carbon in α-iron was measured for temperatures above 823 °K. This result contrasts sharply with the lack of pressure dependence obtained by relaxation measurements at low temperatures.

(ii) Analysis of the data in accordance with the empirical approach of Eq. (5) suggests a temperature-dependent activation volume varying from 5 cm^3/mole at 889 °K to 8 cm^3/mole at 1000 °K.

(iii) Analysis of the data in accordance with the two-mechanism model proposed in Ref. 4 suggests a temperature-independent activation volume of 10 cm^3/mole for high-temperature-diffusion mechanism.

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[1] A. J. Bosman, P. E. Brommer, and G. W. Rathenau, Physica 26, 533 (1960); 23, 1001 (1957).

[2] J. Bass and D. Lazarus, J. Phys. Chem. Solids 23, 1820 (1962).

[3] R. P. Smith, Trans. AIME 224, 105 (1962).

[4] C. G. Homan, Acta Met. 12, 1071 (1964).

[5] C. G. Homan and J. F. Cox (unpublished).

[6] H. M. Strong, in *Progress in Very High Pressure Research*, edited by F. P. Bundy, W. R. Hibbard, Jr., and H. M. Strong (Wiley, New York, 1961), p. 182.

[7] F. Simon, Trans. Faraday Soc. 33, 65 (1937).

[8] L. Salter, Phil. Mag. 45, 369 (1954); J. Gilvarry, Phys Rev. 102, 308 (1956).

[9] J. P. Nickol, H. F. Meiners, K. H. Moore, and W. Eppenstein, *Analytical Laboratory Physics* (Edwards, Ann Arbor, Mich., 1956).

[10] R. W. Keyes, *Solids Under Pressure* (McGraw-Hill New York, 1963), p. 80.

[11] D. Ye. Temkin, Fiz. Metal. Metalloved. 29, 589 (1970).

[12] J. E. Hilliard and J. W. Cahn, in Ref. 6, p. 109.

[13] T. G. Nilan, Trans. AIME 239, 898 (1967).

[14] J. E. Hilliard and W. R. Tully, ASD Technical Report No. TDR-16-21, Pt. 1, 1961 (unpublished).

[15] J. F. Frye, E. E. Stansbury, and D. L. McElroy, Trans. AIME 167, 219 (1953).

[16] L. S. Darken and R. M. Fisher, *Decomposition of Austenite by Diffusional Processes* (Interscience, New York, 1962), p. 249.

PHYSICAL REVIEW B VOLUME 5, NUMBER 12 15 JUNE 1972

Nearly-Free-Electron Susceptibility of Noble Metals[*]

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Theoretical calculations of the magnetic susceptibility of solid and liquid noble metals are presented. The effective shape of the Fermi surface of solid metals is taken into account by using the simple "eight-cone" model by Ziman. The interference function of liquid metals is evaluated according to the procedure given by Ashcroft and Lekner. A model potential recently proposed by the authors allows completion of the calculations. We find that, when electron correlations are taken into account, good agreement with the available experimental data generally results. The resulting estimates of the shift in susceptibility on melting are also confirmed by experiment.

I. INTRODUCTION

Recently tractable expressions for the magnetic susceptibility of simple metals have been obtained by many authors through the use of the pseudopotential formalism.[1–5] We have shown in a preceding paper[6] the applicability of these expressions to noble metals also, for which some reliable pseudopotentials exist[7–10]; we have also carried out a simple calculation of the nonoscillatory diamagnetic susceptibility of the noble metals Cu, Ag, and Au.

In this paper we present the results of a more complete calculation of the nonoscillatory magnetic susceptibility of solid and liquid metals Cu, Ag, and Au. While for the liquid metals the calculation does not offer any trouble once accurate pseudopotentials and the liquid-structure factor are known, for the solid metals some difficulties arise because of the distorted Fermi surface. Actually, as is well known, the Fermi surface of the solid noble metals is so much distorted from a spherical shape as to contact the (111) faces of the Brillouin zone.[11]

Since it is not possible to treat the Fermi surface as a sphere, a revision of the existing expressions for the spin paramagnetism[1] and for the orbital diamagnetism[5] of conduction electrons is needed. On the other hand, this revision is made easier by a simple model of the energy surfaces of the noble metals, the "eight-cone" model, devised by Ziman[12] about eleven years ago. Many reliable results for the calculated transport properties of the noble metals were given, in the past, by use of this model. Using the "eight-cone" model, we have obtained expressions for the magnetic susceptibilities of the noble metals which are consistent with both the known topological properties and the existing theories.

