for the Boltzmann factor. According to Fong's theory, however, C_{4v} sites should dominate C_{2v} sites at all temperatures up to the melting point of the crystal.[5] Either the binding energies used in the calculation are wrong or the populations are uncorrelated with the spectrum. Regardless, any attempt to utilize the fluorescent spectrum in determining the site distributions must start with the correct identification of the lines.

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Knight-Shift Calculations in Liquid Magnesium

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The Knight shift K_s and nuclear spin-relaxation time T_1 have been calculated in liquid Mg using the pseudopotential theory. The results of this calculation show that both K_s and T_1T are independent of temperature T within the error in our calculation. The calculated value of K_s at the melting temperature (651 °C) is $(0.10 \pm 0.005)\%$ which compares well with the recent experimental measurement $(0.112 \pm 0.004)\%$ made between -196 and 230 °C. From this evidence, it can be concluded that there is no significant change of K_s upon melting, contrary to what has been observed in Cd. The theoretical value of the Korringa ratio, $(K_s^2 T_1 T)_{\text{theor}} / (K_s^2 T_1 T)_{\text{ideal}}$, departs from its ideal value of unity by about 17%. This departure is attributed to the different role of exchange enhancement on the uniform and nonuniform spin paramagnetic susceptibilities.

I. INTRODUCTION

In this paper, we have investigated the temperature T dependence of the Knight shift K_s and nuclear spin-relaxation time T_1 in liquid Mg. Mg is a divalent metal and has hexagonal-close-packed (hcp) structure similar to Be and Cd. In general, these metals exhibit very interesting band structure and hyperfine properties.[1] The nuclear-magnetic-resonance properties of this divalent group have been extensively studied both experimentally[2-4] and theoretically[5,6] in the solid state. It is interesting to note that Cd shows a strong temperature dependence[4] of K_s, K_{an} (anisotropic Knight shift), and T_1T in the solid state. On the other hand, K_s in Mg[3] and presumably Be[2] is independent of temperature. Furthermore, K_s and T_1T in liquid Cd[4] exhibit no temperature dependence. The source of the temperature dependence has been explained in the solid[5] to be mainly due to the role of electron-phonon interactions and in the liquid[7] through the temperature dependence of the observed ionic interference functions. However, no such investigations have been made either in liquid Be or Mg. We will extend the theory developed earlier[8] for liquid Cd, to study the nuclear-magnetic-resonance properties of liquid Mg and attempt to understand the liquid-state properties as compared to those in the solid state.

The purpose of the present work is to calculate K_s and T_1 using pseudopotentials[9] and interference functions[10-12] in liquid Mg. The role of the Korringa constant and the effects involving the exchange interactions among conduction electrons in liquid Mg will also be discussed. In Sec. II, we will outline the theory of K_s and T_1 pertinent to liquid Mg, and in Secs. III and IV, we will, respectively, present and discuss the results.

II. RESUMÉ OF THE THEORY

A perturbation formulation of K_s and $T_1 T$ in the liquid metals using the nonlocal pseudopotentials has been recently carried out.[8] We will apply this theory to calculate the spin density up to second order in perturbation theory for liquid Mg using the local pseudopotential. For the sake of brevity, we will, however, outline a few basic steps in the theory, as they pertain to the particular case of liquid Mg. The expression for the Knight shift[13] is written as

$$K_s = \tfrac{8}{3}\pi\chi_s N\Omega_0 \mathcal{G} \ , \tag{1}$$

where χ_s, Ω_0, and N are, respectively, the Pauli spin paramagnetic susceptibility, ionic volume, and number of ions in the entire liquid under consideration. The spin density $\mathcal{G}$ in the liquid can be expressed as

$$\mathcal{G} = \langle (1/N)\textstyle\sum_i |\psi_{k_F}(\vec{R}_i)|^2\rangle \ . \tag{2}$$

In Eq. (2), $\psi_{k_F}(\vec{R}_i)$ is the value of the conduction-electron wave function, normalized over the entire volume of the liquid $N\Omega_0$ at the $\vec{R}_i$th ion site. As mentioned in the earlier paper,[8] the spin density $\mathcal{G}$ needs to be averaged over all the dynamic ion sites. A Fermi-surface averaging is not needed since the Fermi surface in the liquid is generally assumed to be spherical.

