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Pseudopotential Form Factor and Interionic Potential in Simple Metals: Many-Electron Effects*

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We construct a pseudopotential form factor and a metallic interionic potential using Shaw's nonlocal model potential and the many-electron screening due to Singwi *et al.* for eight simple metals. We have particularly examined the role of many-electron effects and found them to contribute significantly to the pseudopotential form factor in the region of $k_F < q < 2.2k_F$ and to be essential in determining a realistic interionic potential. In addition, we have studied the effects of exchange and correlation on the residual resistivity due to vacancies, the resistivity of liquid metals, the interatomic force constants, and the sound velocity. The inclusion of many-electron effects invariably improves the agreement between theory and experiment.

I. INTRODUCTION

Pseudopotential theory has proven to be a versatile and useful technique in understanding various properties of metals.[1,2] It is now possible to investigate such diverse properties as lattice dynamics, cohesive energy, optical absorption, and transport properties once an accurate pseudopotential is known for the metal. The basic starting point for investigating these properties is the pseudopotential form factor which consists of the ionic part (bare-ion pseudopotential) and the contribution from the conduction electrons resulting in the screening of the bare-ion pseudopotential. The bare-ion potential can be constructed in a semiempirical way, Ashcroft's[3] form factor is a typical example, or from first-principles considerations using results extrapolated from atomic spectroscopic data; the Heine-Abarenkov model potential[4] and the optimized model potential by Shaw[5] are good examples here. The contribution to the form factor due to the conduction electrons is generally treated in the self-consistent-field (SCF) approximation and incorporated through the use of a dielectric function either in the Hartree form or in a modified form, which includes the exchange and correlation effects (many-electron effects) among the conduction electrons. Since recent work on the interionic potential,[6,7] interatomic force constants,[7] and phonon spectra[8-10] have demonstrated within the local pseudopotential scheme the importance of many-electron effects, we wish to further investigate these effects in a nonlocal pseudopotential scheme. In Sec. II, we describe the procedure for constructing the pseudopotential form factor and the interionic potential which contain both the desired nonlocal bare-ion potential and the self-consistently determined many-electron screening. Results are presented here for eight simple metals. In addition, we have particularly examined and assessed the role of the exchange and correlation effects in influencing various properties such as the residual resistivity due to vacancies, the resistivity of liquid metals, the interatomic force constants, and sound velocity. Details of such investigations are given in Sec. III. Our concluding remarks are presented in Sec. IV.

II. PSEUDOPOTENTIAL FORM FACTOR AND INTERIONIC POTENTIAL

We begin constructing the pseudopotential form factor with Shaw's nonlocal Hartree results. Shaw's bare-ion model potential $w_q^b(\vec{k})$ consists of two parts, a local contribution v_q and a nonlocal contribution $F(\vec{k}, \vec{q})$:

$$w_q^b(\vec{k}) = v_q + F(\vec{k}, \vec{q}) \ . \tag{1}$$

Shaw then proceeded to include the contribution due to the conduction electrons using the Hartree screening via the familiar Hartree (or Lindhard) dielectric function $\epsilon_H(q)$,

$$\epsilon_H(q) = 1 + \chi_H(q) \ , \tag{2}$$

with

$$\chi_H(q) = \frac{4\pi Z e^2}{\Omega_0 q^2} \left(\tfrac{2}{3} E_F\right)^{-1} \left(\frac{1}{2} + \frac{4k_F^2 - q^2}{8k_F q} \ln \left| \frac{2\vec{k}_F + \vec{q}}{2\vec{k}_F - \vec{q}} \right| \right) , \tag{3}$$

and the screened pseudopotential form factor becomes

$$w_q^H(\vec{k}) = \frac{v_q + v_{dq}}{\epsilon_H(q)} + F(\vec{k}, \vec{q}) + g(\vec{q}) \ , \tag{4}$$

where v_{dq} is the local contribution due to the depletion hole as defined by Shaw and $g(q)$ represents the screening due to the nonlocal part of the bare-ion potential and is therefore related to $F(\vec{k}, \vec{q})$ and $\epsilon_H(q)$.

One now needs to include the exchange and correlation effects among the conduction electrons. In the SCF approximation, this can be easily accomplished by using a modified dielectric function $\epsilon(q)$,[11,4] which differs from the Hartree result in the following manner:

$$\begin{aligned} \epsilon(q) &= 1 + [1 - f(q)][\epsilon_H(q) - 1] \\ &= 1 + [1 - f(q)]\, \chi_H(q) \ , \end{aligned} \tag{5}$$

with $f(q)$ accounting for the many-electron correction. [$f(q) = 0$ corresponds to Hartree screening.] The corresponding many-electron contribution to the pseudopotential form factor then becomes[9]

$$\Delta w_q(\vec{k}) = -\,[f(q)/\epsilon(q)]\,[w_q^H(\vec{k}) - w_q^b(\vec{k})] , \tag{6}$$

and the desired pseudopotential form factor takes the form

$$w_q(\vec{k}) = w_q^H(\vec{k}) + \Delta w_q(\vec{k}) \ . \tag{7}$$

The problem now is knowing $f(q)$ accurately. Using various approximations, numerous authors have suggested forms for approximating the many-electron effects. Of them, the Hubbard-Sham[11] approximation, which considers only the exchange effects, yields

$$f(q)_{\text{HS}} = q^2 / 2(q^2 + k_F^2 + k_s^2) , \tag{8}$$

and a similar version by Geldart and Vosko[12] gives

$$f(q)_{\text{GV}} = q^2 / 2(q^2 + \zeta k_F^2) \ . \tag{9}$$

For a more satisfactory $f(q)$, one must improve the above approximations by including the Coulomb correlation effects. Indeed, this has been successfully carried out recently by Singwi *et al.*[13] in the problem of the electron liquid. Their method consists of using a local-field correction, which depends on the pair correlation function, and solving in a self-consistent manner the set of equations that couples the dielectric function $\epsilon'(q)$ (defined by the potential seen by a test charge) and the pair correlation function. In terms of the functions of $f(q)$ and $\chi_H(q)$ appearing in Eq. (5) for the modified dielectric function $\epsilon(q)$, $\epsilon'(q)$ is given by[13,7]

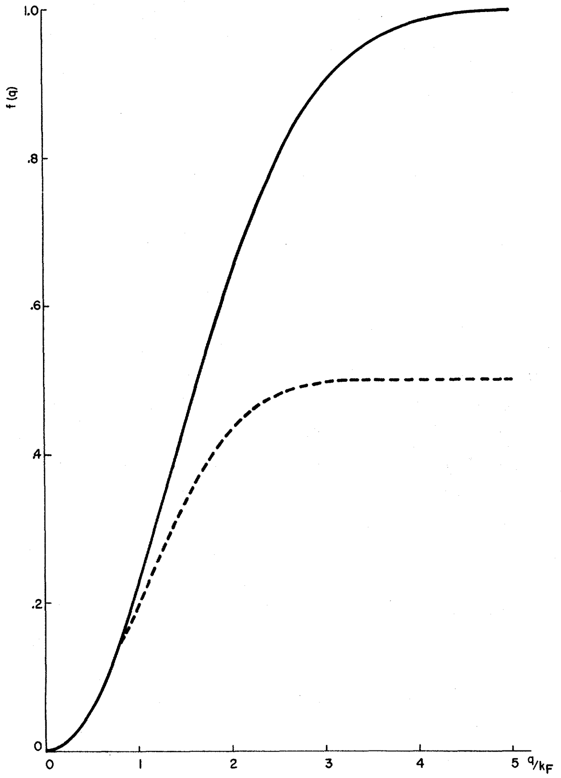

FIG. 1. Plot of the $f(q)_{\text{SP}}$ function (dashed line) and $f(q)_{\text{SSTL}}$ function (solid line) for sodium metal.