The geometry of the "eight-cone" model is outlined in Sec. II. In Sec. III we derive suitable expressions and evaluate the spin and diamagnetic susceptibility of the solid noble metals. In Sec. IV an analogous calculation is carried out for the liquid metals. The effect of electron correlations is taken into account in Sec. V and a comparison is made with the available experimental data.

II. "EIGHT-CONE" MODEL

To start our calculation, we need to know an analytical representation for the Fermi surfaces of the solid noble metals. This is easily accomplished using Ziman's[12] phenomenological model, the "eight-cone" model. This model is quite simple; in fact, since we know that the Fermi surfaces of the noble metals keep far away from all zone boundaries but the (111) planes, we can make the shape of the energy surfaces depend on a single parameter, which can be interpreted as the pseudopotential form factor, or one-half the s-p band gap at L [the center of the nearest (111) zone face]. In this way the integral expressions over the Fermi surface which enter in the calculation of the diamagnetic and spin susceptibilities can be evaluated by elementary methods. In order to make the calculation of Sec. III clear we shall give here a brief account of the "eight-cone" model.

The first Brillouin zone is supposed to be made up of eight circular cones, pointing into the center along the diagonals of a cube. Each cone subtends the solid angle $4\pi/8$, so that its vertex angle is $\cos^{-1}(\frac{3}{4})$. The axis of the cone is a vector $\vec{p}=\frac{1}{2}\vec{G}$, where $\vec{G}$ is the vector of the reciprocal lattice corresponding to the nearest hexagonal (111) zone face. The free Fermi surface would have a radius $k_F = 0.902p$.

Taking the local z axis in the $\vec{p}$ direction, the expression for the one-electron energy $E_{\vec{k}}$ can be easily shown to be

$$E_{\vec{k}}=\frac{\hbar^2}{2m}(k_x^2+k_y^2)+\frac{\hbar^2}{m}f(k_z)\,, \tag{2.1}$$

where

$$f(k_z)=\tfrac{1}{2}p^2+\tfrac{1}{2}(p-k_z)^2-[U_{\vec{G}}^2+p^2(p-k_z)^2]^{1/2}\,, \tag{2.2}$$

and $V_{\vec{G}}=\hbar^2 U_{\vec{G}}/m$ is the Fourier component of the lattice pseudopotential. Introducing, as in Ziman's paper,[12] dimensionless variables $x\equiv k_x/p$, $y\equiv k_y/p$, $z\equiv k_z/p$, $\epsilon\equiv E_{\vec{k}}/(\hbar^2p^2/m)$, and $u\equiv U_{\vec{G}}/p^2$, formulas (2.1) and (2.2) are more conveniently written as

$$\epsilon=\tfrac{1}{2}(x^2+y^2)+f(z)\,, \tag{2.3}$$

$$f(z)=\tfrac{1}{2}+\tfrac{1}{2}(1-z)^2-[u^2+(1-z)^2]^{1/2}\,. \tag{2.4}$$

Since on the cone

$$x^2+y^2=\tfrac{7}{9}z^2\,, \tag{2.5}$$

one finds that each energy surface cuts the side surface of the cone at some ordinate z_1, so that

$$\epsilon=\tfrac{7}{18}z_1^2+f(z_1)\,. \tag{2.6}$$

This same energy surface will either cut the z axis at some point z_2 given by

$$\epsilon=f(z_2) \tag{2.7}$$

or meet the zone boundary at $z_2=1$.

III. SUSCEPTIBILITY OF SOLID METALS

We shall first derive an expression for the chemical potential in the case of a single Bragg-reflection plane. We start from

$$N=(1/4\pi^3)\int d^3k\,F(E)\,, \tag{3.1}$$

where $F(E)$ is the Fermi function, N is the number of electrons per unit volume, $N=(2m\zeta_0)^{3/2}/3\pi^2\hbar^3$, and ζ_0 is the free-electron chemical potential.

The volume (in units of p^3) lying inside a fraction of $\frac{1}{8}$ of the Fermi surface is the sum of the volume of a right circular cone, of height z_1 and semiangle $\cos^{-1}(\frac{3}{4})$, i.e., $(7\pi/27)z_1^3$, plus the volume

$$\pi\int_{z_1}^{1}(x^2+y^2)dz=2\pi\int_{z_1}^{1}[\epsilon_F-f(z)]\,dz\,, \tag{3.2}$$

where $\epsilon_F=\zeta/(\hbar^2p^2/m)$. The integral goes from z_1 to 1, since the Fermi surface is known to contact the (111) zone boundary.

