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# Enhancement of the Korringa Constant in Alkali Metals by Electron-Electron Interactions

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The theory of Moriya is extended to include electron-electron interaction potentials with a strong momentum dependence. This extension is based on recent theoretical studies of the electron-gas response. It is shown that the observed enhancement of the Korringa relation in alkali metals can be attributed almost entirely to electron-electron interactions described by an effective interaction potential derived from the pair-correlation function for a low-density electron gas.

#### I. INTRODUCTION

In the alkali metals, the s-contact hyperfine interaction is the dominant mechanism coupling nuclear spins with the conduction electrons. Consequently, one might expect that the Knight shift K and the spin-lattice relaxation time  $T_1$  would satisfy the well-known Korringa relation<sup>1</sup>

$$K^2 T_1 T = S = (\gamma_e / \gamma_n)^2 (\hbar / 4\pi k_B)$$
, (1.1)

where  $\gamma_e$  and  $\gamma_n$  are the electronic and nuclear gyromagnetic ratios, respectively. However, experimental values of  $K^2T_1T$  are typically 60% higher than predicted by (1.1). Since (1.1) was derived in the independent-particle approximation, this discrepancy has traditionally been attributed to electron-electron interactions. <sup>2,3</sup> The experimental and theoretical situation has been reviewed in a recent paper by Narath and Weaver, <sup>4</sup> and these authors concluded that the data could not be adequately explained by Moriya's theory, in which electron-electron interactions are assumed to have zero range.

Narath and Weaver<sup>4</sup> have given a rather complete discussion of various possible explanations for the remaining discrepancy between theory and experiment. Of these explanations, perhaps the most appealing (and the only one we consider explicitly in this paper) is that a zero-range interaction potential is not realistic, and should be replaced by an effective interaction obtained from detailed theoretical studies of electron-gas response. Actually, Narath and Weaver<sup>4</sup> did consider this possibility briefly. They introduced an effective potential (in momentum space) of the form suggested

by Hubbard<sup>5</sup> (a screened Coulomb potential in real space) and found for Na a screening parameter of about  $2k_F$ . However, they concluded that the result had only qualitative significance, primarily because they felt that approximations made in deriving an expression for the enhancement factor limited the result to potentials with constant Fourier transforms (that is, with no momentum dependence). We have concluded, on the basis of recent studies of electron-gas response, <sup>6</sup> that constraints on the effective interaction potential are less restrictive than suggested by Narath and Weaver. <sup>4</sup>

There exist in the recent literature various expressions for the effective exchange-correlation potentials which are thought to be reasonable approximations at metallic densities. We demonstrate in this paper that when these results are used in Moriya's theory of Korringa enhancement, essentially all of the experimentally observed enhancement can be attributed to electron-electron interactions. This conclusion is based on the observation that Stoner enhancement factors determined by equating theoretical and experimental Korringa enhancement are found to predict correctly the observed enhancement of the susceptibility in sodium and lithium.

### II. THEORY AND CALCULATIONS

Since the relevant theory has been clearly reviewed by Narath and Weaver, <sup>4</sup> we will confine the present discussion to a summary of the results pertinent to our calculations. We will, however, consider in some detail the validity of two essential approximations involved in obtaining the results we have used, introducing in this context results

from a recent series of papers on the dielectric response of an electron gas.  $^{7-10}$ 

In the presence of electron-electron interactions, the Knight shift is enhanced relative to the independent particle result  $K_0$  by the Stoner factor  $(1 - \alpha)^{-1}$ :

$$K = K_0/(1-\alpha)$$
, (2.1)

where  $\alpha$  is related to the strength of the effective electron-interaction potential  $V(\bar{\mathbf{q}})$  and the density of states at the Fermi level  $\rho_0(E_F)$  by  $\alpha = V(0)\rho_0(E_F)$ . Following the Moriya theory, <sup>2,3</sup> one obtains a similar expression for the enhanced spin-lattice relaxation time

$$T_1^{-1} = (T_{1,0})^{-1} \langle [1 - \alpha \overline{V}(\overline{q})F(\overline{q})]^{-2} \rangle$$
 (2.2)