The spin density $\mathcal{G}$ in Eq. (2) can be simplified to the form

$$\begin{aligned}\mathcal{G} &= O_{k_F}{}^2\langle (1/N)\textstyle\sum_i |\phi_{k_F}(\vec{R}_i)|^2\rangle \\ &= O_{k_F}{}^2 P_F \ ,\end{aligned} \tag{3}$$

where

$$O_{k_F}{}^2 = \frac{1}{N_{k_F}}\Big(1-\sum_{ns} b_{ns}(\vec{k}_F)\,\Theta_{ns}(0)\Big)^2 \tag{4}$$

and $\phi_{k_F}(\vec{R}_i)$ is the pseudo-wave-function with momentum k_F. N_{k_F} in Eq. (4) is the normalization factor. $\Theta_{ns}(0)$ corresponds to the value of the core function "ns" at the origin, and

$$b_{ns}(\vec{k}) = \langle \Theta_{ns}(\vec{r})|e^{i\vec{k}\cdot\vec{r}}\rangle \tag{5}$$

is the orthogonalization parameter which measures the overlap of the plane wave with the core state. It should be noted that in deducing Eq. (3) from Eq. (2), one has to make the approximation

$$b_{ns}(\vec{k}) \simeq b_{ns}(\vec{k}_F) \ , \tag{6}$$

i.e., $b_{ns}(\vec{k})$ is a slowly varying function of k. This approximation has been made earlier[6] for solid Cd, and was found to produce 10% enhancement over the value obtained without this approximation. A similar calculation in solid Mg,[14] however, indicates[2] that this approximation influences the spin density by about 1%. As can be seen from Eqs. (3) and (4), the spin density $\mathcal{G}$ contains terms such as $b_{ns}(k_F)\,b_{n's'}(k_F)\,\Theta_{ns}(0)\,\Theta_{n's'}(0)$. For a multicore system, the orthogonal parameters $b_{ns}(k)$ for the inner cores are slowly varying functions of k, whereas for the outer cores, they vary appreciably with k. In addition, $b_{ns}(k)$ have smaller values for the inner cores than those of the outer ones. On the other hand, $\Theta_{ns}(0)$ is the largest for the innermost core. Thus, there is a competition between $b_{ns}(k_F)$ and $\Theta_{ns}(0)$ as to which core will contribute most to the spin density. It is generally found that the outermost ns core contributes most to the spin density. Thus the approximation in deducing Eq. (3) will be more valid for metals for which $b_{ns}(k)$ corresponding to the outermost ns core varies slowly with k for the momentum region of interest.

Using Eq. (3), the Knight shift in Eq. (1) can be rewritten as

$$K_s = \tfrac{8}{3}\pi\chi_s N\Omega_0 O_{k_F}{}^2 P_F \ , \tag{7}$$

where we define P_F to be the pseudospin density, i.e.,

$$P_F = (1/N)\langle \textstyle\sum_i |\phi_{k_F}(\vec{R}_i)|^2\rangle \ ; \tag{8}$$

the pseudofunction $\phi_{k_F}(\vec{R}_i)$ is then expanded by perturbation theory up to second order,

$$\phi_{k_F}(\vec{R}_i) = \phi_{k_F}^{(0)}(\vec{R}_i) + \phi_{k_F}^{(1)}(\vec{R}_i) + \phi_{k_F}^{(2)}(\vec{R}_i) \ , \tag{9}$$

where $\phi_{k_F}^{(0)}$, $\phi_{k_F}^{(1)}$, and $\phi_{k_F}^{(2)}$ are respectively, the standard zero-, first-, and second-order perturbation terms.[15] The pseudospin density P_F in Eq. (8) can now be expressed in terms of the various perturbation orders as

$$P_F = P_F(00) + P_F(01) + P_F(11) + P_F(02) \ , \tag{10}$$

where

$$P_F(00) = (1/N)\langle \textstyle\sum_i |\phi_{k_F}^{(0)}(\vec{R}_i)|^2\rangle \ , \tag{11}$$

$$P_F(01) = (1/N)\langle \textstyle\sum_i 2\,\mathrm{Re}\,\phi_{k_F}^{(0)}(\vec{R}_i)^*\phi_{k_F}^{(1)}(\vec{R}_i)\rangle \ , \tag{12}$$

$$P_F(11) = (1/N)\langle \textstyle\sum_i |\phi_{k_F}^{(1)}(\vec{R}_i)|^2\rangle \ , \tag{13}$$

$$P_F(02) = (1/N)\langle \textstyle\sum_i 2\,\mathrm{Re}\,\phi_{k_F}^{(0)}(\vec{R}_i)^*\phi_{k_F}^{(2)}(\vec{R}_i)\rangle \ . \tag{14}$$