TABLE I. Pseudopotential form factor $w_q(k_F)$ (in Ry) for eight simple metals.

q/k_F	Li	Be	Na	Mg	Al	K	Cd	In
0.00	−0.231 28	−0.705 48	−0.158 90	−0.349 64	−0.573 28	−0.103 86	−0.367 34	−0.423 68
0.10	−0.228 11	−0.694 75	−0.156 72	−0.344 70	−0.564 60	−0.102 06	−0.359 63	−0.416 81
0.20	−0.224 67	−0.676 16	−0.154 85	−0.337 61	−0.549 54	−0.100 90	−0.353 46	−0.407 86
0.30	−0.218 97	−0.646 08	−0.151 75	−0.326 00	−0.525 19	−0.098 93	−0.343 21	−0.393 28
0.40	−0.211 01	−0.605 72	−0.147 40	−0.310 11	−0.492 46	−0.096 19	−0.329 13	−0.373 61
0.50	−0.200 91	−0.556 71	−0.141 83	−0.290 37	−0.452 66	−0.092 72	−0.311 50	−0.349 51
0.60	−0.188 66	−0.500 91	−0.135 03	−0.267 22	−0.407 33	−0.088 45	−0.290 69	−0.321 86
0.70	−0.174 43	−0.440 31	−0.127 09	−0.241 33	−0.358 19	−0.083 46	−0.267 18	−0.291 51
0.80	−0.158 39	−0.376 97	−0.118 04	−0.213 38	−0.306 97	−0.077 77	−0.241 57	−0.259 49
0.90	−0.140 80	−0.312 74	−0.108 00	−0.184 17	−0.255 45	−0.071 45	−0.214 39	−0.226 79
1.00	−0.121 94	−0.294 34	−0.097 13	−0.154 50	−0.205 15	−0.064 61	−0.186 41	−0.194 29
1.10	−0.102 18	−0.188 15	−0.085 60	−0.125 20	−0.157 44	−0.057 32	−0.158 24	−0.162 72
1.20	−0.081 91	−0.130 20	−0.073 68	−0.096 99	−0.113 38	−0.049 78	−0.130 51	−0.132 67
1.30	−0.061 48	−0.076 24	−0.061 59	−0.070 49	−0.073 75	−0.042 13	−0.103 78	−0.104 49
1.40	−0.041 31	−0.026 67	−0.049 61	−0.046 29	−0.038 97	−0.034 60	−0.078 44	−0.078 33
1.50	−0.021 77	0.018 33	−0.037 98	−0.024 69	−0.009 30	−0.027 35	−0.054 82	−0.054 05
1.60	−0.003 07	0.058 84	−0.026 96	−0.005 95	0.015 28	−0.020 61	−0.033 07	−0.031 40
1.70	0.014 52	0.095 03	−0.016 71	0.009 85	0.034 94	−0.014 54	−0.013 31	−0.009 96
1.80	0.030 92	0.127 21	−0.007 43	0.022 72	0.049 96	−0.009 28	0.004 59	0.010 86
1.90	0.046 06	0.155 80	0.000 83	0.032 78	0.060 66	−0.004 92	0.020 75	0.031 68
2.00	0.060 09	0.181 46	0.008 07	0.040 29	0.067 53	−0.001 53	0.035 43	0.053 35
2.10	0.066 95	0.188 20	0.013 08	0.043 71	0.068 82	0.001 37	0.043 66	0.062 23
2.20	0.071 70	0.190 75	0.016 88	0.044 94	0.067 26	0.003 45	0.049 76	0.068 82
2.30	0.074 79	0.190 16	0.019 60	0.044 42	0.063 59	0.004 80	0.054 00	0.073 38
2.40	0.076 44	0.186 97	0.021 36	0.042 55	0.058 28	0.005 45	0.056 72	0.076 39
2.50	0.076 91	0.181 76	0.022 30	0.039 62	0.051 83	0.005 53	0.058 13	0.077 86
2.60	0.076 39	0.174 89	0.022 55	0.035 87	0.044 54	0.005 19	0.058 41	0.078 11
2.70	0.075 02	0.166 79	0.022 22	0.031 51	0.036 78	0.004 45	0.057 79	0.077 20
2.80	0.072 98	0.157 75	0.021 39	0.026 77	0.028 80	0.003 48	0.056 38	0.075 38
2.90	0.070 39	0.148 04	0.020 21	0.021 84	0.020 81	0.002 32	0.054 39	0.072 72
3.00	0.067 39	0.137 94	0.018 71	0.016 78	0.013 00	0.001 02	0.051 91	0.069 37
3.10	0.064 03	0.127 65	0.016 98	0.011 80	0.005 55	−0.000 35	0.049 05	0.065 39
3.20	0.060 44	0.117 36	0.015 11	0.006 96	−0.001 44	−0.001 70	0.045 90	0.060 95
3.30	0.056 69	0.107 21	0.013 12	0.002 33	−0.007 84	−0.003 09	0.042 51	0.056 12
3.40	0.052 86	0.097 38	0.011 07	−0.001 98	−0.013 61	−0.004 39	0.039 03	0.050 99
3.50	0.048 98	0.087 93	0.008 97	−0.005 92	−0.018 66	−0.005 61	0.035 49	0.045 63
3.60	0.045 17	0.078 96	0.006 93	−0.009 48	−0.022 96	−0.006 72	0.031 91	0.040 20
3.70	0.041 37	0.070 55	0.004 91	−0.012 61	−0.026 48	−0.007 76	0.028 38	0.034 74
3.80	0.037 71	0.062 75	0.003 00	−0.015 29	−0.029 28	−0.008 60	0.024 95	0.029 32
3.90	0.034 23	0.055 61	0.001 14	−0.017 55	−0.031 33	−0.009 36	0.021 58	0.024 03
4.00	0.030 89	0.049 10	−0.000 58	−0.019 31	−0.032 65	−0.009 94	0.018 38	0.018 95
4.10	0.027 76	0.043 22	−0.002 14	−0.020 63	−0.033 33	−0.010 40	0.015 37	0.014 15
4.20	0.024 80	0.038 04	−0.003 60	−0.021 56	−0.033 37	−0.010 70	0.012 51	0.009 69

TABLE I. *(Continued)*

q/k_F	Li	Be	Na	Mg	Al	K	Cd	In
4.30	0.022 10	0.033 45	−0.004 88	−0.022 06	−0.032 89	−0.010 86	0.009 86	0.005 57
4.40	0.019 58	0.029 47	−0.006 00	−0.022 18	−0.031 89	−0.010 88	0.007 44	0.001 89
4.50	0.017 32	0.026 05	−0.007 00	−0.021 94	−0.030 47	−0.010 82	0.005 24	−0.001 33
4.60	0.015 28	0.023 15	−0.007 88	−0.021 42	−0.028 69	−0.010 62	0.003 25	−0.004 09
4.70	0.013 46	0.020 71	−0.008 46	−0.020 62	−0.026 63	−0.010 32	0.001 49	−0.006 37
4.80	0.011 86	0.018 67	−0.008 96	−0.019 58	−0.024 35	−0.009 92	−0.000 07	−0.008 17
4.90	0.010 42	0.017 01	−0.009 32	−0.018 36	−0.021 91	−0.009 44	−0.001 39	−0.009 49
5.00	0.009 20	0.015 69	−0.009 52	−0.017 02	−0.019 41	−0.008 90	−0.002 52	−0.010 40

$$\epsilon'(q) = 1 + \chi_H(q)/[1 - f(q)\chi_H(q)] \; . \qquad (10)$$

This immediately reveals that $\epsilon(q)$ and $\epsilon'(q)$ are related by

$$\epsilon'(q) = \epsilon(q)/[1 - f(q)\chi_H(q)] \qquad (11)$$

and are, in general, not the same unless for the special case of Hartree screening, namely, $f(q) = 0$. The work of Singwi *et al.* dealt with solving a self-consistent $\epsilon'(q)$. Through Eq. (10), one immediately obtains the self-consistent $f(q)$ which can then be used to obtain the many-electron correction to the pseudopotential form factor.