The brackets  $\langle \ \rangle$  indicate that the enhancement factor is to be averaged over all scattering momenta q connecting states on the Fermi surface. The function  $\overline{V}(\overline{\mathbf{q}}) = V(\overline{\mathbf{q}})/V(0)$  appearing in (2.2) is a normalized interaction potential. If we approximate the Fermi surface by a sphere we obtain for  $F(\overline{\mathbf{q}})$  the usual Lindhard function

$$F(\eta) = \frac{1}{2} \left( 1 + \frac{4 - \eta^2}{4\eta} \ln \left| \frac{2 + \eta}{2 - \eta} \right| \right)$$
, (2.3)

where  $\eta = q/k_F$  is the scattering momentum scaled by the Fermi momentum.

Now, if we take the Knight shift  $K_0$  and the spinlattice relaxation time  $T_{1,0}$  computed in the independent-particle approximation to be related by the Korringa constant S in (1.1), then, following Moriya,  $^3$  we can define a Korringa enhancement factor  $K(\alpha)$  by the relation

$$K^2T_1T = SK(\alpha)^{-1}$$
 (2.4)

By combining (2.1) and (2.2) we obtain an explicit expression for  $K(\alpha)$ :

$$K(\alpha) = \frac{(1-\alpha)^2}{2} \int_0^2 d\eta \, \eta [1-\alpha \, \overline{V}(\eta) F(\eta)]^{-2} \,, \quad (2.5)$$

where we have expressed the average over a spherical Fermi surface explicitly.

The approximations required in the derivation of (2.5) are discussed by Narath and Weaver. 4 We concentrate here on two fundamental assumptions which have been shown to be less restrictive<sup>6</sup> than had been thought previously, particularly in the case of free-electron-like simple metals. The first of these is the assumption that exchange and correlation between conduction electrons can be described by an effective potential  $V(\vec{q})$  depending only on the momentum q transferred during the interaction. Such a local function  $V(\overline{q})$  obviously cannot give an exact description of the exchangecorrelation potential, but it has been demonstrated in recent work<sup>7-10</sup> that such an approximation has reasonable justification at metallic densities. Furthermore, model potential theories of metallic

properties based on such an approximation for the exchange-correlation potential have been found to give excellent agreement with experiment.  $^{11,12}$  We should emphasize that this success in calculating properties such as phonon spectra does not alone constitute a rigorous justification of the q-dependent potential approximation. Furthermore, the theoretical developments we have cited,  $^{7-10}$  while based on plausible assumptions, are difficult to defend rigorously. The theoretical response functions, though asymptotically correct in both longand short-wavelength limits,  $^{8,13}$  are still uncertain in the intermediate wave-number region around  $q = 2k_F$  which is most critical for calculations of metallic properties.

The second, and related, assumption is that the susceptibility for an interacting electron gas can be written in the form

$$\chi(\vec{\mathbf{q}}, \omega) = \frac{\chi_0(\vec{\mathbf{q}}, \omega)}{1 - V(q)\chi_0(\vec{\mathbf{q}}, \omega)} \quad . \tag{2.6}$$

Clearly, if V(q) is taken to be frequency dependent, (2.6) is a canonical form which requires no approximation whatever and in essence simply defines  $V(q,\omega)$ . The work of Singwi<sup>9</sup> and co-workers indicates that (2.6) follows directly from a natural extension of random-phase approximation (RPA), and that V(q) is given by

$$V(q) = (4\pi/q^2) G(q) , \qquad (2.7)$$

where G(q) is a function coupled to the pair-correlation function g(r) by a simple set of transform relations. 10 A result similar to (2.6) is obtained from the work of Kleinman<sup>7</sup> and of Langreth<sup>8</sup> [there is a subtle formal difference 13, 14 between the approach of these two authors and that of Singwi et al., which, for the present purpose, we can take into account by the selection of an appropriate G(q) in<sup>13</sup> (2.7)]. The essential point to note here is that the recent derivations of (2.6) do not confine the result to situations in which V(q) is a constant. Hence, the constraint on V(q) imposed in the Narath-Weaver work can be lifted with some confidence. In particular, we know that an electronelectron dielectric function obtained directly from  $\chi(\bar{q}, \omega)$  of the form given in (2.6) leads to screenedmodel potentials which appear to provide accurate descriptions of properties such as phonon spectra for both monovalent and polyvalent simple metals. 11,12 There is good reason to expect that the same approach can be applied successfully in the present problem.

