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Non-rigid-muffin-tin calculations of the electron-phonon interaction in simple metals

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The Gaspari-Gyorffy theory for calculating the electron-phonon interaction λ is extended to incorporate a correction to the rigid-muffin-tin approximation (RMTA). This correction is achieved by constructing a potential which has the correct asymptotic behavior at large distances and reduces to essentially a uniform potential well inside the muffin-tin sphere. This method is particularly applicable to the simple metals where the usual RMTA underestimates λ. The results obtained without any adjustable parameter are in better agreement with the experimental data than those obtained by the RMTA.

I. INTRODUCTION

The Gaspari-Gyorffy (GG) theory[1,2] has been successful[3,4] in calculating the phonon-mediated electron-electron interaction for transition metals in terms of first-principles band-structure results. However, application of the theory to simple metals gives a systematic underestimation of the electron-electron attraction.[3-5] To trace out the sources of this discrepancy one must examine the various approximations entering the derivation of the GG theory. The first such approximation is the so-called spherical approximation (SA) which assumes a spherical averaging of the Fermi-surface integrals. The SA has been tested[4] and shown to contribute insignificant errors (2% or less) to the calculation. Another approximation is the so-called local approximation (LA) which neglects the phonon-mediated attraction between two electrons from different atoms. Recently, Rietschel[6] examined the validity of the local approximation in detail. The conclusion from Rietschel's[6] work is that the LA is adequate when the umklapp electron-phonon scattering is large, while for normal processes the LA overestimates the electron-electron attraction. Thus the corrections to the LA will tend to further increase the discrepancy between theoretical results and experimental data. Hence, one has to conclude that the theoretical underestimation of the electron-electron attraction in simple metals is mainly due to the rigid-muffin-tin approximation (RMTA), in which the local environment of a vibrating atom is approximated by rigidly displacing the muffin-tin potential for that atom.

II. THEORY

In order to proceed with our theory for removing the RMTA we will recall that Rietschel[6] expressed the Eliashberg function $\alpha^2(\omega)F(\omega)$ in terms of an integral in $\vec{q}$ space involving an on-Fermi-sphere electron-ion pseudopotential $V(q)$ given, in atomic units, by

$$V(q)=\frac{-1}{\pi n_t(E_F)}\left[\frac{E_F}{E_F^0}\right]^{1/2}\times\sum_l\left[\frac{n_l n_{l+1}}{n_l^{(1)}n_{l+1}^{(1)}}\right]^{1/2}A_{l,l+1}(E_F)\times\sum_{l'=0}^{l}(2l'+1)P_{l'}\left[1-\frac{q^2}{2k_F^2}\right]. \tag{1}$$

In Eq. (1), E_F^0 is the free-electron Fermi level, E_F is the Fermi energy n_l, $n_l^{(1)}$ are the partial density of states at the Fermi level for the solid and the free scatterer, respectively, and n_t is the total density of states per spin per atom; $A_{l,l+1}(E_F)$ is given by

$$A_{l,l+1}(E_F)=\int_0^{\infty} dr\, r^2 R_l \frac{dU}{dr} R_{l+1} , \tag{2}$$

where R_l is the radial wave function and U is the potential associated with each moving ion. An equivalent expression for the electron-phonon pseudopotential $V(q)$ has been obtained by Allen and Lee.[7] In this formalism the LA is equivalent to the replacement (in the expression for α^2F) of a phonon-dependent factor by an appropriate average value.[6] The calculation of the potential U is a very difficult problem because it requires the knowledge of the electronic response to the motion of one (or more) ions. It has been shown[8] that U must satisfy the sum rule

$$U_t(\vec{r})=\sum_i U(\vec{r}-\vec{R}_i)+\text{const} , \tag{3}$$

where $U_t(\vec{r})$ is the total periodic crystalline potential, $\vec{r}$ is the position vector of the electron, and $\vec{R}_i$ is the equilibrium position vector of the ith ion. Furthermore, Heine *et al.*[9] have proved by employing linear response theory that

$$\lim_{q\to 0} V(q)=-\frac{Z}{2n_t(E_F)} , \tag{4}$$

where Z is the valency. It must be noted that Eq. (4) remains true[9] even if many-body effects are included. For real anisotropic solids, where in general V is a function of two wave vectors $\vec{k}$ and $\vec{q}$, Eq. (4) remains valid on the average,[9] i.e.,

$$\lim_{q\to 0} 2\sum_k V_k(q)\delta(E_k-E_F)=-Z . \tag{5}$$

Thus any approximation which produces a $\vec{k}$-independent $V(q)$ must satisfy Eq. (4). On the other hand, Eq. (4) being a linear response result may not be valid if the potential U is very strong as, e.g., in the case of transition metals.[10]