It should be mentioned that Shaw and Pynn[9] have recently also sought to improve Shaw's nonlocal Hartree pseudopotential by incorporating the many-electron effects in a phenomenological way. The $f(q)$ function they have adopted is given by

$$f(q)_{\rm SP} = \tfrac{1}{2}(1 - e^{-q^2/\beta k_F^2}) + (\gamma q^2/k_F^3)\, e^{-\alpha q^2/\gamma k_F} \; , \qquad (12)$$

with $\beta = 2$, $\gamma = 0.0123$, and $\alpha = 0.0538$.

In Fig. 1, we compare $f(q)_{\rm SP}$ with $f(q)$ due to Singwi *et al.* $[f(q)_{\rm SSTL}]$ for sodium metal. Indeed, $f(q)_{\rm SP} \simeq \frac{2}{3} f(q)_{\rm SSTL}$ near $q = 2k_F$ and becomes $\frac{1}{2} f(q)_{\rm SSTL}$ for $q > 3.5k_F$. The large q behavior of $f(q)_{\rm SP}$, namely, $f(q)_{\rm SP} \rightarrow \frac{1}{2}$, is also manifest in $f(q)_{\rm HS}$ and $f(q)_{\rm GV}$, which consider only the exchange effects. The major difference between $f(q)_{\rm SSTL}$ and the other $f(q)$ functions thus lies in the region of $k_F < q < \infty$ and is, of course, due to the inclusion of correlation effects in $f(q)_{\rm SSTL}$.

We have calculated $w_q(k_F)$ [Eq. (7)] in the region of $0 < q < 5k_F$ for eight simple metals. Such results are listed in Table I. In order to assess the significance of the many-electron correction term, we plot in Fig. 2 $\Delta w_q(k_F)$ for sodium, magnesium, and aluminum. Notice that $\Delta w_q(k_F)$ increases as the valence number is increased. In general, we find that $\Delta w_q(k_F)$ peaks around $q = k_F$ and gradually tapers off to zero around $q = 3.5k_F$. Due to the fact that $w_q^H(k_F)$ is large and negative at the origin $[w_q^H(k_F) = -\frac{2}{3}E_F$ at $q = 0]$ and generally has a node in the region of $1.4k_F < q < 2.1k_F$, the correction arising from the electron-electron interaction is extremely important for $k_F < q < 2.2k_F$. Using sodium as an example, we find that $\Delta w_q(k_F)/w_q^H(k_F) \simeq 18\%$ at $q = k_F$ and becomes 50% near $q = 1.8k_F$. It is therefore clear that one cannot ignore these corrections when examining any property that depends on the pseudopotential in the region of $k_F < q < 2.2k_F$. This will be further borne out in Sec. III when we examine in detail the role of many-electron effects in specific cases.

We now turn to the study of interionic potential in metals which was first discussed by Cohen[14] and investigated by Harrison.[1] Following earlier work of Shyu and Gaspari,[15] the interionic poten-

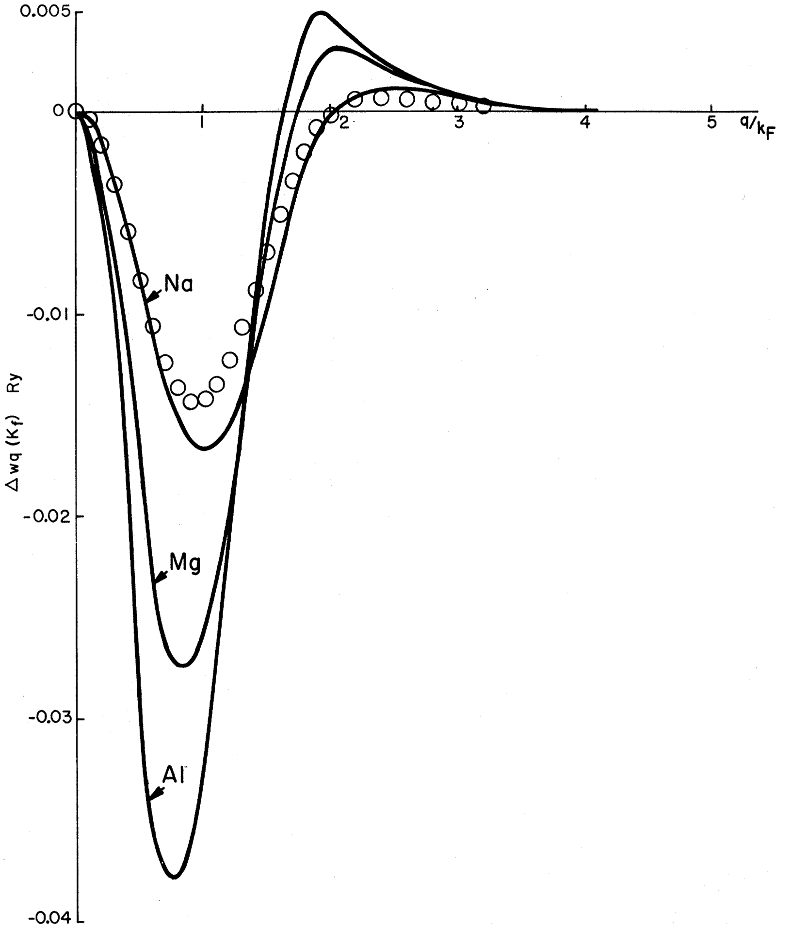

FIG. 2. Many-electron contribution $\Delta\omega_q(k_F)$ to the pseudopotential form factor for sodium, magnesium, and aluminum metals. The circles give $\Delta w_q(k_F)$ in sodium using $f(q)_{\mathrm{SP}}$ screening.

tial $V(r)$ in metals can be written in terms of a direct ion-ion interaction and an indirect ion-electron-ion interaction, which is most easily represented through a $G(q)$ function, first introduced by Cochran[16] in connection with phonon spectra studies:

$$V(r)=\frac{Z^2e^2}{r}-\frac{2Z^2e^2}{\pi}\int_0^{\infty}G(q)\,\frac{\sin qr}{qr}\,dq\ , \tag{13}$$

where $G(q)$ is related to the pseudopotential form factor and the dielectric screening function. One should also remark that this $G(q)$ function is closely related to Harrison's[1] energy-wave-number characteristic in energy-band calculations and is identical to Shaw's[5] normalized energy-wave-number characteristics.

Based on the nonlocal model potential, Shaw has obtained the ion-electron-ion function $G_H(q)$ using Hartree screening. As before, we need to incorporate the many-electron effects. A consideration of such contribution leads to a correction term $\Delta G(q)$ given by[9]

$$\Delta G(q)=\left(\frac{\Omega_0 q^2}{4\pi Z^*}\right)^2\frac{\epsilon_H(q)}{\epsilon(q)}\,f(q)\,[w_q^H(\vec{\mathrm{k}})-w_q^b(\vec{\mathrm{k}})]^2\ . \tag{14}$$

This can be easily calculated using again the

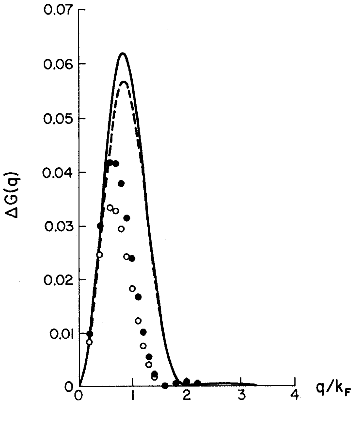

FIG. 3. Many-electron contribution $\Delta G(q)$ to the ion-electron-ion function for sodium (solid line), potassium (dashed line), and aluminum metal (dots). The circles give $\Delta G(q)$ in aluminum using $f(q)_{\mathrm{SP}}$ screening.