It is worth inserting a further word of caution at this point. First, we emphasize again that while (2.6) has the correct leading behavior at both long- and short-wavelength limits, it is definitely not an exact result at intermediate wavelengths. Second, we remark that we are dealing

with a result obtained from density-response theory, in which the susceptibility function  $\chi(\vec{q},\omega)$  is related to dielectric function by

$$\epsilon(\vec{q}, \omega) = 1 - (4\pi/q^2)\chi(\vec{q}, \omega) . \qquad (2.8)$$

In principle, the magnetic-susceptibility function should have precisely the same functional form as (2.6) with a change only in the interaction strength. Note that in Eq. (2.5) the strength of potential has been extracted explicitly in the Stoner parameter  $\alpha$ .

The function  $\overline{V}(\eta)$  appearing in (2.5) describes only the wave-number dependence of the potential. If we adopt the notation of (2.7) we can write  $\overline{V}(\eta)$  as

$$\overline{V}(\eta) = G(\eta)/\gamma \eta^2 \quad , \tag{2.9}$$

where  $\gamma$  is defined as  $\gamma = \lim[G(\eta)/\eta^2]$  as  $\eta \to 0$ , so that  $\overline{V}(0) = 1$ . Note that  $G(\eta)$  is also an implicit function of  $\gamma$ . An explicit expression for  $\gamma$ , appropriate for the dielectric response analysis, can be derived in terms of the exchange-correlation energy  $E_{xc}(\rho_0)$  of an electron gas with density  $Q_0^{10,11}$ .

$$\gamma = \frac{k_F^2}{4\pi e^2} \frac{d^2}{d\rho_0^2} \left[ \rho_0 E_{xc}(\rho_0) \right] . \tag{2.10}$$

If we use the expression for  $E_{xc}(\rho_0)$  given by Nozières and Pines, <sup>15</sup> we obtain

$$\gamma = \frac{1}{4} + 0.0123(\alpha_0 r_s), \quad \alpha_0 = (4/9\pi)^{1/2}.$$
 (2.11)

The first and dominant term in this expression arises from exchange interactions, the second from correlations. Recall that for alkali metals,  $r_s$  ranges between 3 and 6.

We emphasize again that (2.10) is valid in principle only for the compressibility  $\kappa$ . If we apply the compressibility sum rule to (2.8) we obtain

$$\frac{\kappa}{\kappa_F} = \left(1 - \frac{4\alpha_0 \gamma_s}{\pi} \gamma\right)^{-1} , \qquad (2.12)$$

where  $\kappa_F$  is the free-electron compressibility. Comparing this result to the Fermi-liquid theory expression 16

$$\frac{\kappa}{\kappa_{\rm F}} = \frac{m^*}{m} (1 + A_0)^{-1} , \qquad (2.13)$$

which contains only the phonon-enchanced effective mass and the Landau parameter  $A_0$ , we see that if  $\gamma \approx \frac{1}{4}$  then  $A_0 \cong -\alpha_0 r_s/\pi$ , which is approximately correct. <sup>16</sup> Now the long-wavelength limit of the susceptibility is related to the Landau parameter  $B_0$  by an expression similar to (2.13):

$$\frac{\chi}{\chi_F} = \frac{m^*}{m} (1 + B_0)^{-1} . {(2.14)}$$

If we write  $\chi/\chi_F$  in the form of (2.12), with  $\gamma$  re-

placed by  $\gamma'$ ,

$$\frac{\chi}{\chi_F} = \left(1 - \frac{4\alpha_0 r_s}{\pi} \gamma'\right)^{-1} , \qquad (2.15)$$

we find that

$$\gamma' = \gamma + \frac{\pi}{4\alpha_0 r_0} \frac{m}{m^*} (A_0 - B_0)$$
 (2.16)

It is  $\gamma'$  which determines the strength of the potential appropriate to the susceptibility. We have in effect written  $\alpha \simeq (4\alpha_0 r_s/\pi)\gamma'$  in Eq. (2.5).