In the above, the spin density P_F is broken into four parts purposely, because we want to see clearly the role of the various perturbation terms as well as to test the convergence of perturbation theory. Equations (11)–(14) have been derived for numerical evaluation in liquid Cd using the nonlocal pseudopotential. For the case of liquid Mg, we have, however, used the local pseudopotential; reasons for doing so will be discussed in Sec. III. The final expressions appropriate to the first- and

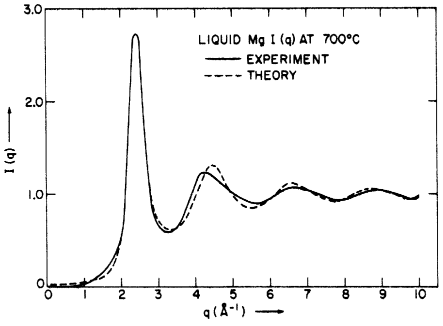

FIG. 1. Comparison between the HS and experimental $I(q)$ for liquid Mg at 700 °C. The experimental $I(q)$ were taken from Ref. (10), and the HS were obtained with the packing density $\eta = 0.47$.

second-order spin densities in Eqs. (12)–(14) are presented in the Appendix.

The spin density in Eq. (10) can also be used to calculate the nuclear spin-lattice-relaxation time[13] through the equation

$$1/T_1 T = \tfrac{16}{9}\pi^3\hbar^3\gamma_e{}^2\gamma_n{}^2 g^2(\epsilon_F)\, k_B (N\Omega_0 O_{k_F}{}^2 P_F)^2, \quad (15)$$

where γ_e and γ_n are, respectively, the electron and nuclear gyromagnetic ratios, k_B is the Boltzmann constant, and $g(\epsilon_F)$ is the band density of states per conduction electron. Had there been no complication due to the exchange enhancement, exchange core polarization, and orbital effects, we could have obtained $T_1 T$ using a calculated K_s and the Korringa relation

$$(K_s{}^2 T_1 T)_{\text{ideal}} = \left(\frac{\hbar}{4\pi k_B}\right)\left(\frac{\gamma_e}{\gamma_n}\right)^2 . \quad (16)$$

The ratio between $T_1 T$ calculated in this way and that of the experimental value will be utilized to analyze the importance of the core polarization and exchange enhancement effects.

III. COMPUTATION AND RESULTS

For the calculation of the Knight shift and nuclear spin-relaxation time in liquid metals, we require a knowledge of the interference function $I(q)$ and the pseudopotential form factors $v(q)$ of the ions. In the case of liquid Mg we have used both the experimental and theoretical $I(q)$. The experimental[10] $I(q)$ were taken from the work of Lukens and Wagner, and theoretical[11,12] ones were obtained from the hard-sphere (HS) model based on the Percus-Yevic theory.[16] Unfortunately, the experimental $I(q)$ are available only at one temperature (700 °C) close to the melting point, and the temperature dependence of $I(q)$ has not yet been measured. We have, therefore, used the HS model[11,12] for the temperature-dependence study of K_s and $T_1 T$. The packing-density parameter η was determined by comparing the HS and experimental $I(q)$ at 700 °C. Five temperatures appropriate to the available density data were selected; the relevant information is given in Table I. For Mg, the suitable packing density was found to have the value 0.47. It can be seen from Fig. 1 that the agreement between the HS and experimental $I(q)$ is very good. A comparison between the spin densities using both of these $I(q)$ at 700 °C will be made in Sec. IV. The HS $I(q)$ at five temperatures are plotted in Fig. 2.

Next we discuss the choice of the pseudopotential required to calculate the first- and second-order spin densities. Recently, Ritter and Gardner[17] have discussed the critical dependence of the calculated spin density on the choice of the potential in liquid Na. Ballentine,[18] in his calculation of the electronic structure of several liquid metals, noticed that the liquid-metal system behaves like a free-electron gas if the first node of the pseudopotential lies in the neighborhood of the main peak of the liquid interference function. Shaw and Smith[19] have pointed out that the use of nonlocal pseudopotentials, through their strong angular dependence, eliminates the above critical dependence of the results on the position of the node of the pseudopotential form factor. The latter viewpoint can still be achieved[20] with local pseudopotentials, if one makes use of the form of the pseudopotential over a large range [Eq. (A5)] and carries out the principal-value integration as suggested earlier.[8] However, for

TABLE I. Particle density, hard-sphere diameter, and various terms contributing to spin density in liquid Mg as a function of temperature.