Taking into account these results and the expression (2.4) for $f(z)$, Eq. (3.1) easily gives

$$\epsilon_0=(\tfrac{9}{2})^{1/3}\Bigg(\tfrac{7}{27}z_1^3+(2\epsilon_F-1)(1-z_1)+(1-z_1)[(1-z_1)^2+u^2]^{1/2}-\tfrac{1}{3}(1-z_1)^3+u^2\ln\left|\frac{(1-z_1)+[(1-z_1)^2+u^2]^{1/2}}{u}\right|\Bigg)^{2/3}\,, \tag{3.3}$$

where ϵ_0 is the free Fermi energy in dimensionless units, $\epsilon_0=\zeta_0/(\hbar^2p^2/m)$.

By the knowledge of the pseudopotential form factor u it is possible, using Eqs. (2.6) and (3.3), to calculate z_1 and ϵ_F by a reiteration process or by a graphical interpolation method. The diamagnetic and spin susceptibilities are then evaluated in terms of z_1 and ϵ_F.

For the spin susceptibility one simply has

$$\chi_P = \mu_B^2 N(\zeta) = \mu_B^2 \frac{1}{4\pi^3\hbar} \int \frac{dS}{v} , \tag{3.4}$$

where μ_B is the Bohr magneton and $N(\zeta)$ is the density of states in energy at the Fermi surface.

For the "eight-cone" model surface we have

$$v = (\hbar p/m)\{x^2 + y^2 + [f'(z)]^2\}^{1/2} , \tag{3.5}$$

and Eq. (3.4) gives

$$\chi_P = \frac{e^2 p}{mc^2\pi^2} \int_{z_1}^{1} dz = \frac{e^2 p}{mc^2\pi^2} (1 - z_1) \tag{3.6}$$

and

$$\chi_P = \chi_P^{\text{free}} (4p/k_F)(1 - z_1) , \tag{3.7}$$

where χ_P^{free} is the spin susceptibility of free electrons. Now, to derive an expression for the diamagnetic susceptibility χ_L suitable for solid noble metals, we start from the general expression given by Misra, Mohanty, and Roth,[13] which we simply adapt to our case in order to take into account the effective shape of the Fermi surface. Taking also into account the cubic symmetry of the problem, we obtain in our notations

$$\chi_L = \frac{e^2}{12m^2c^2\pi^3} \left[\frac{\hbar^2}{4} \int d^3k\, F'(E) - \hbar^2 u^2 \int d^3k \frac{F'(E)}{[(1-z)^2+u^2]^{3/2}} \left(\frac{1}{6} - \frac{k_\rho^2}{8p^2[(1-z)^2+u^2]^{1/2}}\right) - \frac{mu^2}{4p^2} \int d^3k \frac{F(E)}{[(1-z)^2+u^2]^2} \left(1 - \frac{k_\rho^2}{p^2[(1-z)^2+u^2]^{1/2}}\right)\right] , \tag{3.8}$$

where the local z axis is parallel to the axis of the cone, $F'(E)$ is the derivative of the Fermi function $F(E)$, and k_ρ is the component of the k momentum normal to the z axis.

The integrals are to be extended to each cone and then multiplied by 8 to get the total contribution to the diamagnetic susceptibility. Using cylindrical coordinates and the fact that at zero temperature $F'(E) = -\delta(E - \zeta)$, we have for the first term χ_1 in Eq. (3.8)

$$\chi_1 = -\frac{e^2 p}{3\pi^2 mc^2} \int_{z_1}^{1} dz \int d\left(\frac{\hbar^2 k_\rho^2}{2m}\right) \delta\left(\frac{\hbar^2 k_\rho^2}{2m} + \frac{\hbar^2}{m} f(k_z) - \zeta\right) . \tag{3.9}$$

