and observed γ_e's. Also, for Au the agreement is quite satisfactory. A calculation[83] of $d\ln[N(E_F)]/d\ln V$ for Au gave 1.23, which overestimates the experimental γ_e by about the same amount that our result underestimates it.

TABLE VII. Results for γ_e.

Element	$\frac{d\ln[N(E_F)]}{d\ln V}$	$\frac{\lambda}{1+\lambda}\left[\frac{d\ln\lambda}{d\ln V}\right]$	Calc.	γ_e Thermal expansion[b]
Li	0.25	−0.37	−0.12	
Al	0.09±0.1	0.93	1.02	1.60
Nb	1.1[a]	0.31	1.41	1.5
Pd	1.67	0.57	2.24	2.22
Au	0.63	0.67	1.30	1.6
Pb	0.82±0.1	2.75	3.57	1.7

[a] Reference 2.

[b] Reference 81.

Pb is the only case in Table VII where there is a serious discrepancy between calculated and observed γ_e's. In this case the thermal-expansion result is less accurate due to the low Θ and large lattice Grüneisen parameter γ_G, and more precise measurements were found to be necessary.[81] From both the pressure dependence of the critical field[84] and the volume change[82] at T_c larger values of γ_e were found, viz., 4.6±0.8 and 3.1±0.8, respectively.[85] Our result is within these values and confirms the high value of γ_e for Pb.

In concluding the discussion of our results for γ_e, we find satisfactory agreement with direct experimental results in all cases except perhaps for Al. This observation gives further support that our results for $N(E_F)$, q, and B are consistent.

VII. CONCLUDING REMARKS

The main result of this paper is the demonstration of the usefulness of Eq. (8) to study the pressure dependence of λ. For this purpose we have obtained accurate measurements of the electrical resistance of Li, Pd, Au, and Pb as a function of pressure and temperature in a region around 0 °C and band-structure results for these metals and for Al including the volume dependence of $N(E_F)$, $m_{\rm op}$, $\langle v^2\rangle^{1/2}$, and ω.

It is found that Eq. (8) provides a straightforward way of obtaining $d\ln\lambda/dp$ that appears to be very general. Together with our previous results and published results for ω of La, we have investigated five superconductors, i.e., Al, Pb, V, Nb, and La, and in all cases the change of T_c with pressure calculated from our results for $\lambda(p)$ is rather close to the experimental observation. In this calculation we have used accepted values of μ^*, $\lambda(0)$, γ_G, and Θ, but there is no further element-specific assumption. In fact, except for La and V, the agreement with the experimental dT_c/dp is within about 0.02 K/GPa and we have argued that spin fluctuations for V and the La calculation of q are likely reasons for the larger discrepancies in these cases. In particular, our result for $\lambda(p)$ of V suggests that the small increase of T_c with pressure for this metal is due to suppression of spin fluctuations. As demonstrated by the results for Nb, one can also obtain small pressure variations from Eq. (8), smaller, e.g., than those resolved in tunneling experiments.

The electronic Grüneisen parameter γ_e was calculated from the volume dependence of $N(E_F)$ and λ, and compared to literature results of low-temperature thermal-expansion measurements. The agreement is generally good, which gives further support to the consistency of our theoretical and experimental results. For Al, however, this agreement is somewhat less convincing.

The method of determining $d\ln\lambda/dp$ is not limited to superconductors. We have obtained results for Au, Pd, and Li. For Au it is found that $\lambda(p)$ decreases with pressure. For Pd and bcc Li it is predicted that pressure may induce superconductivity.

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