Temperature in °C	Particle density in $Å^{-3}$	Hard-sphere diameter in Å	$2J_L$	J_L^2	$J_L'(1)$	$J_L'(2)$	$J_L'(3)$	$2J_L'$	$J_L^2 + 2J_L$
651	0.0390	2.845	−0.658	0.108	−0.172	0.002	0.043	−0.254	−0.146
700[a]	0.0307	2.868	−0.638	0.102	−0.161	0.002	0.054	−0.210	−0.108
700[b]	0.0307	2.868	−0.613	0.094	−0.149	0.002	0.035	−0.224	−0.130
750	0.0364	2.910	−0.605	0.092	−0.146	0.002	0.063	−0.162	−0.070
850	0.0340	2.978	−0.560	0.078	−0.123	0.002	0.084	−0.074	0.004
1000	0.0298	3.112	−0.494	0.061	−0.084	0.003	0.128	−0.094	−0.033

[a] J_L's are computed using HS $I(q)$.

[b] J_L's are computed using experimental $I(q)$.

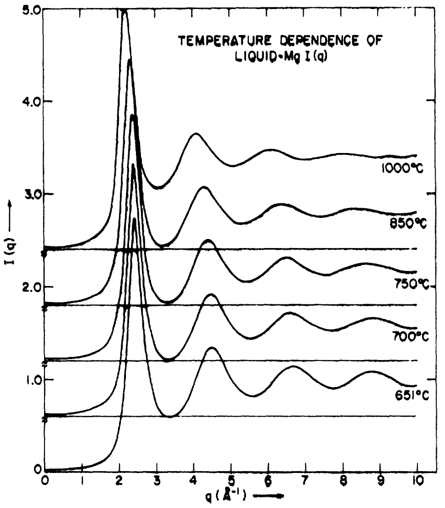

FIG. 2. Temperature dependence of HS $I(q)$ for liquid Mg calculated for five temperatures.

metals, such as Cd, the additional effort required for the nonlocal calculation cannot be avoided since Cd possesses *d* cores which have rather large overlap integrals. Additionally, the nonlocality of the pseudopotential in Cd has been shown[21] to be very important in interpreting the band structure and Fermi-surface dimensions in the solid state.

However, Mg does not have any *d* cores and the 1*s*, 2*s*, and 2*p* cores are fairly localized. Kimball *et al.*[22] found that both the nonlocal and local pseudopotentials in solid Mg yielded results in good agreement with the de Haas-van Alphen and magnetoresistance studies of the Fermi surface. Further, the spin densities calculated at one point on the Fermi surface of solid Mg using both the local and nonlocal pseudopotentials were in good agreement (within 5%) with each other (this was found by one of the authors, viz., P. J., after actual computations). We have, therefore, used the local pseudopotential form factors to calculate the spin density. This choice, in particular, simplifies to a large extent the amount of computational effort involved. For our calculation, we have used both the local-pseudopotential form factors $v(q)$ of Kimball *et al.*[22] and the model potential of Animalu and Heine.[9] The perturbation spin densities obtained using the local pseudopotential form factors $v(q)$ were found to be negative and about 60% of the zero-order spin density. This would indicate a substantial amount of *p* character in the electronic wave functions in the liquid. This conclusion seems rather unphysical since the Fermi electrons in Mg in the solid state exhibit strong *s* character.[1,23]

It should be pointed out that these local-pseudopotential form factors were obtained at the Fermi surface for four values of K [$(10\bar{1}0)$, (0002), $(10\bar{1}0)$, $(10\bar{1}2)$] and then fitted to an analytical form:

$$v(K) = A(K - K_0)\,e^{-B(K-K_0)},$$

where A, B, and K_0 are constants. In the solid state, K has to be the magnitude of a reciprocal-lattice vector, and therefore it is discontinuous. However, in the liquid state the periodicity of the lattice structure is absent and K takes continuous values, i.e., q. While the above form of $v(K)$ for $0.8 < q < 1.25a_0^{-1}$ may be quite accurate, its validity for all values of q ranging from 0 to ∞ is very uncertain. We have, therefore, used the model potential of Animalu and Heine[9] which at least does not possess this uncertainty.