TABLE II. Ion-electron-ion function $G(q)$ for eight simple metals.

q/k_F	Li	Be	Na	Mg	Al	K	Cd	In
0.0	1.000 00	1.000 00	1.000 00	1.000 00	1.000 00	1.000 00	1.000 00	1.000 00
0.1	0.991 27	0.986 75	0.992 19	0.988 41	0.985 95	0.991 89	0.990 50	0.987 71
0.2	0.965 40	0.947 92	0.969 04	0.954 30	0.944 80	0.967 88	0.962 37	0.951 66
0.3	0.923 31	0.886 14	0.931 31	0.899 55	0.879 51	0.928 85	0.916 87	0.894 27
0.4	0.866 51	0.805 56	0.880 20	0.827 18	0.794 57	0.876 18	0.855 97	0.819 23
0.5	0.797 02	0.711 29	0.817 39	0.741 06	0.695 75	0.811 73	0.782 28	0.731 22
0.6	0.717 37	0.609 03	0.744 90	0.645 75	0.589 36	0.737 75	0.699 01	0.635 37
0.7	0.630 48	0.504 52	0.665 12	0.546 06	0.481 79	0.656 77	0.609 71	0.536 86
0.8	0.539 63	0.403 02	0.580 74	0.446 82	0.378 79	0.571 60	0.518 12	0.440 49
0.9	0.448 26	0.309 09	0.494 64	0.352 47	0.285 13	0.485 18	0.427 92	0.350 23
1.0	0.359 83	0.226 16	0.409 74	0.266 69	0.204 17	0.400 50	0.342 46	0.269 12
1.1	0.277 59	0.156 48	0.328 91	0.192 26	0.137 78	0.320 34	0.264 53	0.199 05
1.2	0.204 37	0.101 21	0.254 70	0.130 82	0.088 39	0.247 26	0.196 23	0.140 88
1.3	0.142 31	0.060 34	0.189 15	0.082 84	0.049 20	0.183 12	0.138 82	0.094 51
1.4	0.092 75	0.033 06	0.133 70	0.047 80	0.024 56	0.129 23	0.092 75	0.059 22
1.5	0.056 13	0.017 80	0.089 04	0.024 32	0.010 12	0.086 14	0.057 76	0.033 81
1.6	0.032 03	0.012 52	0.055 10	0.010 44	0.003 45	0.053 53	0.032 94	0.016 91
1.7	0.019 11	0.014 63	0.031 14	0.003 88	0.001 92	0.030 41	0.016 98	0.007 02
1.8	0.015 12	0.021 24	0.015 81	0.002 26	0.003 40	0.015 50	0.008 21	0.002 54
1.9	0.016 83	0.028 55	0.007 34	0.003 23	0.005 63	0.006 81	0.004 67	0.002 00
2.0	0.017 94	0.028 73	0.003 58	0.004 19	0.006 36	0.002 59	0.003 79	0.002 71
2.1	0.015 90	0.022 93	0.002 25	0.004 29	0.005 70	0.001 22	0.003 40	0.002 62
2.2	0.015 30	0.020 18	0.001 79	0.004 33	0.005 15	0.000 68	0.003 46	0.002 78
2.3	0.014 84	0.017 85	0.001 93	0.004 22	0.004 53	0.000 78	0.003 74	0.002 94
2.4	0.014 20	0.015 63	0.002 22	0.003 88	0.003 82	0.001 03	0.003 95	0.002 95
2.5	0.013 36	0.013 53	0.002 47	0.003 41	0.003 06	0.001 24	0.004 05	0.002 84
2.6	0.012 36	0.011 57	0.002 61	0.002 86	0.002 35	0.001 33	0.004 03	0.002 60
2.7	0.011 24	0.009 75	0.002 60	0.002 28	0.001 70	0.001 32	0.003 86	0.002 37
2.8	0.010 04	0.008 12	0.002 46	0.001 73	0.001 15	0.001 21	0.003 60	0.001 96
2.9	0.008 87	0.006 67	0.002 24	0.001 24	0.000 73	0.001 03	0.003 29	0.001 68
3.0	0.007 70	0.005 42	0.001 94	0.000 84	0.000 44	0.000 83	0.002 96	0.001 31
3.1	0.006 62	0.004 37	0.001 64	0.000 54	0.000 24	0.000 64	0.002 62	0.001 01
3.2	0.005 62	0.003 48	0.001 32	0.000 31	0.000 12	0.000 47	0.002 29	0.000 76
3.3	0.004 71	0.002 76	0.000 98	0.000 16	0.000 08	0.000 34	0.001 97	0.000 57
3.4	0.003 85	0.002 18	0.000 76	0.000 10	0.000 09	0.000 25	0.001 71	0.000 41
3.5	0.003 23	0.001 69	0.000 53	0.000 06	0.000 13	0.000 20	0.001 50	0.000 30
3.6	0.002 66	0.001 32	0.000 35	0.000 08	0.000 18	0.000 19	0.001 31	0.000 20
3.7	0.002 16	0.001 03	0.000 23	0.000 13	0.000 22	0.000 19	0.001 14	0.000 16
3.8	0.001 76	0.000 80	0.000 12	0.000 18	0.000 26	0.000 24	0.001 04	0.000 14
3.9	0.001 41	0.000 62	0.000 07	0.000 21	0.000 30	0.000 28	0.000 97	0.000 13
4.0	0.001 15	0.000 49	0.000 03	0.000 26	0.000 32	0.000 34	0.000 93	0.000 12
4.1	0.000 93	0.000 38	0.000 04	0.000 30	0.000 32	0.000 40	0.000 92	0.000 13
4.2	0.000 76	0.000 28	0.000 06	0.000 32	0.000 31	0.000 45	0.000 91	0.000 15

TABLE II. (*Continued*)

q/k_F	Li	Be	Na	Mg	Al	K	Cd	In
4.3	0.000 62	0.000 22	0.000 09	0.000 33	0.000 29	0.000 49	0.000 88	0.000 16
4.4	0.000 51	0.000 17	0.000 11	0.000 32	0.000 26	0.000 52	0.000 88	0.000 17
4.5	0.000 40	0.000 14	0.000 14	0.000 30	0.000 22	0.000 51	0.000 88	0.000 17
4.6	0.000 33	0.000 11	0.000 18	0.000 28	0.000 19	0.000 51	0.000 91	0.000 17
4.7	0.000 27	0.000 09	0.000 21	0.000 25	0.000 15	0.000 52	0.000 90	0.000 16
4.8	0.000 22	0.000 07	0.000 23	0.000 21	0.000 11	0.000 49	0.000 93	0.000 15
4.9	0.000 18	0.000 06	0.000 24	0.000 18	0.000 08	0.000 44	0.000 90	0.000 14
5.0	0.000 15	0.000 06	0.000 25	0.000 14	0.000 06	0.000 39	0.000 92	0.000 12

self-consistent result of Singwi *et al.*, namely, $f(q)_{\mathrm{SSTL}}$. Results of $\Delta G(q)$ are illustrated in Fig. 3 for sodium, potassium, and aluminum metals. It is seen that $\Delta G(q)$ generally peaks around $q = 0.8k_F$ and becomes negligibly small after $q > 2.2k_F$. For comparison, we have also plotted $\Delta G(q)$ arising from using $f(q)_{\mathrm{SP}}$ for aluminum metal, and it is seen to give a smaller value for $\Delta G(q)$ as anticipated.