Integrating this expression over the Fermi surface, we obtain

$$\chi_1 = -\frac{e^2 p}{3\pi^2 mc^2} (1 - z_1) . \tag{3.10}$$

As may be easily seen from Eqs. (2.6) and (2.7), χ_1 gives the Landau diamagnetism for free electrons if one takes the correct limit $1 - z_1 \to z_2 - z_1 = k_F/4p$ for a spherical Fermi surface. On the same basis it is a matter of algebraical derivation to obtain the correct result for the second and third terms in Eq. (3.8). We will limit ourselves to reporting the final result,

$$\chi_L = \chi_L^{\text{free}} (4p/k_F)(1 - z_1 - u^2 I + \tfrac{7}{18} u^2 H) , \tag{3.11}$$

where χ_L^{free} is the nonoscillatory diamagnetic susceptibility of free electrons

$$I = \frac{1 - z_1}{u^2} \frac{1}{[(1-z_1)^2+u^2]^{1/2}} \left(\frac{(\epsilon_F - \frac{1}{2})^2}{u^2} - \frac{u^2}{4} - \frac{1}{3}\right) - \frac{1}{3u^4} \frac{(1-z_1)^3}{[(1-z_1)^2+u^2]^{3/2}} (\epsilon_F - \tfrac{1}{2} + \tfrac{1}{2}u^2)^2 + \tfrac{1}{4} \ln\left|\frac{(1-z_1) + [(1-z_1)^2+u^2]^{1/2}}{u}\right| , \tag{3.12}$$

and H is a very complicated expression which results from integrating the third term into the cone for z varying from zero to z_1. For this reason we will report here only the terms of H which give a significant contribution to χ_L,

$$H \simeq \frac{1}{2u^2} \left[\frac{1+u^2}{u} \left(\tan^{-1}\frac{1}{u} - \tan^{-1}\frac{1-z_1}{u}\right) + \frac{z_1^2 - z_1(1+u^2)}{(1-z_1)^2+u^2}\right] - \tfrac{7}{18} \ln\left|\frac{1+(1+u^2)^{1/2}}{(1-z_1) + [(1-z_1)^2+u^2]^{1/2}}\right| . \tag{3.13}$$

As we have succeeded in obtaining the contribution to susceptibility from the nearest (111) $\vec{G}$ vectors, it would be very simple to take into account, by means of a nondegenerate calculation, the contribution given by the more distant reciprocal-lattice vectors. However, as they usually contribute about 1% of the total value,[1,5] we neglect them with a

TABLE I. Susceptibility corrections for solid metals.

	u^a	Δ_L	Δ_P	u^b	Δ_L	Δ_P
Cu	0.20	−0.70	0.57	0.142	−0.96	0.50
Ag	0.168	−0.89	0.54	0.14	−1.03	0.51
Au	0.188	−0.79	0.56	0.15	−0.95	0.52

[a] From de Haas–van Alphen measurements (see Ref. 12).
[b] From optical measurements (see Refs. 14 and 15).

TABLE II. Parameters which enter in Eq. (4.5).

	r_1	r_2	A	V_0
Cu	1	1.815	0.50	1.90
Ag	1	2.38	0.68	2.95
Au	1	2.60	0.50	2.66

TABLE III. Susceptibility corrections for liquid metals.

	Δ_L	Δ_P
Cu	−0.26	0.29
Ag	−0.36	0.35
Au	−0.39	0.40

very small error.

To emphasize the deviations from the free-electron values we write

$$\chi_P = \chi_P^{\text{free}}(1+\Delta_P)\,, \quad \chi_L = \chi_L^{\text{free}}(1+\Delta_L)\,.$$

We have calculated Δ_P and Δ_L for solid noble metals using for u both the values deduced from de Haas–van Alphen experiments, as reported in Ziman,[12] and the values deduced from the optical measurements of the band gap at L.[14,15]

As may be seen in Table I, the results are nearly similar for the two sets of experimental u values, both giving almost a vanishing diamagnetic susceptibility for the conduction electrons.

IV. SUSCEPTIBILITY OF LIQUID METALS

The expressions for spin and diamagnetic susceptibility of liquid metals have been recently calculated in the pseudopotential formalism by Timbie and White.[16] However, these expressions can be also briefly derived from the analog expressions for solid metals[1,5] by going to the correct continuum limit for the reciprocal-lattice sums $\sum_{\vec{G}} \to (\Omega/8\pi^3)\int d^3q\,|S(q)|^2$, where Ω is the volume and $S(q)$ is the liquid-structure factor. If we write $\chi_P = \chi_P^{\text{free}} \times (1+\Delta_P)$, we obtain from Abe's expression[1]

$$\Delta_P = -\frac{3}{32\xi_0^2}\int_0^\infty dk\, I(k)\, v^2(k)\, G_P(k)\,, \tag{4.1}$$

$$G_P(k) = 2k\ln\left|\frac{k+2}{k-2}\right| - \frac{8k^2}{k^2-4}\,. \tag{4.2}$$

Here $k = q/k_F$, $I(k) = N|S(k)|^2$ is the interference function for the liquid, and $v(k)$ is the pseudopotential form factor.