We have plotted these local-pseudopotential[22] and model-potential[9] form factors in Fig. 3. It can be seen that these two kinds of form factors compare very well in the momentum transfer region $0.8 < q < 1.25a_0^{-1}$. Kimball *et al.*[22] have obtained excellent agreement with the Fermi-surface data by using $v(q)$, where q lies in the above region. However, for the calculation of spin density in the liquid state, it will be shown later (for example, in Fig. 4) that the momentum transfer region $\frac{3}{2}k_F < q < 3k_F$ ($k_F = 0.727a_0^{-1}$ for Mg) happens to be the most important region. It is clear from Fig. 3 that these two kinds of form factors are very different from each other in this region, the local-pseudopotential form factors being stronger. In view of these arguments, we have used the model-potential form factors for our present calculation.

The various terms in Eqs. (A1)-(A11) evaluated numerically using the model-potential form factors of Animalu and Heine[9] and the liquid interference functions[10-12] are presented in Table I for all the temperatures. We shall first compare the various terms in the second-order spin density. The (11) term (J_L^2) has opposite sign to the (02)

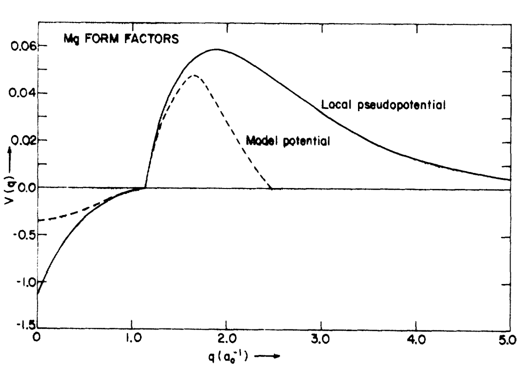

FIG. 3. Pseudopotential form factors (in units of rydbergs) for liquid Mg. The solid curve represents the local-pseudopotential form factors of Kimball *et al.*, while the broken curve represents the model-potential form factor. Note that the positive and negative scales are clearly different in the figure.

term (J_L') and is smaller in magnitude. The net contribution to the spin density from the second order is, therefore, negative but small. Among the three terms of J_L' [see Eq. (A6)], the $J_L'(1)$ term contributes most to the spin density and bears an opposite sign to that of $J_L'(2)$ and $J_L'(3)$. If the major contribution to these terms would have arisen from the region around the singularity ($k' = k_F$), then one would expect $J_L'(1)$ and $J_L'(3)$ to nearly cancel out while $J_L'(2)$ would be the only surviving term from the second order. However, the major contribution to J_L and various terms in J_L' comes from a region $\frac{3}{2}k_F < q < 3k_F$. This can be seen from Fig. 4, where we have plotted the integrand of the first-order contribution (i.e., integrand of $2J_L$) as a function of q. Similar behavior was observed for the integrands of the second-order terms contributing to the spin density.

It is interesting to note that the contributions from various second-order terms are individually smaller than the first-order contribution. In addition, cancellation among various second-order terms makes the net second-order contribution about a factor of 8 smaller than that of the first order. In Table II, we have presented the zero-, first-, and second-order contributions to the spin density for the five temperatures under study. The smallness of the second-order spin density compared to the first order shows a definite trend for convergence. The higher-order contributions to the spin density are expected to be still smaller since the major contributions arise from a momentum range $\frac{3}{2}k_F < q < 3k_F$, and the energy denominators increase rapidly with higher order of perturbation terms. This demonstration of convergence is important and gives us confidence in using the pseudopotential perturbation theory.