For the purpose of the present calculation, we have introduced the following ansatz. We have used two forms of  $G(\eta)$ , both derived from independent studies of electron-gas response, and both depending implicitly on the parameter  $\gamma$ . We then regard (2.9) as a parametrized function specifying the wave-number dependence of the interaction, and we use the value  $\gamma$  [Eq. (2.11)] which is appropriate to the actual derivation of the  $G(\eta)$  functions. In effect, this ansatz assumes that the wave-number dependence of  $\overline{V}(\eta)$  is a general property of the interacting system and the strength of the potential alone is determined by the details of the response being considered. As a test that this approximation does not lead to serious inconsistency we later compare the  $\gamma'$  obtained theoretically from (2.16) with that obtained from  $\gamma' = \alpha \pi / 4\alpha_0 r_s$  where we use the  $\alpha$  deduced by comparing the theoretical and experimental  $K(\alpha)$ .

The first of the effective potentials we have considered is a result due to Kleinman<sup>7</sup> which can be written as

$$\overline{V}_{k}(\eta) = \frac{1}{2} \left[ 1 + 1/(1 + \gamma \eta^{2}) \right]. \tag{2.17}$$

The second is a result derived by Shaw<sup>10</sup> using a pair-correlation function valid for a low-density electron gas (a physical example of such a system is an alkali metal). The function  $G(\eta)$  is given in terms of the Dawson integral D(x), a standard tabulated function, <sup>10,17</sup> and the resulting  $\overline{V}(\eta)$  is

$$\overline{V}_s(\eta) = \frac{1}{\gamma \eta^2} \left[ 1 - \frac{2\beta}{\eta} D\left(\frac{\eta}{2\beta}\right) \right], \quad \beta^2 = (6\gamma)^{-1}. \quad (2.18)$$

These two functions  $\overline{V}(\eta)$  are compared with  $\overline{V}\equiv 1$  in Fig. 1. At very short wavelengths  $(\eta-\infty)$ ,  $\overline{V}_k(\eta)+\frac{1}{2}$ , whereas  $\overline{V}_s(\eta)+0$ . This difference arises from the fact that Kleinman<sup>7</sup> and Langreth<sup>8</sup> have included self-energies in the noninteracting susceptibility  $\chi_0(\overline{q},\omega)$  which enters Eq. (2.6). <sup>13,14</sup> What is most important for the present work is the behavior of  $\overline{V}(\eta)$  in the range  $0\leq \eta \leq 2$ . It is clear from Fig. 1 that both Eqs. (2.17) and (2.18) deviate appreciably from  $\overline{V}=1$  over this momentum range.

The evaluation of  $K(\alpha)$  requires only a simple numerical integration, the accuracy of which we can test by comparing the results for  $\overline{V}=1$  with those given by Narath and Weaver. We carry out

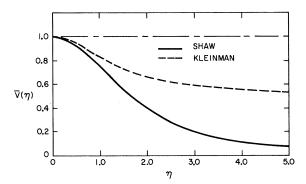


FIG. 1. Comparison of three models of the normalized effective interaction potential  $\overline{V}(\eta)$  as a function of  $\eta$ .

a separate calculation for each of the alkali metals, using Eq. (2.11) to determine the appropriate  $\gamma$ .