In an analogous way we write $\chi_L = \chi_L^{\text{free}}(1+\Delta_L)$ for the diamagnetic susceptibility and obtain from the Misra and Roth expression[5] in the nondegenerate case

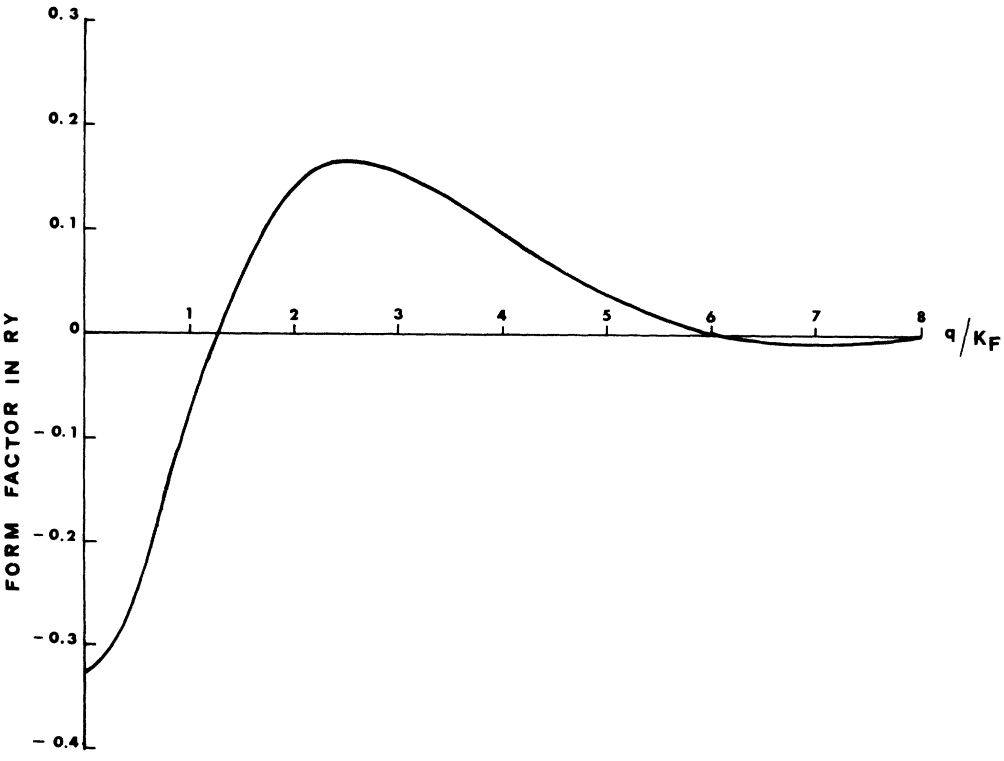

FIG. 1. Pseudopotential form factor for copper at liquid density.