IV. DISCUSSIONS AND CONCLUSIONS

For the evaluation of the absolute value of the Knight shift, we need the magnitude of the Pauli spin paramagnetic susceptibility χ_s. Unfortunately, χ_s has not been measured either for solid or liquid Mg. We have, therefore, used the calculated free-electron value

$$\chi_s^{\text{free}} = 0.98 \times 10^{-6} \text{ cgs volume units,} \tag{17}$$

and then corrected this χ_s^{free} for the electron-electron exchange and correlation effects through the Silverstein theory.[24] Assuming the effective-mass ratio $m^*/m = 1$ for liquid Mg, the exchange enhancement of the uniform susceptibility turned out to be

$$\eta_s = 1.35 \ . \tag{18}$$

Thus, the free-electron exchange enhanced susceptibility is

$$\chi_s = 1.32 \times 10^{-6} \text{ cgs volume units .} \tag{19}$$

The direct contribution to Knight shift, K_s^d, can now be calculated for the five temperatures using the spin densities in Table II, the spin susceptibility in Eq. (19), and the enhancement factor $O_{k_F}{}^2$ in Eq. (4). To evaluate $O_{k_F}{}^2$, we have calculated the orthogonalization integrals $b_t(k_F)$ in Eq. (5) using the Hartree-Fock atomic core functions for Mg tabulated by Mann.[25] The densities of the ns core functions Θ_{ns} were also taken from tables given by Mann. Thus, for Mg

$$O_{k_F}{}^2 = 108.36 \ . \tag{20}$$

In view of the convergence of the total spin density in Table II, we believe that our calculated Knight shift using χ_s from Eq. (19) can be accurate only up to second place of the decimal. Thus, for the first three temperatures, i.e., 651, 700, and 750 °C, we find that $K_s^d = 0.07 \pm 0.005\%$. However, for the next two higher temperatures, i.e., 850 and 1000 °C, $K_s^d = 0.08 \pm 0.005\%$. From these results we conclude that K_s^d in liquid Mg is almost temperature independent within the error of our calculation. For the exchange-core-polarization contribution to the Knight shift, K_s^{cp}, we have taken

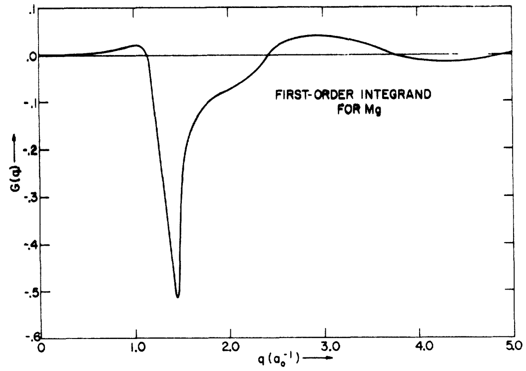

FIG. 4. Integrand of first-order contribution to spin density (i.e., integrand of $2J_L$) showing the momentum region from which the maximum contribution results.

TABLE II. Contributions to spin densities (in units of $1/N\Omega_0$) from zero-, first-, and second-order perturbation terms.

Temperature in °C	First order	Second order	Zero order	Total
650	−0.408	−0.056	1.0	0.536
700[a]	−0.396	−0.042	1.0	0.562
700[b]	−0.380	−0.050	1.0	0.570
750	−0.375	−0.027	1.0	0.598
850	−0.347	0.002	1.0	0.655
1000	−0.306	−0.013	1.0	0.681

[a] Refers to the HS $I(q)$.

[b] Refers to the experimental $I(q)$.

the one-OPW result, namely, 0.03%, and have considered it to be insensitive to the temperature in comparison to K_s^d (see, for example, Ref. 14). Thus the total K_s is about 0.10%.

Unfortunately, no experimental measurement on K_s is available for liquid Mg. However, recent experimental study[3] on K_s ($0.112 \pm 0.004\%$) in solid Mg from -196 to 230 °C shows no variation of K_s with temperature. The predicted results indicate that K_s in liquid Mg apparently does not undergo a significant discontinuous change upon melting, contrary to what has been experimentally observed in Cd.[4] This apparent difference between Mg and Cd may be attributed to the different degree of free-electron behavior as is exhibited by the shapes of the Fermi surfaces in these two metals.[21, 22, 26] Mg possesses all the segments of the Fermi surface (i.e., monster, lens, butterflies, cigars, and caps) that can be constructed from the Harrison model[9] for the free electrons. On the other hand, Cd possesses only the lens and monster which have substantial p character at low temperatures. With the rise of temperature, these segments become more s-like[5] and butterflies start appearing. Since Mg is a free-electron-like metal even at low temperatures, the Fermi surface and the angular character of the electrons are not expected to change appreciably.