Upon combining $\Delta G(q)$ with $G_H(q)$, we have now the appropriate ion-electron-ion $G(q)$ function, which includes both the nonlocal potential and the many-electron screeening,

$$G(q) = G_H(q) + \Delta G(q) \ . \tag{15}$$

Values of $G(q)$ are presented in Table II for eight simple metals. They represent not only the most convenient input function for generating the interionic potential but also for investigating phonon spectra.[8] In Figs. 4–8 we have plotted the interionic potential $V(r)$ for eight simple metals generated by the above $G(q)$ function. They show the long-range oscillatory behavior expected of the metallic interaction. To determine the extent of influence exerted by the many-electron effects on the interionic potential, we have also calculated $V(r)$ using $G(q)$ functions resulting from Hartree screening and Shaw-Pynn screening. It is seen that in the Hartree case there is a significant change in the shape of the interionic potential corresponding to the first few neighbor distances. This has been noted by Shyu and Gaspari[6] and by Shaw and Pynn[9] earlier and can be understood here in terms of the behavior of $\Delta G(q)$ function and its contribution to the interionic potential. Later, through an analysis of the interatomic force constants and sound velocity, we will further demonstrate that the inclusion of many-electron effects is essential in obtaining a realistic potential.

III. ANALYSIS AND COMPARISON WITH EXPERIMENT

In order to assess the importance of electron-electron interactions we choose to study four specific cases. They are the residual resistivity due to vacancies, the resistivity of liquid metals, the interatomic force constants, and the longitudinal sound velocity.

A. Resistivity of Vacancies in Simple Metals

Basically one needs to find the scattering potential due to the presence of vacancies. This is easily accomplished using again the linear screening approach, which treats the crystal potential as a superposition of the individually screened pseudopotentials. If one neglects the lattice distortion and assumes the vacancy concentration is small so that one has essentially a collection of singly isolated vacancies, one can easily derive the resistivity of vacancies using the standard

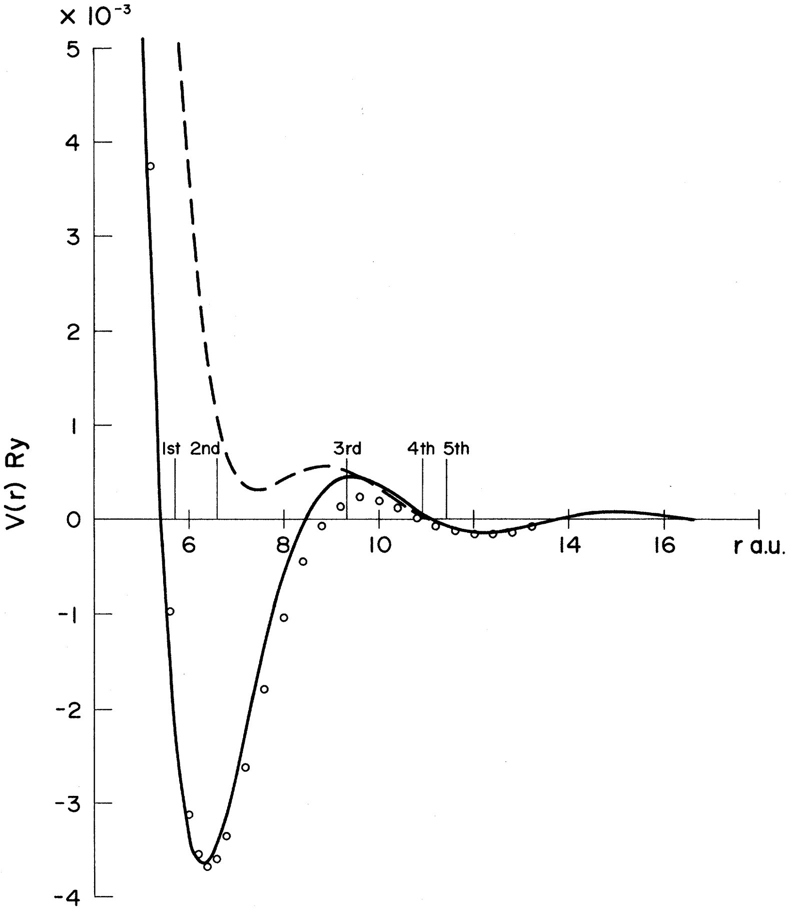

FIG. 4. Interionic potential $V(r)$ as a function of the interionic separation r in lithium metal based on the self-consistent screening [circles, $f(q)_{\mathrm{SP}}$ screening; dashed line, Hartree screening].

scattering theory with the missing pseudopotential associated with the vacancy serving as the perturbation. The final result is[1]

$$\rho_v=\frac{3\pi m\Omega_0}{8e^2\hbar E_F}\,\frac{1}{N}\int_0^2 |\langle\vec{k}+\vec{q}|w|\vec{k}\rangle|^2_{E_F}\left(\frac{q}{k_F}\right)^3 d\left(\frac{q}{k_F}\right), \tag{16}$$

where $\langle\vec{k}+\vec{q}|w|\vec{k}\rangle|_{E_F}$ is simply the individual pseudopotential form factor corresponding to scattering on the Fermi surface and the factor $1/N$ is usually expressed in terms of atomic percentage so one can set $N=100$.

Based on our earlier analysis, Eq. (16) immediately reveals that the resistivity of vacancies ρ_v will depend sensitively on the many-electron screening. To determine the exact extent of such influence, here we calculate ρ_v using for the pseudopotential form factor both $w_q^H(k_F)$ and $w_q(k_F)$ as described in Sec. II. Our results which are listed in Table III show that in general the many-electron contribution to ρ_v is about 16–33% and is more important for metals of large r_s values, such as Na and K. For comparison, we have also calculated ρ_v using pseudopotential form factor with many-electron screening included in the Shaw-Pynn manner [via $f(q)_{\mathrm{SP}}$ function] as described in Sec. II. This yields a resistivity larger than the Hartree result but is somewhat smaller than the one obtained using $f(q)_{\mathrm{SSTL}}$ which is to be attributed to the underestimation of the correlation effects in the $f(q)_{\mathrm{SP}}$ function. No reasonable comparison between theory and experiment is possible here due to the lack of experimental results although there is some information regarding Al which gives ρ_v a value of 2.2 $\mu\Omega$ cm/at.%[17] and 3.0 $\mu\Omega$ cm/at.%.[18] It should be mentioned that Harrison[19] has calculated ρ_v in Al to be 0.8 $\mu\Omega$ cm/at.% using an orthogonalized-plane-wave (OPW) form factor with Hartree screening. His result compares fairly well with ours.

We reiterate here that many-electron effects are important in determining ρ_v although a meaningful comparison of theory and experiment will require the availability of experimental results in these metals and a refinement of the theoretical model to include effects of lattice distortion which could conceivably be large owing to the long-range nature of the interionic force in these metals.