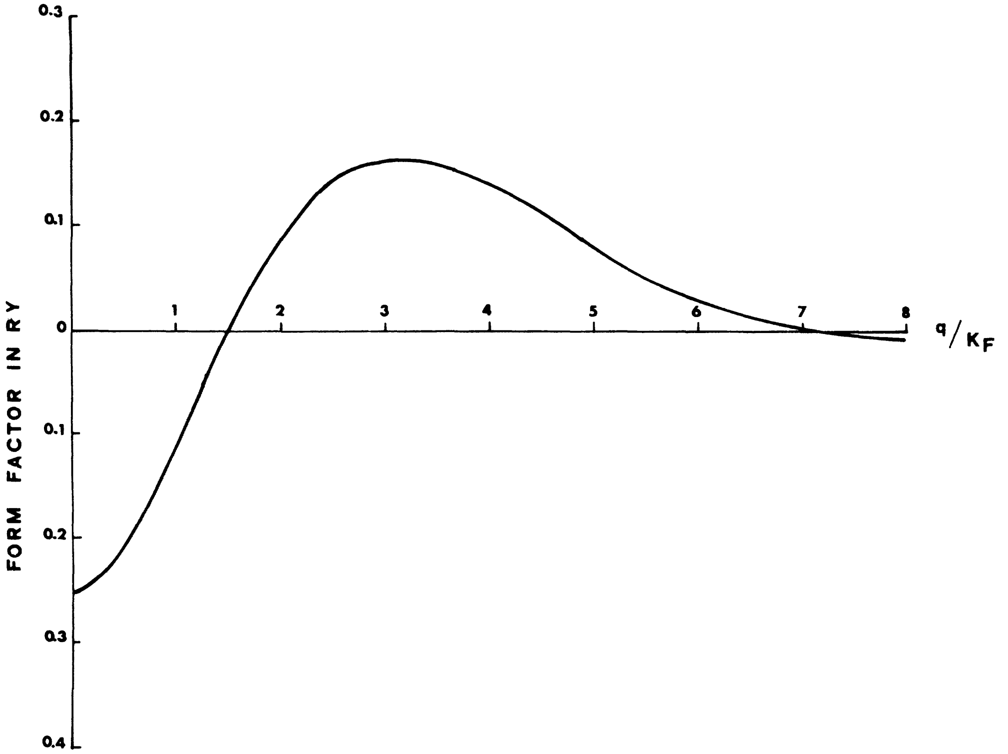

FIG. 2. Pseudopotential form factor for silver at liquid density.

$$\Delta_L = -\frac{3}{32\xi_0^2}\int_0^\infty dk\, I(k)\, v^2(k)\, G_L(k)\ , \qquad (4.3)$$

$$G_L(k) = \frac{2}{k}(k^2+2)\ln\left|\frac{k+2}{k-2}\right| - \frac{8}{3}\,\frac{24-22k^2+3k^4}{(k^2-4)^2}\ . \qquad (4.4)$$

Once these expressions have been obtained, the basic requisite for investigating the magnetic properties of liquid noble metals is the knowledge of suitable interference functions and pseudopotential form factors.

The interference functions we use are calculated by means of the Percus Yevick theory, according to the procedure outlined in Ashcroft and Lekner.[17]

The packing density is 0.45 for Ag and Au and 0.456 for Cu. The pseudopotential form factors are taken from a semiempirical model potential recently proposed by the present authors,[8]

$$v(q) = -\frac{4\pi e^2}{\Omega_0\epsilon(q)q^2}\Big(\cos(qr_2) + \frac{A}{q}[\sin(qr_2) - \sin(qr_1) - qr_2\cos(qr_2) + qr_1\cos(qr_1)] - \frac{V_0}{q}[\sin(qr_1) - qr_1\cos(qr_1)]\Big)\ , \qquad (4.5)$$

where Ω_0 is the volume per ion and $\epsilon(q)$ is the Hartree dielectric function. The values of the parameters r_1, r_2, A, and V_0 appropriate to the liquid noble metals are reported on Table II in atomic units. As may be seen in Figs. 1–3, these form factors converge properly for $q \gg k_F$.

The results of the calculation are given in Table III. The integrals which appear in Eqs. (4.1) and (4.3) are evaluated first by integrating numerically on each side of $k=2$ and then calculating analytically the contribution of the divergences at $k=2$ as principal value.[16]

V. COMPARISON WITH EXPERIMENT AND DISCUSSION

Before comparing calculated susceptibilities with experiment we must give a brief account of the effect of the exchange and correlation of the electrons. Unfortunately, in the case of the diamagnetic susceptibility, the effect of the exchange and correlation is not well understood at metallic densities.[18,19]

TABLE IV. Correlation corrections for noble metals.