#### III. RESULTS AND DISCUSSION

We consider first the case of exchange enhancement alone  $(\gamma = \frac{1}{4})$ , and compare the  $K(\alpha)$  obtained using the two effective potentials (2.17) and (2.18) with the zero-range results of Narath and Weaver. Numerical values for  $K(\alpha)$  are given in Table I. It is clear from a plot of these results (Fig. 2) that use of a realistic exchange potential leads to a substantial reduction in  $K(\alpha)$ , particularly in the intermediate  $\alpha$  range. An increase in  $\gamma$  tends to further reduce  $K(\alpha)$  at a given  $\alpha$ , though reduction is not dramatic as illustrated in Fig. 3.

The next step is to determine by interpolation the value of  $\alpha$  for which the theoretical and experimental enhancement factors  $K(\alpha)$  agree. We list in Table II the results obtained using the two expressions for the interaction potential,  $\overline{V}_k(\eta)$  and  $\overline{V}_s(\eta)$ , and compare them to the Narath-Weaver re-

TABLE I. Comparison of  $K(\alpha)$  obtained with three different effective potentials.  $\overline{V}=1$  is the case treated by Narath and Weaver (Ref. 4).  $\overline{V}_k$  and  $\overline{V}_s$  are the Kleinman and Shaw expressions discussed in the text [Eqs. (2.17) and (2.18)]. These results are for exchange enhancement only,  $\gamma=\frac{1}{4}$ .

α		$K(\alpha)$	
	$\overline{V}$ = 1	$\overline{V} = V_k$	$\overline{V} = V_{\mathcal{S}}$
0.0	1.000	1.000	1.000
0.1	0.9566	0.9339	0.9231
0.2	0.9078	0.8622	0.8415
0.3	0.8523	0.7843	0.7550
0.4	0.7886	0.6993	0.6632
0.5	0.7147	0.6063	0.5657
0.6	0.6277	0.5043	0.4621
0.7	0.5234	0.3922	0.3525
0.8	0.3950	0.2692	0.2370
0.9	0.2307	0.1357	0.1171
1.0	0.0000	0.0000	0.0000

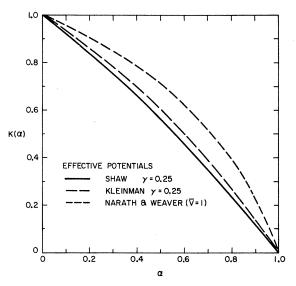


FIG. 2. Korringa enhancement factor  $K(\alpha)$  as a function of  $\alpha$  computed using the three interaction potentials discussed in the text.

sults. Typically, the new values of  $\alpha$  obtained using the Shaw potential (for example) are smaller by approximately 30%.

As a check on the suitability of our choice of  $\gamma$ , we compute the parameter  $\gamma'$  defined in Eq. (2.16) using theoretical Landau parameters given by Rice. <sup>18</sup> There is some uncertainty in the values of  $A_0$ ,  $B_0$ , and  $m^*/m$ , and this in turn leads to some variation in the computed  $\gamma'$ . In Table III we give two sets of parameters for Na and the resulting  $\gamma'$ . For comparison we compute  $\gamma'$  from the value of  $\alpha^s$  given in Table II using the approximate result that  $\alpha \cong (4\alpha_0 r_s/\pi)\gamma'$ . The value we obtain lies midway between the two theoretical results. We make a similar comparison for K and find a slightly greater discrepancy than for Na. However, the Landau parameters we have used are rather uncertain for various reasons discussed by Rice, <sup>18</sup>

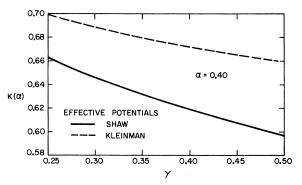


FIG. 3. Variation of  $K(\alpha)$  as a function of the parameter  $\gamma$  for  $\alpha$  = 0.4. Results for the Kleinman and Shaw interaction potentials are given.

and consequently we regard the agreement as satisfactory. The conclusion we draw from the results of Table III is that the use of a  $\gamma$  appropriate to density-response theory to describe the q dependence of the potential is a reasonable procedure and leads to susceptibility parameters  $\gamma'$  which are substantially in agreement with theoretical values.