The RMTA assumes that U is equal to the muffin-tin potential U_{MT} determined usually by an augmented plane wave (APW) or Korringa-Kohn-Rostoker (KKR) band-structure calculation. By setting $U=U_{\text{MT}}$ in Eq. (2) one obtains[1,2] that

$$A_{l,l+1}^{\text{RMTA}}=\sin(\delta_l-\delta_{l+1}) , \tag{6}$$

where δ_l are phase shifts at $E=E_F$ corresponding to the muffin-tin potential U_{MT}. It must be pointed out that the RMTA choice for U automatically satisfies Eq. (3). However, the RMTA does not in general satisfy Eq. (4). The physical reason for this failure is the following: The $q=0$ condition [Eq. (4)] reflects the fact that at large distance $|r-R_i|$ the ionic potential U is behaving (at least in the weak limit) as a screened Coulomb potential, i.e.,

$$\lim_{|r-R_i|\to\infty} U(r-R_i)=-\frac{Ce^{-q_{\text{TF}}r}}{r} , \tag{7}$$

where q_{TF} is the Thomas-Fermi wave vector given by (in atomic units)

$$q_{\text{TF}}^2=(12/r_{\text{WS}}^3)n_t(E_F) , \tag{8}$$

where r_{WS} is the Wigner-Seitz radius. Actually, the Fourier transform of the rhs of Eq. (7), divided by the atomic volume $4\pi r_{\text{WS}}^3/3$, gives in the limit $q\to 0$ just $-Z/2n_t(E_F)$ if C is chosen, in atomic units, as $2Z$. The RMTA, by assuming that $U_{\text{MT}}=0$ for $|\vec{r}-\vec{R}_i|>r_{\text{MT}}$ (where r_{MT} is the muffin-tin radius), does not have the correct behavior for large $|\vec{r}-\vec{R}_i|$ and hence is not expected to produce a $V(q)$ which will behave correctly at $q=0$. Note that one can write

$$U=U_{\text{MT}}+U_c^* , \tag{9}$$

where $U_c^*(\vec{r}-\vec{R}_i)=\text{const}$ for $\vec{r}-\vec{R}_i$ within the Wigner-Seitz cell and zero outside, without violating Eq. (3). This freedom of the additive constant has been employed[7,11,12] in the literature to improve the RMTA in conjunction with the additional simplifying approximation of replacing the Wigner-Seitz cell by a muffin-tin sphere. A variant of this approach that utilizes phase shifts fitted to the Fermi-surface measurements was recently proposed by Coleridge.[13] A different point of view to treat screening in transition rather than simple metals was taken by Pettifor.[14]

In the present work we combine the idea of adding a constant-potential well to the muffin tin, with the correct asymptotic behavior given by Eq. (7). Thus we write (by taking from now on R_i equal to zero)

$$U(r)=U_{\text{MT}}(r)+U_c(r)+U_1(r) , \tag{10}$$

where

$$U_c(r)=U_0\{(r/r_{\text{MT}})\exp[q_{\text{TF}}(r-r_{\text{MT}})]+1\}^{-1} . \tag{11}$$

$U_c(r)$ is a simple function which, for $q_{\text{TF}}(r_{\text{MT}}-r)>>1$, reduces to a constant-potential well of depth U_0, while, for $q_{\text{TF}}(r-r_{\text{MT}})>>1$, behaves as the rhs of Eq. (7). Because of the tail in $U_c(r)$, the sum $U_{\text{MT}}(r)+U_c(r)$ does not satisfy Eq. (3). The last term in Eq. (10), $U_1(r)$, has been added as to ensure the validity of Eq. (3). Without loss of generality we took $U_1(r)=0$ for $r>r_{\text{MT}}$ and $U_1(0)=0$. We found that the contribution of the term $U_1(r)$ to our final results is of the order of 5% or less.