In computing the relaxation time $T_1 T$ using the Korringa relation[27] and the calculated K_s, it should be recalled that the value of K_s was derived using the exchange enhanced χ_s. Since exchange enhancement effects on uniform and nonuniform χ_s are different, one has to divide the K_s values by the enhancement factor η_s and then utilize the Korringa relation to obtain $T_1 T$. The values of $T_1 T$ obtained in this manner are 130 ± 10 deg sec for the first three temperatures. The electron-electron exchange and correlation effects on the relaxation time, η_M, are incorporated using the Moriya theory,[28] i.e.,

$$(T_1 T)_{\mathrm{Moriya}} = (T_1 T)/\eta_M \,, \tag{21}$$

where for liquid Mg

$$\eta_M = 1.57 \,. \tag{22}$$

Thus the corrected relaxation time 82 ± 7 deg sec is also independent of temperature. The theoretical Korringa ratio then becomes

$$(K_s^2 T_1 T)_{\mathrm{theor}} / (K_s^2 T_1 T)_{\mathrm{ideal}} = 1.17 \,, \tag{23}$$

which departs from the noninteracting value of unity by 17%. This difference is probably due to the different role of exchange enhancement effect on the uniform and nonuniform χ_s. To establish this point unequivocally, it will be worthwhile to study other metals with particular reference to η_s and η_M.

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APPENDIX

Following the procedure developed in the earlier paper, we now write down the explicit forms for the various spin densities as stated in Eqs. (11)–(14). These spin-density functions are applicable to the local pseudopotentials, and are much simpler than those for the nonlocal pseudopotentials. We can readily show that for liquid Mg,

$$(N\Omega_0) P_F(00) = 1 \,, \tag{A1}$$

$$(N\Omega_0) P_F(01) = [\Omega_0/(2\pi)^3] 2\,\mathrm{Re} J_L \,, \tag{A2}$$

$$(N\Omega_0) P_F(11) = [\Omega_0^2/(2\pi)^6] |J_L|^2 \,, \tag{A3}$$

$$(N\Omega_0) P_F(02) = [\Omega_0^2/(2\pi)^6] 2\,\mathrm{Re} J_L' \,. \tag{A4}$$

The expressions for the various J_L''s are found to be

$$J_L = 2\pi \mathcal{P} \int_0^\infty \frac{k'^2 dk'}{k_F^2 - k'^2} \int_{-1}^1 I\left((k_F^2 + k'^2 - 2k_F k' x)^{1/2}\right) \times v\left((k_F^2 + k'^2 - 2k_F k' x)^{1/2}\right) dx \,,$$

which also can be written as

$$J_L = \frac{\pi}{k_F} \mathcal{P} \int_0^\infty I(q)\, v(q) \ln \left| \frac{q - 2k_F}{q + 2k_F} \right| q\, dq \tag{A5}$$

and

$$J_L' = J_L'(1) + J_L'(2) + J_L'(3) \,, \tag{A6}$$

where

$$J_L'(1) = \frac{\pi}{k_F} \mathcal{P} \int_0^\infty I(q) v(q) F(q) \ln \left| \frac{q - 2k_F}{q + 2k_F} \right| q\, dq \,, \tag{A7}$$

$$J_L'(2) = -2\pi \mathcal{P} \int_0^\infty \frac{I(q)\, |v(q)|^2}{q^2 - 4k_F{}^2}\, dq \,, \tag{A8}$$

$$J_L'(3) = -4\pi v(0) \mathcal{P} \int_0^\infty \frac{I(q) v(q)\, dq}{q^2 - 4k_F{}^2} \,, \tag{A9}$$

where $\mathcal{P}$ means principal part. Here, the interference function $I(q)$ and the total pseudopotential $V(r)$ have forms

$$I(q) = (1/N) \left\langle \textstyle\sum_i \sum_\nu e^{i\vec{q} \cdot (\vec{R}_i - \vec{R}_\nu)} \right\rangle \tag{A10}$$

and

$$V(\vec{r}) = \textstyle\sum_\nu v(|\vec{r} - \vec{R}_\nu|) \,, \tag{A11}$$

where $v(|\vec{r} - \vec{R}_\nu|)$ is the potential of the single ion.

The function $F(q)$ is given by

$$F(q) = \frac{\pi}{q} \mathcal{P} \int_0^\infty q'\,dq'\,I(q')\,v(q') \ln \left| \frac{k_F^2 - q'^2 - q^2 - 2qq'}{k_F^2 - q'^2 - q^2 + 2qq'} \right| . \tag{A12}$$

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