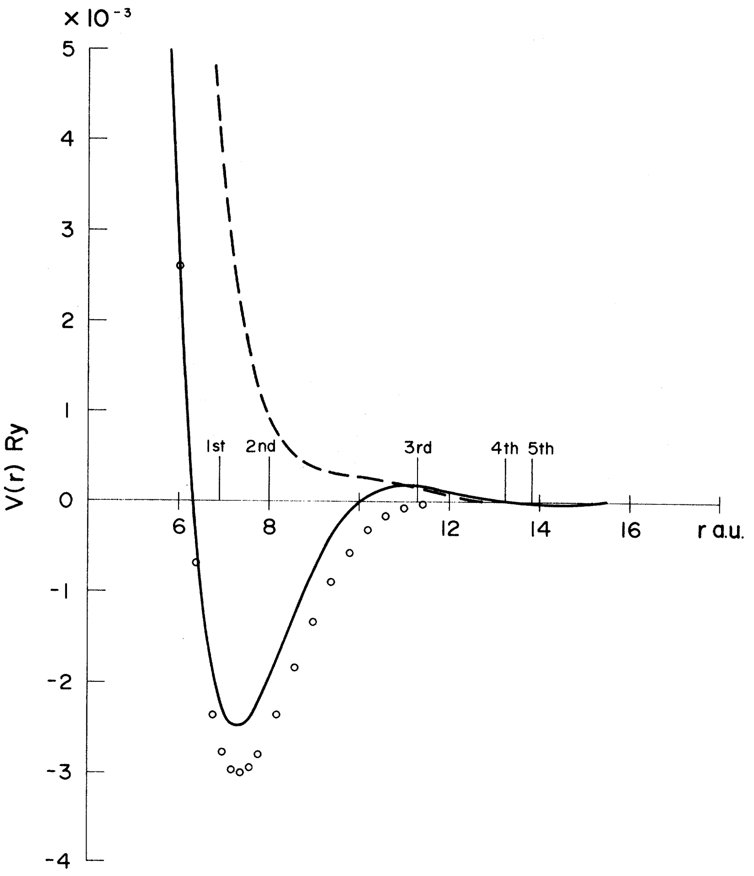

FIG. 5. Interionic potential in sodium metal based on the self-consistent screening [circles, $f(q)_{\mathrm{SP}}$ screening; dashed line, Hartree screening].

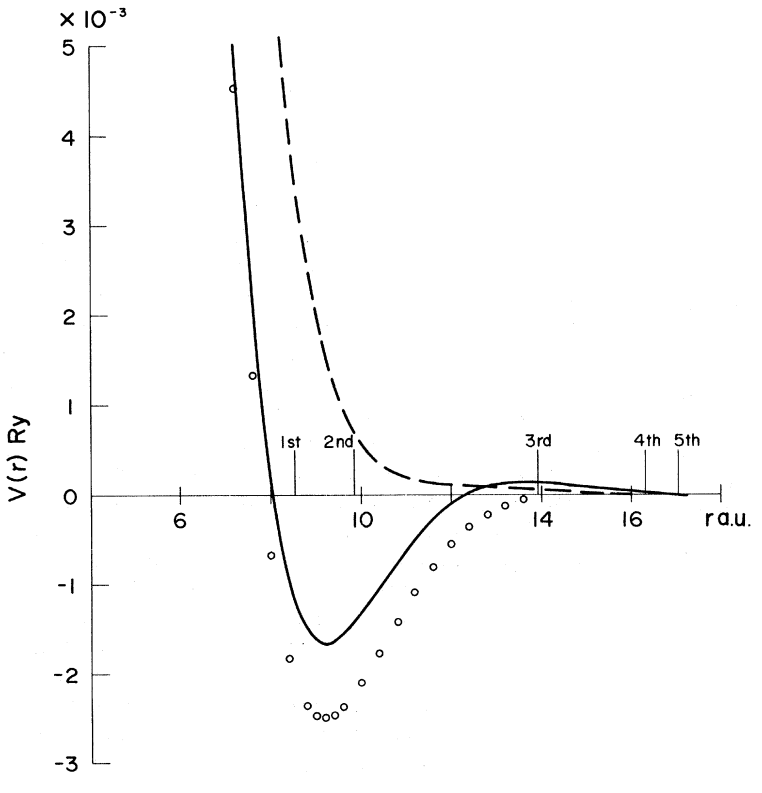

FIG. 6. Interionic potential in potassium metal based on the self-consistent screening [circles, $f(q)_{\mathrm{SP}}$ screening; dashed line, Hartree screening].

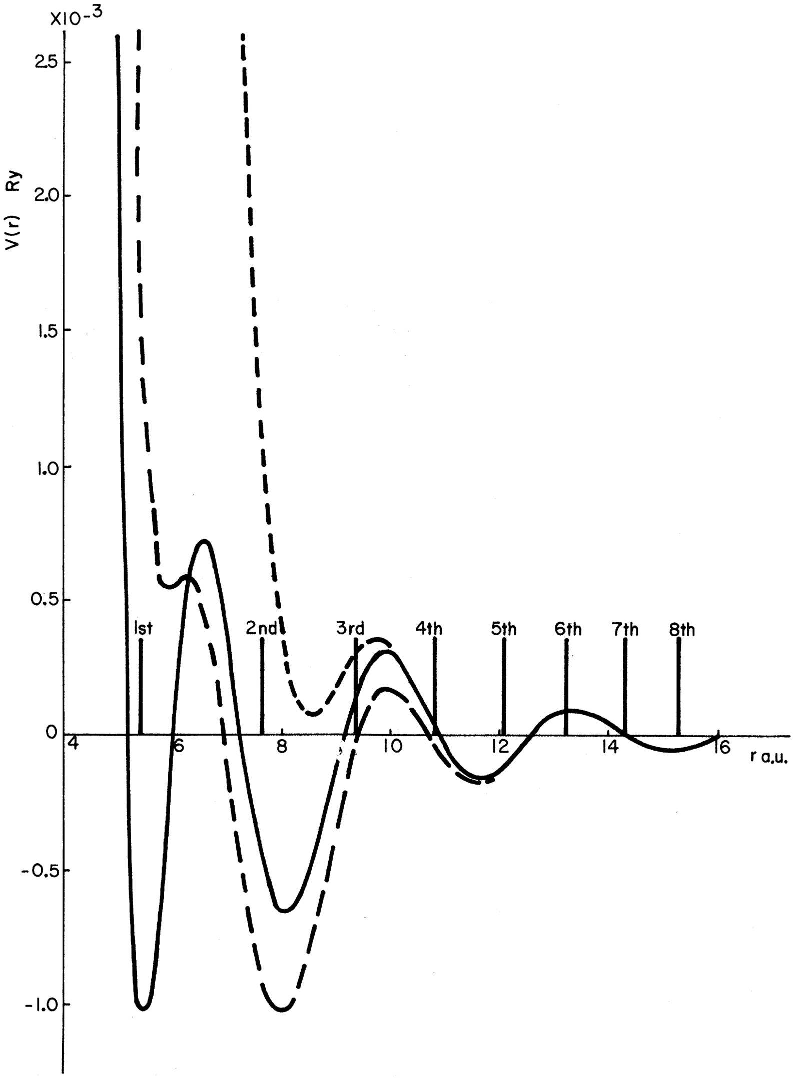

FIG. 7. Interionic potential in aluminum metal based on the self-consistent screening [dashed line, $f(q)_{\text{SP}}$ screening; short dashed line, Hartree screening].

B. Resistivity of Liquid Metals

The situation here is similar to Sec. III A. One needs to find the scattering potential arising out of the ionic arrangement in the liquid state. Using the pseudoatom approach, Ziman[20] has formulated this problem in terms of an individual pseudopotential associated with the properly screened ion and a structure factor which describes the ionic configuration in the liquid metal. His formula for the resistivity of the liquid metal is as follows:

$$\rho_{\text{liq}} = \frac{3\pi m \Omega_0}{8e^2 \hbar E_F} \int_0^2 a(q) \left| \langle \vec{k} + \vec{q} | w | \vec{k} \rangle \right|^2_{E_F} \left(\frac{q}{k_F} \right)^3 d\left(\frac{q}{k_F} \right) , \tag{17}$$

where $a(q)$ is the liquid structure factor and all density-dependent parameters are to be evaluated at the appropriate liquid density.