Thus in what follows we omit the contribution of $U_1(r)$ by taking it as zero.

Combining Eqs. (2), (10), and (11) we obtain

$$A_{l,l+1}=\sin(\delta_l-\delta_{l+1})+\int_0^\infty dr\, r^2 R_l \frac{dU_c}{dr} R_{l+1}\ . \quad (12)$$

The yet undetermined parameter U_0, which characterizes the strength of the correction to the RMTA, will be obtained by requiring the validity of Eq. (4). Combining Eqs. (1), (4), (11), and (12) we obtain the following linear equation for U_0:

$$\left[\frac{E_F}{E_F^0}\right]^{1/2}\frac{1}{\pi n_t(E_F)}\left[\sum_l (l+1)^2\left[\frac{n_l n_{l+1}}{n_l^{(1)}n_{l+1}^{(1)}}\right]^{1/2}\sin(\delta_l-\delta_{l+1})-U_0 q_{\mathrm{TF}}\right.$$
$$\left.\times\sum_l (l+1)^2\left[\frac{n_l n_{l+1}}{n_l^{(1)}n_{l+1}^{(1)}}\right]^{1/2}\int_0^\infty dr\, r^2 R_l R_{l+1}\frac{(1+q_{\mathrm{TF}}r)e^{q_{\mathrm{TF}}(r-r_{\mathrm{MT}})}/r_{\mathrm{MT}}}{[(r/r_{\mathrm{MT}})e^{q_{\mathrm{TF}}(r-r_{\mathrm{MT}})}+1]^2}\right]$$
$$=\frac{Z}{2n_t(E_F)}\ . \quad (13)$$

In the first summation the $l>3$ terms are negligible due to the fact that $\delta_l\approx 0$ for $l>3$. In the second summation one has to include terms up to $l=10$ in order to obtain convergence for all cases. Thus we need the ratios $n_l/n_l^{(1)}$ for $l>3$ as well. These quantities were not given in Ref. 3 (the results of which are used in the present study), and are usually not available from band-structure calculations. We have calculated $n_l/n_l^{(1)}$ for $l>3$ assuming plane-wave behavior of the wave functions. This assumption, following Rietschel,[6] leads to the formula

$$\frac{n_l}{n_l^{(1)}}=\frac{n_t(E_F)}{n_0(E_F)} \quad (14)$$

with

$$n_0(E_F)=\frac{V}{4\pi^2 N}E_F^{1/2}\ , \quad (15)$$

where V/N is the unit-cell volume.

Equation (14) probably underestimates the ratio $n_l/n_l^{(1)}$, which as a result, produces an overestimation of U_0. In the integral of Eq. (13) we have approximated R_l by the following expression:

$$R_l(r_{\mathrm{MT}},E_F)=j_l(k_F r_{\mathrm{MT}})\cos\delta_l + y_l(k_F r_{\mathrm{MT}})\sin\delta_l\ , \quad (16)$$

where $k_F=E_F^{1/2}$ and j_l, y_l are spherical Bessel and Newmann functions, respectively. We have checked this approximation in Na, K, and Pb by using the actual APW wave function and found errors of less than 5%. Also, since by construction our potential U_c produces significant correction only near r_{MT}, it was sufficiently accurate to start the integration at the value $r_{\mathrm{MT}}-1/q_{\mathrm{TF}}$ and terminte it at $r\approx 10$ a.u.

Having determined U_0 we see that the correction to the RMTA is achieved by replacing $\sin(\delta_l-\delta_{l+1})$ with $A_{l,l+1}$ as given by Eq. (12). This replacement is now made in the original GG formula for the electron-mass-enhancement factor, i.e.,

$$\lambda=\eta/m\langle\omega^2\rangle\ , \quad (17a)$$

$$\eta=\frac{E_F}{\pi^2 n_t(E_F)}\sum_l \frac{2(l+1)n_l n_{l+1}}{n_l^{(1)}n_{l+1}^{(1)}}A_{l,l+1}\ . \quad (17b)$$

III. RESULTS AND DISCUSSION

The Fermi energy E_F, the total density of state (DOS) $n_t(E_F)$, the partial DOS ratios $n_l/n_l^{(1)}$, and the phase shift functions $A_{l,l+1}^{\mathrm{RMTA}}=\sin(\delta_l-\delta_{l+1})$ required for the present calculations were taken from Refs. 3 and 5 and are reproduced in Table I for the 15 metals indicated. In Table I we also show the present results for the plasmon energy Ω_p, for q_{TF} and U_0, and for the intermediate quantities $A_{l,l+1}$ given by Eq. (12).