	r_s	$\delta_{\mathrm{ex+cor}}$
Cu	2.67	−0.21
Ag	3.01	−0.22
Au	3.00	−0.22

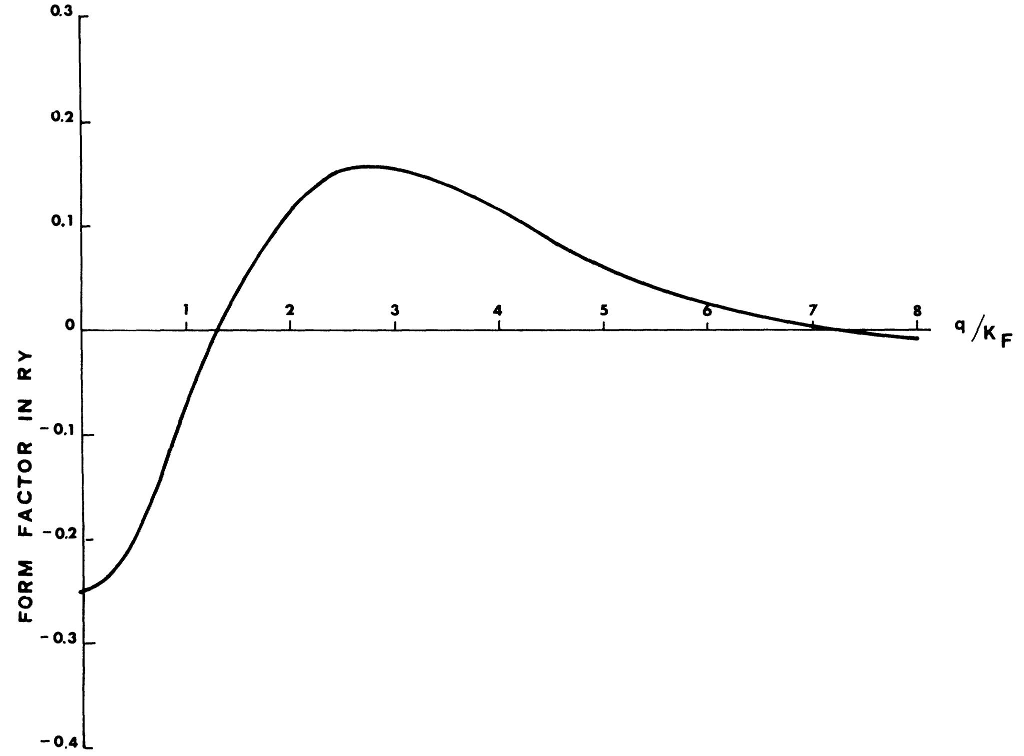

FIG. 3. Pseudopotential form factor for gold at liquid density.

However, a recent calculation by Isihara and Tsai,[19] who evaluate the exchange and correlation contribution to χ_L to second order in the interparticle spacing r_s, would give very small corrections at densities of interest here ($r_s \simeq 3$). For these reasons we do not take into account any correlation correction to χ_L and will limit ourselves to consider the corrections to χ_P only.

Including the exchange and correlation effects,[20] the spin susceptibility becomes

$$\chi_P = \chi_P^{\text{free}} \left(1 + \delta_{\text{ex+cor}} - \frac{\Delta_P}{1+\Delta_P}\right)^{-1} , \qquad (5.1)$$

where $\delta_{\text{ex+cor}}$ can be estimated from Silverstein's work[20] and we have replaced m/m^* in Silverstein's expression by $(1+\Delta_P)^{-1}$, the free-electron-to-band-mass ratio. Correlation corrections to χ_P are reported in Table IV for the solid noble metals. At liquid densities the values of $\delta_{\text{ex+cor}}$ are practically unchanged. In Table V our theoretical values for the total electronic susceptibility χ_E are listed and compared with the available experimental data.[21-23]

Since no direct experimental measurements of either the diamagnetic or the spin susceptibility of noble metals are available, the experimental values of χ_E have been obtained in an indirect way from the relation

$$\chi_E = \chi_T - \chi_i ,$$

TABLE V. Electronic susceptibility of solid and liquid noble metals[a](10^{-6}emu/g).

	Liquid χ_E			Solid χ_E				$\chi_{\text{liq}} - \chi_{\text{sol}}$		
	Free	Calc.	Expt.	Free	Calc.[b]		Expt.	Calc.[b]		Expt.
Cu	0.070	0.160	0.10	0.072	0.243	0.236	0.22	−0.083	−0.076	−0.12
Ag	0.052	0.134	0.09	0.055	0.188	0.186	0.21	−0.054	−0.052	−0.10
Au	0.029	0.078	0.07	0.030	0.103	0.101	0.16	−0.025	−0.023	−0.07

[a] The experimental values of χ_E in the liquid and of $\chi_{\text{liq}} - \chi_{\text{sol}}$ are taken from Ref. 21; the experimental values of χ_E in the solid have been obtained from Ref. 22.

[b] The first column refers to the u value deduced from de Haas–van Alphen experiments (see Ref. 12), the second to the u value from optical measurements (see Refs. 14 and 15).

where χ_T is the measured total magnetic susceptibility and χ_i is the susceptibility of the ion cores.

In spite of the general good agreement between experiment and theory, we wish to point out that same caution must be adopted in examining the experimental values of χ_E. Indeed, as pointed out by Cusack,[21] the uncertainty here is rather large, particularly in subtracting χ_i.

