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Effects of pressure on superconducting properties of simple metals†

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Abstract. First principles studies of the superconducting behaviour under pressure of the simple metals Al and Pb have been made. Good agreement is obtained with the experimental volume derivative of the transition temperature in Al and, for higher compressions, upward deviations are predicted to occur from the linear relationship with volume observed at low pressures. In Pb, the relative rates of decrease under pressure of T_c, Δ_0, and $2\Delta_0/k_BT_c$ show the same trends as experiment, while in Al the ratio $2\Delta_0/k_BT_c$ is found not to vary significantly with compression.

1. Introduction

The superconductivity of simple metals is now understood theoretically to high precision (see, for instance, Parks 1969). In this paper we calculate the pressure dependence of the superconducting parameters of Al and Pb and assess the extent to which quantitative first principles calculations of transition temperatures are now possible.

Many experimental studies of the effects of pressure on superconductivity have been made in the last fifteen years, and the results for simple metals have been summarized by Smith and Chu (1967). They showed that, over the range of pressures so far covered, the transition temperatures, T_c, of simple metals decrease linearly with volume, Ω. In Al, the measurements extend to compressions of almost 3%, for which T_c is decreased by 40%, and in Pb a decrease of 50% is found for the maximum compression of 20%. Extrapolating these curves, they predicted the eventual suppression of superconductivity by pressure. In addition, it has been found (Franck and Keeler 1968, Galkin and Svistunov 1968) that in Pb the ratio $2\Delta_0/k_BT_c$ decreases under pressure at about the same rate as does T_c itself. The relative experimental pressure derivatives are included in table 1.

The most detailed calculations of the superconducting properties of metals that have been performed to date are those of Carbotte and Dynes (1968). They calculated electron–phonon coupling functions from the model electron–ion potentials of Animalu and Heine (1965, to be referred to as AH) and experimental phonon dispersion curves, and thence the zero temperature energy gap at the gap edge, Δ_0, from the strong coupling theory of superconductivity. These calculations were extended to variable volume by Trofimenkoff and Carbotte (1969, 1970) by scaling the phonon frequencies by the measured change in sound velocities and rescreening the potential. They obtained good agreement with experimental values of Δ_0, T_c and their volume derivatives for both Al and Pb.

We have shown (Coulthard 1970, to be referred to as I) that local AH potentials can be used to predict quite reliably the phonon frequencies and their pressure derivatives in the simple metals Na, K and Al, but that the calculations are not adequate for Pb. Dynamic electron–phonon coupling functions $\alpha^2(\nu)F(\nu)$ calculated from these potentials and frequencies have also been found to be satisfactory (Coulthard 1971, preceding paper, to be referred to as II). This then suggests that a semi-quantitative explanation of the observed superconducting behaviour of Al under pressure can be given, without recourse to other experimental data, by using these coupling functions in the strong coupling theory. While

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Table 1. Calculated pressure dependence of Δ_0 and T_c in Pb

Compression (%)	λ	T_c	Δ_0	$\frac{2\Delta_0}{k_B T_c}$
0	1·71	7·19	1·35	4·34
5	1·50	6·65	1·19	4·14
$-\frac{d \ln X}{dP}$ (10^{-6} bar^{-1})	calc.[a]	3·7	5·8	2·3
	expt.[b]	$4·9 \pm 0·2$	$10·1 \pm 0·8$	$5·2 \pm 0·6$

[a] Pressure derivatives (for bulk metal) obtained from volume dependence via P–Ω equation of Munson and Barker (1966).

[b] Franck and Keeler (1968); thin film.

similar calculations in Pb can indicate only the trends of T_c and Δ_0, the difference in their volume derivatives is most likely associated just with the greater strength of the electron–phonon coupling and should therefore be apparent even if the calculation of the coupling is approximate. Our results confirm these expectations.

2. Theory and calculation procedure

The strong coupling theory of superconductivity in simple metals is well known (Schrieffer 1964) so we just review the resulting gap equations here. The electron–phonon interaction is treated, according to the analogue for superconductors of Migdal's (1958) approximation, to $O(m/M)^{1/2}$, where m and M are the electron and ion masses respectively, and the Coulomb interactions between electrons are also included. Anisotropies in the electron self-energy, which arise from those in the electron–phonon interaction, band structure, and phonon density of states, are relatively small in the simple metals (Bennett 1965). Averaging over these, equations for the renormalization function $Z(\omega)$ and the gap function $\Delta(\omega)$ at the Fermi surface are obtained. At zero temperature, these are

$$\{1 - Z(\omega)\}\omega = \int_{\Delta_0}^{\infty} d\omega' \, \mathrm{Re}\left[\frac{\omega'}{\{\omega'^2 - \Delta^2(\omega')\}^{1/2}}\right] K_-(\omega, \omega')$$

$$\Delta(\omega) = \frac{1}{Z(\omega)} \int_{\Delta_0}^{\infty} d\omega' \, \mathrm{Re}\left[\frac{\Delta(\omega')}{\{\omega'^2 - \Delta^2(\omega')\}^{1/2}}\right] \{K_+(\omega, \omega') - \mu^* \theta(\omega_c - \omega')\} \qquad (1)$$

where $\mathrm{Im}\,[Z(\omega)\{\omega^2 - \Delta^2(\omega)\}^{1/2}] > 0$,

$$K_\pm(\omega, \omega') = \int_0^{\infty} d\nu \, \alpha^2(\nu) F(\nu) \left(\frac{1}{\omega' + \omega + \nu + i\delta} \pm \frac{1}{\omega' - \omega + \nu - i\delta}\right)$$

and $\alpha^2(\nu) F(\nu)$ is the effective electron–phonon coupling function defined in equation (1) of II. The electron–electron Coulomb pseudopotential μ^* has the form (Schrieffer 1964)

$$\mu^* = \frac{N(0)V}{1 + N(0)V \ln(\epsilon_F/\omega_c)} \qquad (2)$$

where V is an average over the Fermi surface of the screened Coulomb interaction between electrons, $N(0)$ is the electron density of states at the Fermi surface, excluding electron–phonon renormalization effects, and ω_c is a cut-off frequency of order $5\omega_D$, where ω_D is the Debye energy. As in II, we neglect the Coulomb vertex corrections and quasi-particle renormalization factors in $\alpha^2(\nu) F(\nu)$ and μ^*.

The gap equations at nonzero temperature are more complicated than (1) but have the same general form (Scalapino *et al.* 1965), so we will not give them here. The gap edge at temperature T, Δ_T, is defined by

$$\Delta_T = \mathrm{Re}\,\Delta(\omega = \Delta_T) \qquad (3)$$