Using these results and Eq. (17b) we obtain the quantity η shown in the second column of Table II. In the first column we reproduced for comparison the results of η_{RMTA}. The values of $m\langle\omega^2\rangle$ were obtained by using a parabolic $\alpha^2(\omega)F(\omega)$ approxi-

TABLE I. Input and intermediate quantities entering in the present calculations. Symbols are defined in the text.

Metal	E_F (Ry)	n_t (Ry/atom spin)$^{-1}$	Ω_p (eV)	q_{TF}	$n_s/n_s^{(1)}$	$n_p/n_p^{(1)}$	$n_d/n_d^{(1)}$	$n_f/n_f^{(1)}$	n_t/n_0
Li	0.290	3.40	6.53	1.091	0.955	1.751	1.450	3.167	1.73
Na	0.247	3.04	7.53	0.818	1.005	1.137	1.075	1.120	1.06
K	0.159	5.26	4.19	0.738	1.200	1.178	1.037	0.934	1.07
Rb	0.146	6.44	3.71	0.737	1.441	1.141	1.159	0.848	1.12
Mg	0.402	3.18	8.83	1.006	0.905	0.988	1.515	1.738	1.25
Ca	0.286	12.26	2.69	1.480	0.230	3.881	1.888	3.942	3.22
Be	0.814	0.44	3.00	0.631	0.502	0.089	0.626	0.083	0.35
Zn	0.611	2.14	10.85	1.063	1.262	0.733	1.462	1.417	1.13
Cd	0.512	2.48	9.32	0.951	1.336	0.718	1.381	1.146	0.99
Al	0.618	2.39	12.33	1.046	0.960	0.591	1.296	1.762	1.09
Ga	0.525	1.85	11.82	0.880	1.239	0.444	0.769	1.938	0.84
Pb	0.365	3.48	9.02	0.924	1.164	0.698	1.158	1.933	1.11
In	0.409	2.27	9.93	0.798	1.299	0.434	0.739	1.880	0.78
Cu	0.598	1.96	8.97	1.113	0.564	0.862	0.928	0.842	1.26
Ag	0.517	1.74	9.23	0.879	0.602	0.951	0.776	0.529	0.84

mation which leads to

$$\langle\omega^2\rangle=\tfrac{1}{2}\Theta_D^2\ , \tag{18}$$

where Θ_D is the Debye temperature. For Pb and In we used also the accurate values of $\langle\omega^2\rangle$ based[15] on the experimental determination of $\alpha^2(\omega)F(\omega)$ from tunneling data. Comparison of these accurate values with the ones based on Eq. (18) shows a discrepancy of about 25% which is a typical measure of the errors in the $m\langle\omega^2\rangle$ column in Table II. Although for some of the materials in Table II one can use an $F(\omega)$ based on experimentally determined dispersion relations, we have not done so because in order to reveal certain trends we think that one must use consistent values for all the metals examined. However, one must keep in mind these possible errors in $m\langle\omega^2\rangle$, comparing theoretical values of λ with experimental ones.

In the next three columns of Table II we present theoretically determined values of λ: $\lambda_{\mathrm{RMTA}}^{\mathrm{theor}}$ is the RMTA value resulting from the division of η_{RMTA} by $m\langle\omega^2\rangle$; $\lambda_{\mathrm{present}}^{\mathrm{theor}}$ is our present result found from η_{present} and $m\langle\omega^2\rangle$; $\lambda_{\mathrm{pseud}}^{\mathrm{theor}}$ presents results based on pseudopotential calculations summarized and reviewed in Ref. 16, except for Be which was taken from Ref. 17. It must be pointed out that when APW pseudopotentials are used a correction of the type shown in Eq. (9) has been employed.[5,7,11–13] However, in this approach, the correction of U_c^* has been treated as a correction to the crystalline muffin-tin potential, which shifts E_F to a new value such that Eq. (4) is satisfied. This shifting of E_F produces a respective change in the wave functions, in contrast to our method where the wave functions remain unchanged.