Our main interest is again in determining the many-electron contribution. In evaluating ρ_{liq}, we have used as before three separate pseudopotential form factors corresponding to Hartree, $f(q)_{\text{SP}}$, and $f(q)_{\text{SSTL}}$ screening. Theoretically, these pseudopotential form factors should be recomputed for the correct liquid density here. Since it is known[21] that this density correction will only affect the final result by a few percent, we have ignored this modification here. For $a(q)$, we have chosen the theoretical Ashcroft-Lekner[22] result with the packing parameter $\eta = 0.45$. Our results in Table IV show that many-electron effects contribute about 9–38% to ρ_{liq} and are essential in bringing the theoretical value to closer agreement with experiment. Except for Li and Cd, the agreement between theory and experiment is generally very good, in spite of the uncertainties in the pseudopotential, structure factor, and experimental measurements.

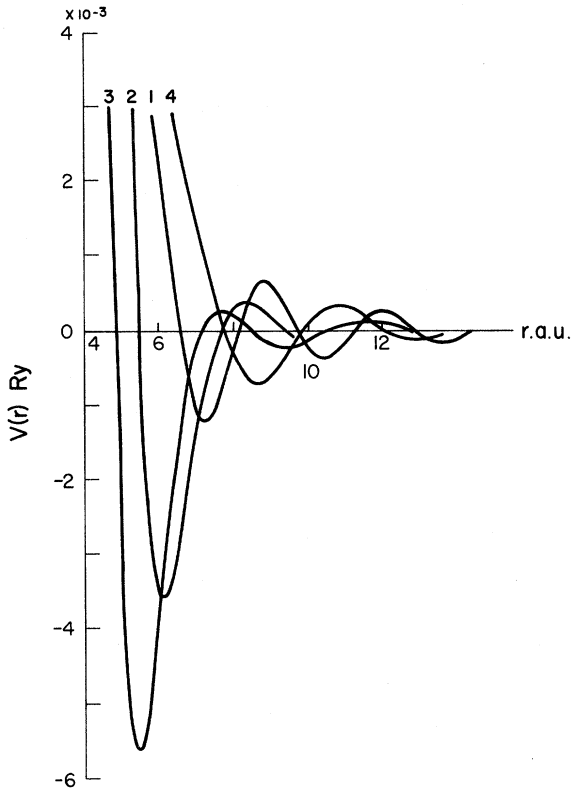

FIG. 8. Interionic potential in beryllium (curve 1), magnesium (curve 2), cadmium (curve 3), and indium metal (curve 4).

C. Interatomic Force Constants

We choose to analyze the interatomic force constants here since they are related to the shape of the interionic potential, namely, the first and second derivatives of the interionic potential. Furthermore, results of the neutron scattering measurement on phonon spectra have often been analyzed in terms of the Born–von Kármán force constants evaluated at different lattice sites which are merely various linear combinations of the tangential force constant k_t and radial force constant k_r given by

$$k_t=\frac{1}{r}\frac{dV}{dr}=-\frac{e^2}{r^3}-\frac{2e^2}{\pi r^2}\int_0^\infty G(q)\left(\cos qr-\frac{\sin qr}{qr}\right)dq\;, \qquad (18)$$

$$k_r=\frac{d^2V}{dr^2}=\frac{2e^2}{r^3}-\frac{2e^2}{\pi r}\int_0^\infty G(q) \times\left(\frac{2\sin qr}{qr^2}-\frac{2\cos qr}{r}-q\sin qr\right)dq\;. \qquad (19)$$

Knowing $G(q)$, one can easily calculate k_t and k_r to form the proper Born–von Kármán force constants (interatomic force constants) and compare with experiments. Indeed, this is carried out here with our $G(q)$ function for cubic metals such as lithium, sodium, potassium, and aluminum where experimental force constants exist from

TABLE III. Resistivity of vacancies in simple metals.

Metal	r_s (a.u.)	ρ_v ($\mu\Omega$ cm/at.%) Hartree $f(q)=0$	$f(q)_{\mathrm{SP}}$	$f(q)_{\mathrm{SSTL}}$
Li	3.22	0.578	0.719	0.763
Be	1.87	0.522	0.591	0.621
Na	3.99	0.774	1.061	1.138
Mg	2.64	0.572	0.717	0.767
Al	2.07	0.526	0.632	0.673
K	4.87	1.028	1.451	1.531
Cd	2.58	0.721	0.910	0.981
In	2.41	0.882	1.089	1.167

TABLE IV. Resistivity of liquid metals (in units of $\mu\Omega$ cm).

Metal	Theory Hartree $f(q)=0$	$f(q)_{\mathrm{SP}}$	$f(q)_{\mathrm{SSTL}}$	Expt[a]
Li	13.8	15.1	15.8	25
Be	63.5	67.5	69.8	• • •
Na	6.1	8.6	9.5	9.6
Mg	19.2	22.3	23.9	27.4
Al	18.9	21.9	23.4	24.2
K	8.9	13.2	14.4	13.0
Cd	14.4	18.1	20.0	33.7
In	27.0	34.0	37.4	33.1

[a] See Ref. 22.

TABLE V. Interatomic force constants (dyn/cm) for lithium metal

Shell	Type of atoms	Interatomic force const	Hartree $f(q)=0$	Theory $f(q)_{SP}$	Theory $f(q)_{SSTL}$	Expt[a]
1	$\frac{1}{2}a(1, 1, 1)$	K_{xx}	3047	3082	3041	2320 ± 32
		K_{xy}	4581	3983	3832	2520 ± 58
2	$\frac{1}{2}a(2, 0, 0)$	K_{xx}	4219	3037	2723	678 ± 71
		K_{yy}	−295	94	144	153 ± 48
3	$\frac{1}{2}a(2, 2, 0)$	K_{xx}	−137	−306	−319	−285 ± 28
		K_{zz}	−15	21	9	110 ± 40
		K_{xy}	122	−327	−327	−152 ± 46
4	$\frac{1}{2}a(3, 1, 1)$	K_{xx}	108	62	98	185 ± 33
		K_{yy}	−5	−8	−9	−116 ± 22
		K_{xy}	14	9	13	22 ± 27
		K_{yz}	42	26	40	−113 ± 34
5	$\frac{1}{2}a(2, 2, 2)$	K_{xx}	51	46	57	158 ± 20
		K_{xy}	63	56	71	−89 ± 57
6	$\frac{1}{2}a(4, 0, 0)$	K_{xx}	21	22	30	−266 ± 63
		K_{yy}	6	7	7	8 ± 38
7	$\frac{1}{2}a(3, 3, 1)$	K_{xx}	−30	−33	−35	−3 ± 18
		K_{zz}	−1	−1	−1	−8 ± 12
		K_{xy}	−33	−37	−38	−22 ± 13
		K_{xz}	−11	−12	−13	30 ± 27

[a] H. G. Smith, G. Dolling, R. M. Nicklow, P. R. Vijayaraghavan, and M. K. Wilkinson, in Proceedings of the Conference on Inelastic Neutron Scattering, Copenhagen, Denmark, 1968, p. 149 (unpublished).

neutron scattering data. Such results are given in Tables V–VIII together with force constants calculated based on $G(q)$ functions determined using Hartree screening and Shaw-Pynn screening. In general, we find that the inclusion of many-electron effects invariably improves the agreement between theory and experiment although excellent agreement is only achieved in sodium and potassium metal. The slight disagreement in aluminum metal could be due to the neglect of anharmonic effects there. In lithium metal, however, the much too large theoretical force constants could be attributed to the neglect of modeling the $l = 1$ component in Shaw's nonlocal bare-ion potential as first

TABLE VI. Interatomic force constants (dyn/cm) for sodium metal.