To evaluate the internal self-consistency of our results, we compare the values of  $\alpha$  given in Table II with the Stoner parameters obtained independently from electronic susceptibility measurements. As a specific example, we consider sodium metal. The value of  $\alpha$  determined by Narath and Weaver<sup>4</sup> from susceptibility data and Ham's <sup>19</sup> effective mass is  $\alpha = 0.42 \pm 0.03$ . We plot in Fig. 4 the theoretical  $K(\alpha)$  over this range of  $\alpha$  for the three models we have been considering, and on the same plot we indicate the experimental  $K(\alpha)$  for sodium. The intersection of experimental and theoretical enhancement factors occurs well within the specified range of  $\alpha$  for the Shaw model but not for either of the other two.

A similar approach could be used for lithium metal, for which susceptibility data are also available. However, there are two complicating factors: (i) The effective mass for lithium is less certain than it is for sodium and (ii) there is a substantial p core-polarization contribution to the lithium Knight shift. 20 It is therefore tempting to turn the argument around and use the  $\alpha$  determined from a theoretical prediction of the Korringa enhancement in lithium to estimate the band effective mass. The result we obtain using the susceptibility data for lithium is  $m^* = 1.52 \pm 0.07$ , a slightly smaller value than the  $m^* = 1.66$  calculated by Ham. <sup>19</sup> However, this calculation of  $m^*$  may be somewhat misleading since we have yet to take account of p-state contirbutions. Gaspari et al. 20 have calculated the p core-polarization contribution to the Knight shift, and they obtain a 23% reduction from the s-state contribution. Using the Shaw model to calculate  $K(\alpha)$ , we find that this reduction corresponds to a 60% decrease in  $\alpha$  and consequently a decrease in the effective mass to  $m^* = 0.86$ . Since various

TABLE II. Values of  $\alpha$  obtained by equating the experimental enhancement factor taken from the work of Narath and Weaver (NW) with theoretical calculations of  $K(\alpha)$  using Kleinman (K) and Shaw (S) interaction potentials. The new values are compared to the  $\overline{V}=1$  results of NW.

Metal	γ	$K(\alpha)_{\text{expt}}$	$\alpha^{NW}$	$\alpha^{\mathrm{K}}$	α <sup>S</sup>
Li	0.271	0.637	0.59	0.462	0.420
Na	0.275	0.625	0.60	0.474	0.431
K	0.281	0.614	0.61	0.484	0.440
Rb	0.283	0.617	0.61	0.479	0.436
Cs	0.286	0.578	0.65	0.519	0.474

TABLE III. Comparison of the parameter  $\gamma'$  computed from (2.16) and the corresponding value computed from the results of Table II assuming  $\gamma' = \pi \alpha^S/4\alpha_o \gamma_s$ . The Landau parameters and effective masses used in the theoretical calculation are taken from Rice (Ref. 18).

Metal	$A_0$	$\boldsymbol{B}_0$	$m^*/m$	γ′	$\pi \alpha^S / 4\alpha_0 r_s$	
Na	-0.62	-0.14	1.26	0.131	0.163	
	-0.45	-0.17	1.19	0.186		
K	-0.58	-0.24	1.11	0.188	0.135	

independent calculations<sup>19,21</sup> have shown that the Fermi-level density of states in lithium is considerably greater than the corresponding free-electron density of states, we conclude that this  $m^*$  is unrealistic. This conclusion is further supported by Hodgson's<sup>22</sup> measurement of the optical mass for lithium,  $m^* = 1.57$ .