The last two columns of Table II present "experimental" values of λ. The column labeled $\lambda_{\mathrm{McMillan}}^{\mathrm{expt}}$ was obtained[15] by inverting the McMillan formula[18] for T_c and by taking T_c from experiment. for Pb and In we also show the values of λ obtained[15] by directly integrating the experimentally determined value of $\alpha^2(\omega)F(\omega)$. In the last column we present $\lambda_{\mathrm{tr}}^{\mathrm{expt}}$ which is obtained from resistivity measurements as follows[19]:

$$\lambda_{\mathrm{tr}}^{\mathrm{expt}}=\frac{\hbar}{8\pi^2 k}\Omega_p^2\frac{d\rho}{dT}\ . \tag{19}$$

ρ is the resistivity, T is the temperature, k is the Boltzmann constant, and Ω_p is the plasma frequency corresponding to the optical effective mass and given (in eV) by[19]

$$\Omega_p^2=19.59(\langle V_F^2\rangle n_t)^{1/2}\ , \tag{20}$$

where V_F is the Fermi velocity calculated from the band-structure results of Refs. 3 and 5. The quantity $\lambda_{\mathrm{tr}}^{\mathrm{expt}}$ is not identical to λ because it contains an extra transport factor of $1-\cos\theta$, which is integrated over the angle θ, where θ and q are related by $q=2k_F\sin(\theta/2)$. In obtaining $\lambda_{\mathrm{tr}}^{\mathrm{expt}}$ we have used Eqs. (19) and (20) with the quantities appearing on its rhs determined from band-structure results. Where no reliable value of Ω_p based on Eq. (20) was available, we have employed either free-electron values of Ω_p, or experimentally determined

TABLE I. *(Continued.)*

Metal	A_{sp}^{RMTA}	A_{pd}^{RMTA}	A_{df}^{RMTA}	A_{sp}	A_{pd}	A_{df}	A_{fg}	U_0 (Ry)
Li	−0.355	0.144	0.004	−0.172	0.220	0.021	0.003	−0.092
Na	−0.130	0.026	0.009	0.112	0.164	0.051	0.010	−0.120
K	−0.139	−0.059	0.032	0.128	0.106	0.079	0.010	−0.086
Rb	−0.131	−0.120	0.046	0.136	0.057	0.096	0.011	−0.079
Mg	−0.016	0.176	0.029	0.162	0.337	0.085	0.016	−0.162
Ca	−0.225	−0.176	0.154	−0.122	−0.090	0.175	0.005	−0.050
Be	−0.504	0.416	0.015	0.252	0.815	0.294	0.149	−1.091
Zn	−0.009	0.292	−0.040	0.177	0.454	0.038	0.028	−0.290
Cd	−0.050	0.280	−0.064	0.147	0.450	0.028	0.037	−0.267
Al	−0.092	0.363	0.062	0.078	0.580	0.165	0.036	−0.309
Ga	0.171	0.536	0.011	0.338	0.810	0.164	0.058	−0.453
Pb	0.404	0.796	−0.004	0.242	1.133	0.185	0.058	−0.436
In	−0.155	0.539	−0.002	0.344	0.860	0.172	0.063	−0.383
Cu	−0.154	0.239	−0.146	0.141	0.361	−0.079	0.025	−0.356
Ag	−0.212	0.173	−0.151	0.043	0.298	−0.072	0.036	−0.284

TABLE II. Results of the present calculations and comparison with experimental values. Symbols are defined in the text.