However, it might be argued that whatever χ_i is, it should not be affected very much by melting, and that therefore the change in the susceptibility at the melting point is a better experimental test of the theory than its magnitude. For this reason the shift in the electronic susceptibility at the melting point $\Delta\chi = \chi_{\text{liq}} - \chi_{\text{sol}}$ is also given in Table V and compared with the experimental value.

The theory predicts the correct sign for the shift and gives a fair account of its magnitude. It should be emphasized again that the error in the experimental values is quite large.

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[1] R. Abe, Progr. Theoret. Phys. (Kyoto) 29, 23 (1963).

[2] A. G. Samoilovich and E. Ya. Rabinovich, Fiz. Tverd. Tela 5, 778 (1963) [Sov. Phys. Solid State 5, 567 (1963)].

[3] M. L. Glasser, Phys. Rev. 134, A1296 (1964).

[4] K. Yamaji and R. Kubo, J. Phys. Soc. Japan 25, 330 (1968).

[5] P. K. Misra and L. M. Roth, Phys. Rev. 177, 1089 (1969).

[6] E. Borchi and S. De Gennaro, Phys. Letters 34A, 19 (1971).

[7] J. A. Moriarty, Phys. Rev. B 1, 1363 (1970).

[8] E. Borchi and S. De Gennaro, Phys. Letters 32A, 301 (1970).

[9] A. Meyer, W. H. Young, and T. M. Hayes, Phil. Mag. 23, 977 (1971).

[10] S. Prakash, Phys. Letters 37A, 177 (1971).

[11] A. B. Pippard, Phil. Trans. Roy. Soc. London A250, 335 (1957).

[12] J. M. Ziman, Advan. Phys. 10, 1 (1961).

[13] P. K. Misra, S. P. Mohanty, and L. M. Roth, Phys. Rev. B 4, 1794 (1971).

[14] I. F. Cornwall, Phil. Mag. 6, 727 (1961).

[15] G. P. Pells and M. Shiga, J. Phys. C 2, 1835 (1969).

[16] J. P. Timbie and R. M. White, Phys. Rev. B 1, 2409 (1970).

[17] N. W. Ashcroft and J. Lekner, Phys. Rev. 145, 83 (1966).

[18] H. Kanazawa and N. Matsudaira, Progr. Theoret. Phys. (Kyoto) 23, 433 (1960).

[19] A. Isihara and J. S. Tsai, Phys. Rev. B 4, 2380 (1971).

[20] S. D. Silverstein, Phys. Rev. 130, 1703 (1963).

[21] N. E. Cusack, Rept. Progr. Phys. 26, 361 (1963).

[22] W. G. Henry and J. L. Rogers, Phil. Mag. 1, 237 (1956).

[23] B. G. Childs and J. Penfold, Phil. Mag. 2, 389 (1957).

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Low-Temperature Heat Capacity of β-Cerium and β-Cerium-Yttrium Alloys[*]

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The low-temperature heat capacity of a nearly pure β-cerium sample (91%β-9%α) and six β-stabilized Ce-Y alloys were determined between 2.5 and 20 °K. Three principal results were obtained. (i) All six alloys showed magnetic ordering characteristic of β-cerium; the ordering temperatures decreased linearly with yttrium concentration. (ii) The magnetic contribution to the heat capacity of β-cerium was found to depend on the cube of the temperature in agreement with spin-wave theory for an antiferromagnetic material. (iii) The entropy associated with magnetic ordering was found to be $R \ln 2$, and is consistent with a crystal field splitting of the $J=\frac{5}{2}$ multiplet into three doublets by the hexagonal lattice.

I. INTRODUCTION

This is the second in a series of papers concerning the physical properties of the low-temperature allotropes of metallic cerium. The first paper[1] was concerned with the low-temperature heat capacity measurement of pure, single-phase α-cerium (collapsed fcc, $a = 4.85$ Å) made at standard pressures. The purpose of this work was to study the β allotrope of metallic cerium (dhcp, $a = 3.68$ Å, $c = 11.92$ Å).

Magnetic-susceptibility[2,3] and neutron-diffraction experiments[4] have established that β-cerium undergoes an antiferromagnetic transition at 12.5 °K. Crystal field effects in β-cerium[5] based on heat-capacity measurements[6,7] have been considered, and an article by Gschneidner and Smoluchowski[8] discussed, among other topics, the electronic