It seems clear that the difficulty here cannot be with the exchange-correlation calculation. If we take the value  $\alpha=0.365$  obtained from Ham's mass and the measured susceptibility and compute the enhancement factor  $K(\alpha)=(1-\alpha)^2$  which is applicable to the extreme limiting case of an effective electron-electron interaction with infinite range [i.e.,  $V(q)=V\delta(q)$ ], we obtain  $K(\alpha)\equiv 0.403$ . This value of  $K(\alpha)$ , which is effectively a theoretical minimum, still exceeds the value  $K(\alpha)=0.376$  obtained by reducing the experimental  $K(\alpha)$  by 41% as suggested by the results of Gaspari  $et\ al.^{20}$ 

There remains the possibility that the calculation of p core-polarization effects may be inaccurate. It is difficult to assess from the analysis given by Gaspari  $et\ al.$  how sensitive their numerical result is to variations in the wave functions or to terms which were neglected when these wave functions were expanded in powers of the Fermi mo-

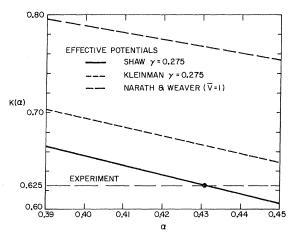


FIG. 4.  $K(\alpha)$  for Na for  $\alpha$  in the range determined by susceptibility measurements (Ref. 4). Results for three interaction potentials are shown, and the experimental enhancement factor (Ref. 4) is indicated explicitly.

TABLE IV. Measured susceptibility for the alkali metals in units of the free-electron susceptibility. The values of  $\alpha$  corresponding to each  $\chi/\chi_F$  are computed using the procedure of Narath and Weaver (Ref. 4), and an effective mass calculated by Ham (Ref. 19).

Metal	Effective	Direct		Spin Wave		Alloy Knight shifts	
	mass <sup>a</sup>	$\chi/\chi_F$	$\alpha$	$\chi/\chi_F$	α	$\chi/\chi_F$	α
Li	1.66	$2.61 \pm 0.12^{b}$	0.365	• • •	•••	• • •	
Na	1.00	$1.72 \pm 0.08^{c}$	0.420	$1.51 \pm 0.06^{d}$	0.337	1.73°	0.422
K	1.09	• • •	• • •	$1.64 \pm 0.05^{d}$	0.335	1.58 <sup>f</sup>	0.310
Rb	1.21	•••	• • •	$1.71 \pm 0.5^{8}$	0.29	1.55f	0.219
Cs	1.76	•••	•••	$2.05 \pm 0.5^{g}$	0.14	h	• • •

<sup>&</sup>lt;sup>a</sup>Reference 19.

<sup>h</sup>Kaeck (Ref. f) found  $\chi/\chi_F$  to be the same for Rb and Cs. If we then use  $\chi/\chi_F = 1.55$  and  $m^* = 1.76$ , we obtain a negative  $\alpha$ 

mentum ( $k_F$  = 0.598 a.u. for lithium). It would be of interest to recompute the p core-polarization contributions to  $K(\alpha)$  using wave functions obtained from Ham's 19 band calculation. It is interesting to note that a 5% increase in the Knight shift due to p core-polarization is required to obtain consistency between Knight-shift and susceptibility measurements if we assume that the exchange-correlation enhancement is given correctly by the present theory.

There exist in the literature values for the susceptibilities of potassium, rubidium, and cesium obtained in various indirect ways. We list in Table IV the results which are available to us at the present time. Direct susceptibility measurements have been made only on lithium and sodium. We feel that these results are quite reliable and have made use of them in the preceding discussion. The spin-wave results are obtained by fitting the excitation spectrum to a theoretical dispersion relation,  $^{16}$  thereby obtaining  $B_0$ . The susceptibility is then computed from (2.14) using measured cyclotron resonance or specific-heat masses. It is worth emphasizing that the susceptibility is obtained rather indirectly and depends on theoretical interpretation of spin-wave data. In the case of the results based on liquid alloy Knight shifts, the susceptibilities are inferred by normalizing to the direct susceptibility measurement for pure sodium. The reliability of this method, which depends on calculated contact densities, is somewhat uncertain. There is a rather obvious test of the method which seems not to have been attempted and that is to measure the Knight shifts of lithium-based alloys in order to see if the direct susceptibility measurement for pure lithium can be verified by extrapolation of the Li-alloy results.