Metal	η_{RMTA}	η_{present} (eV/Å^2)	$m\langle\omega^2\rangle$	$\lambda_{\text{RMTA}}^{\text{theor}}$	$\lambda_{\text{present}}^{\text{theor}}$	$\lambda_{\text{pseud}}^{\text{theor}}$	$\lambda_{\text{McMillan}}^{\text{expt}}$	$\lambda_{\text{tr}}^{\text{expt}}$
Li	0.265	0.250	0.73	0.363	0.34	0.41±0.15		0.40
Na	0.017	0.072	0.52	0.033	0.14	0.16±0.04		0.16[a]
K	0.011	0.021	0.28	0.040	0.08	0.13±0.03		0.14
Rb	0.016	0.016	0.24	0.068	0.07	0.16±0.04		0.19
Mg	0.123	0.53	3.42	0.036	0.15	0.35±0.04		0.32
Ca	0.239	0.19	1.87	0.128	0.10	0.25±0.04		0.02 0.19[b]
Be	0.560	1.79	16.47	0.034	0.11	0.26[c]	0.24±0.01	0.05 2.0[a,b]
Zn	0.544	1.36	6.18	0.088	0.22	0.42±0.01	0.43±0.05	0.67
Cd	0.359	0.91	4.38	0.082	0.21	0.32±0.11	0.42±0.04	0.51
Al	0.590	1.84	4.37	0.135	0.42	0.49±0.05	0.39±0.02	0.41
Ga	0.595	1.93	6.33	0.094	0.30	0.24±0.03	0.42±0.03 1.9±0.3[d]	1.93
Pb	1.199	2.46	2.01 1.55[e]	0.597 0.773[e]	1.22 1.59[e]	1.47±0.30[e]	1.30±0.20 1.55[e]	1.79
In	0.355	1.21	1.19 1.61[e]	0.298	1.02 0.75[e]	0.94±0.15[e]	0.8±0.05 0.805[e]	0.85
Cu	0.456	0.71	6.61	0.069	0.11	0.13±0.04		0.13
Ag	0.288	0.42	4.88	0.059	0.09	0.10±0.04		0.13

[a] Ω_p from the experimental value for the plasmon frequency.

[b] Ω_p from free-electron formula.

[c] From Ref. 17.

[d] Value for amorphous Ga.

[e] Value based on tunneling data (see Ref. 15).

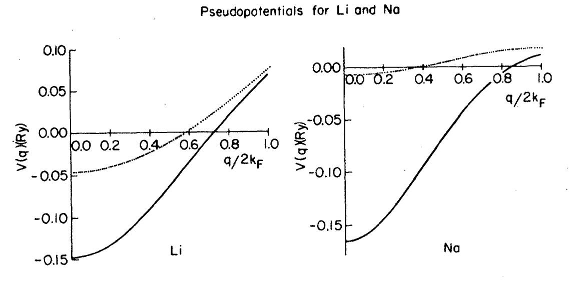

FIG. 1. Plot of the pseudopotential $V(q)$ for Li and Na. Dotted line: RMTA. Solid line: $V(q)$ corrected.

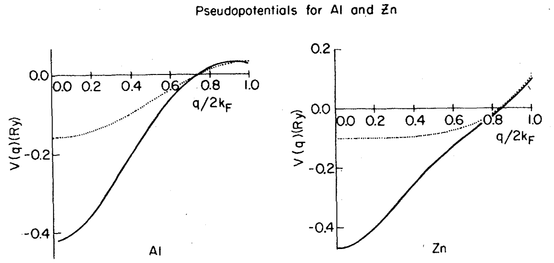

FIG. 3. Plot of the pseudopotential $V(q)$ for Al and Zn. Dotted line: RMTA. Solid line: $V(q)$ corrected.

values for the plasmon frequency as indicated.

The main conclusion to be drawn from the results of Table II is that our correction substantially improves the RMTA. The agreement between the present results and experimental values is particularly impressive for Pb and In, where there is very little uncertainty because of the availabilty of the tunneling data. Good agreement seems to exist also for Al, Ga (within experimental uncertainty), Cu, Ag, Na, and Li. This agreement could worsen if corrections to the LA and accurate phonon-spectra averages (instead of the Debye temperature) would be incorporated. However, these two types of corrections tend to cancel each other so that the results are not expected to change appreciably. For Pb, where the correct phonon averages were used and where the LA is adequate (due to the large umklapp scattering), the agreement between our theoretical result and the experiment is especially impressive. Li seems to be the exception in the sense that our correction slightly reduces the value of $\lambda^{\rm theor}_{\rm RMTA}$ instead of increasing it as in most cases. Similar anomalous behavior is also shown by Rb and Ca. For the rest of the metals, K, Mg, Be, Zn, and Cd, although there is a substantial improvement over the RMTA results, still our values of λ seem to be low. A possible explanation for this remaining discrepancy is that the band structure for Mg, Be, Zn, and Cd was calculated, not in the actual crystal lattice, but in an "equivalent"[3] fcc one. Part of the discrepancy may be also attributed to the uncertainties in the $m\langle\omega^2\rangle$ values.

Some physical insight may be gained by calculating the pseudopotential $V(q)$ as given by Eqs. (1) and (12). In Figs. 1 and 2 we present results for the alkalis, and in Figs. 3 and 4, for some other characteristic cases. One must keep in mind that λ depends strongly on the values of $V(q)$ for large q (due to a q^3 factor in the integrand[6]). On the other hand, our correction to the RMTA value of $V(q)$ for large q is not expected to be reliable. The reason is that our method is physically justified for distances greater than $r_{\rm MT}$, while inside the muffin-tin sphere (where it simply adds an essentially constant potential), it cannot be expected to realistically determine the correction to the RMTA. This behavior in real space implies that our correction is realistic for small q but it cannot be considered reliable for large q. As a result of the above arguments we expect that our method will work better when the large-q corrections to the RMTA values of $V(q)$ are small. This is actually the case as shown in Figs. 3 and 4 for In, Al, and Ag, where our method works very well. The situation is similar for Ga, Pb, and Cu. Figure 3 shows that the large-q correc-

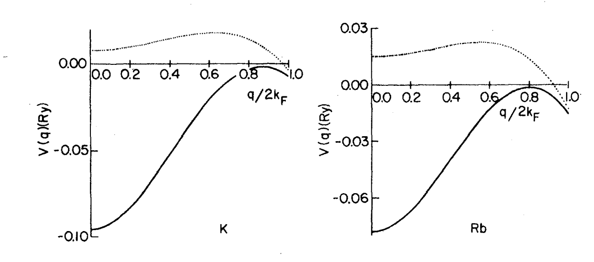

FIG. 2. Plot of the pseudopotential $V(q)$ for K and Rb. Dotted line: RMTA. Solid line: $V(q)$ corrected.

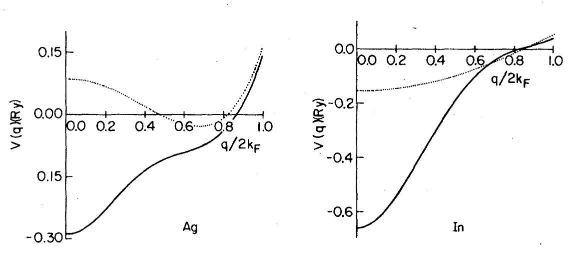

FIG. 4. Plot of the pseudopotential $V(q)$ for Ag and In. Dotted line: RMTA. Solid line: $V(q)$ corrected.

tion to $V(q)$ for Zn is small; yet our corrected value of λ, although an improvement over the RMTA, is still low. As was mentioned before, we attribute this discrepancy for Zn (as well as for Mg, Be, and Cd, where a similar situation appears) to be the fact that the band structure of these materials was calculated not for the actual lattice structure but for an equivalent fcc one.

Figures 1 and 2 show that for large q the correction to the RMTA values of $V(q)$ for the alkalis is not small. This implies that the RMTA does not reproduce the ionic potential correctly even within the muffin-tin sphere. Furthermore, our essentially constant-potential correction within the muffin-tin sphere [and consequently our correction to $V(q)$ for large q] cannot be considered realistic. Because the large-q region contributes strongly to the value of λ, we expect that our correction will not work consistently well for all the alkalis. Indeed, for Na, it works much better than K.

Finally, we have applied our method to transition metals such as V and Nb. We found no significant correction to the RMTA results. This is to be expected since for transition metals, as opposed to simple metals, the electron-phonon scattering takes place almost exclusively within the muffin-tin sphere, and what is happening outside the muffin-tin sphere is of little consequence. Thus, the fact that the RMTA omits the screened potential tail has very little effect on the value of λ.

In conclusion we have developed a simple method to correct the RMTA in nontransition metals. The method is producing results in better than the RMTA agreement with experimental data for several metals without using any adjustable parameter.

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