Several features of Table IV deserve further comment. One is the discrepancy between direct and spin-wave determinations of the susceptibility for sodium. While our calculations are in rather good agreement with the direct measurement, they agree poorly with the spin-wave result. Note also that the spin-wave result for potassium exceeds that for sodium, whereas the opposite trend is indicated by the liquid-alloy results. The enhancement factors  $\alpha$  which we obtain from the various indirect measurements are substantially below those suggested in Table II. In fact, they imply that the effective exchange-correlation potential is approaching the limiting case of infinite range. Part of the difficulty may be due to the selection of effective mass, or to the exclusion of core-polarization effects. However, one thing seems clear, namely, that direct susceptibility measurements for potassium, rubidium, and cesium are essential before a complete test of our model can be made.

Though the situation is still somewhat unclear for lithium, due to uncertainty about the magnitude (and sign) of core-polarization contributions, we can conclude from the sodium results that if a realistic electron-electron interaction potential is used in computing the Korringa enhancement factor  $K(\alpha)$ , one can explain essentially the entire enhancement which is observed experimentally. This conclusion is based on the internal consistency between Korringa and susceptibility enhancement factors which we obtain for sodium. If we assume small core-polarization contributions in lithium, a similar internal consistency is achieved. In our opinion, the uncertainty of the experimental data for the other alkalis rules out further checks on

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cR. T. Schumacher and W. E. Vehse, J. Phys. Chem. Solids 24, 297 (1963).

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Reference value taken from c. Deviation is due to decreased density of the liquid.

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<sup>&</sup>lt;sup>8</sup>These numbers are very crude and should be regarded only as estimates. The value  $B_0 = -0.3 \pm 0.15$  [G. Dunifer (private communication)] was used in both cases. The Azbel-Kaner masses used are from C. C. Grimes *et al.* [Bull. Am. Phys. Soc. 12, 415 (1967)].

the enhancement theory for the present. Our results imply that the additional mechanisms (orbital and dipolar interactions and differential chemical shifts) mentioned (and dismissed) by Narath and Weaver<sup>4</sup> do not play a dominant role in Korringa

enhancement. However, until this is demonstrated by explicit calculations, we would caution against using a Korringa enhancement calculation to test the suitability of a particular exchange-correlation potential.

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PHYSICAL REVIEW B

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## Many-Electron Effects on the Enhancements of the Korringa Constants and Spin-Lattice Relaxation Rates in Alkali Metals\*

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A quantitative explanation of the observed enhancements of the Korringa product and the ratio of Zeeman to dipolar spin-lattice relaxation times in sodium is given. The explanation is based on an extension of the theories of Moriya and Wolff, using for the generalized paramagnetic susceptibility the expression given by the self-consistent theory of Singwi *et al.* of spin correlations in a low-density interacting electron gas. The theory also predicts that the Korringa constant in the alkali metals is almost constant — a result in agreement with experiment.

#### I. INTRODUCTION

It is well known<sup>1</sup> that the many-body effects of electron-electron interactions are manifested in a direct way, at least in simple metals, via the enhancement of the paramagnetic susceptibility over its free-electron value through the so-called Stoner factor  $(1-\alpha)^{-1}$ . It is also known that these correlations lead to an enhancement of the Knight shift  $K_s$  and the nuclear spin-lattice relaxation rates  $T_1^{-1}$ , thereby giving a value for the Korringa constant<sup>2</sup> which is again different from its free-

electron value  $[K_s^2T_1T=(g\mu_B/\nu_n)^2(\hbar/4\pi k_B)\equiv K_c^0]$ . The Korringa relation is valid provided the dominant hyperfine coupling between the conduction electrons and the nuclear spins is of the s type. Recently Narath and Weaver³ have made a careful experimental investigation of the Korringa relation in the alkali and noble metals. These authors have attempted to understand their data in terms of Moriya's theory⁴ which is based on several assumptions: (i) the existence of a spherical Fermi surface, (ii) a  $\delta$ -function electron-electron interaction potential, and (iii) the random-phase approxi-