Shell	Interatomic force const	Hartree $f(q)=0$	Theory $f(q)_{SP}$	Theory $f(q)_{SSTL}$	Expt[a]
1	K_{xx}	1370	1328	1277	1178
	K_{xy}	1991	1548	1461	1320
2	K_{xx}	1532	690	528	472
	K_{yy}	−117	110	115	104
3	K_{xx}	0	−80	−67	−38
	K_{zz}	−9	6	−4	0
	K_{xy}	9	−86	−63	−65
4	K_{xx}	34	19	43	52
	K_{yy}	2	1	2	−7
	K_{xy}	4	2	5	14
	K_{yz}	12	7	16	3
5	K_{xx}	12	10	16	17
	K_{xy}	12	10	17	33

[a] A. D. B. Woods, B. N. Brockhouse, R. H. March, A. T. Stewart, and R. Bowers, Phys. Rev. 128, 1112 (1962).

TABLE VII. Interatomic force constants (dyn/cm) for potassium metal.

Shell	Interatomic force const	Hartree $f(q)=0$	Theory $f(q)_{SP}$	Theory $f(q)_{SSTL}$	Expt[a]
1	K_{xx}	797	771	744	786
	K_{xy}	1168	915	888	895
2	K_{xx}	926	444	394	432
	K_{yy}	−72	56	47	29
3	K_{xx}	−2	−46	−34	−41
	K_{zz}	−3	5	−1	12
	K_{xy}	1	−51	−33	−54
4	K_{xx}	9	2	16	2
	K_{yy}	1	0	0	−4
	K_{xy}	1	0	2	2
	K_{yz}	3	1	6	1
5	K_{xx}	4	3	7	6
	K_{xy}	4	4	8	4

[a] R. A. Cowley, A. D. B. Woods, and G. Dolling, Phys. Rev. 150, 487 (1966).

TABLE VIII. Interatomic force constants (dyn/cm) in aluminum metal.

Shell	Type of Atoms	Interatomic force const	Hartree $f(q)=0$	Theory $f(q)_{\mathrm{SP}}$	$f(q)_{\mathrm{SSTL}}$	Expt[a]
1	$\frac{1}{2}a(1, 1, 0)$	K_{xx}	15623	10411	8788	10107
		K_{zz}	−4207	−925	−232	−1334
		K_{xy}	19830	11337	9019	11444
2	$\frac{1}{2}a(2, 0, 0)$	K_{xx}	3611	1685	1545	2452
		K_{yy}	−295	−77	−95	−529
3	$\frac{1}{2}a(2, 1, 1)$	K_{xx}	−311	−514	−500	−625
		K_{yy}	−61	−87	−89	−182
		K_{xy}	−166	−285	−274	−296
		K_{yz}	−83	−143	−137	−148
4	$\frac{1}{2}a(2, 2, 0)$	K_{xx}	77	45	55	271
		K_{zz}	−27	−24	−29	321
		K_{xy}	104	69	84	−50
5	$\frac{1}{2}a(3, 1, 0)$	K_{xx}	146	161	185	461
		K_{yy}	26	30	32	227
		K_{zz}	11	14	13	198
		K_{xy}	45	49	58	88
6	$\frac{1}{2}a(2, 2, 2)$	K_{xx}	−74	−84	−87	142
		K_{xy}	−76	−87	−90	−109
7	$\frac{1}{2}a(3, 2, 1)$	K_{xx}	36	35	37	−64
		K_{yy}	12	11	12	−94
		K_{zz}	−2	−3	−3	−111
		K_{xy}	29	28	30	36
		K_{xz}	14	14	15	18
8	$\frac{1}{2}a(4, 0, 0)$	K_{xx}	128	142	150	−534
		K_{yy}	2	2	2	−116

[a] G. Gilat and R. M. Nicklow, Phys. Rev. 143, 487 (1966).

suggested by Bortolani and Pizzichini.[23]

D. Sound Velocity

We have further tested the accuracy of the $G(q)$ function by analyzing the sound velocity. Basically one sets up the equation of motion for ions as in studying phonon spectra and obtains the ω-vs-q dispersion relation. The sound velocity s is thus easily derived from $s=\omega/q|_{q\to 0}$. Details of the formalism and calculational procedure have been given earlier by Shyu and Gaspari[24] so only the final results are presented here. Again, results for Hartree screening and Shaw-Pynn screening have been separately obtained. They are all compiled in Table IX and compared with available data from ultrasound measurements.

IV. CONCLUDING REMARKS

We have dealt with the problem of constructing the pseudopotential form factor, which consists of a nonlocal bare-ion potential and a self-consistently determined many-electron screening. In a similar way, an ion-electron-ion $G(q)$ function was constructed to generate the interionic potential in

TABLE IX. Sound velocity in metallic lithium, sodium, potassium, and aluminum.

		Sound velocity (km/sec)			
Metal	Direction of propagation	Hartree $f(q)=0$	$f(q)_{\mathrm{SP}}$	$f(q)_{\mathrm{SSTL}}$	Expt
Li	[100]	8.41	6.74	6.76	•••
	[110]	9.56	8.15	8.18	6.69[a]
	[111]	9.92	8.56	8.60	•••
Na	[100]	3.85	2.90	2.95	2.895[b]
	[110]	4.56	3.81	3.87	3.628[b]
	[111]	4.78	4.07	4.13	•••
K	[100]	2.79	2.16	2.30	•••
	[110]	3.34	2.84	2.96	2.71[c]
	[111]	3.50	3.04	3.16	•••
Al	[100]	8.29	6.18	5.70	•••
	[110]	8.89	6.63	6.05	6.642[d]
	[111]	9.08	6.77	6.16	•••

[a] H. C. Nash and C. S. Smith, J. Phys. Chem. Solids 9, 113 (1959).

[b] M. E. Diederich and J. Trivisonno, J. Phys. Chem. Solids 27, 637 (1966).

[c] W. R. Marquardt and J. Trivisonno, J. Phys. Chem. Solids 26, 273 (1965).

[d] G. N. Kamm and G. A. Alers, J. Appl. Phys. 35, 327 (1964).

metals. Since no arbitrarily adjustable parameter is involved in this calculation, the pseudopotential form factor should serve as meaningful and useful input in studying various properties, such as electronic and optical properties[25] of simple metals. Furthermore, the interionic potential represents the most convenient and basic starting point for investigating lattice relaxation effects around point defects in metals[26] and liquid-metal dynamics.[27]

In addition, we have particularly examined the role of exchange and correlation on the interionic potential. We see that upon inclusion of the many-electron effects, a well-pronounced minimum in $V(r)$ is produced in the region between the first and second neighbors, while such behavior is completely absent if one uses Hartree screening. This minimum in $V(r)$ is well supported by the neutron scattering data on phonon spectra and can be further understood in the following manner. Instead of analyzing it in terms of the interatomic force constants as done earlier, let us use only the tangential force constant which is defined as $k_t = (1/r) \times (dV/dr)$. Now for bcc structure, we have

$$\text{at first neighbor:} \quad k_t(1) = k_{xx}(1) - k_{xy}(1);$$

$$\text{at second neighbor:} \quad k_t(2) = k_{yy}(2) .$$

Using the experimental results on the interatomic force constants derived from neutron scattering measurement listed in Tables VI–VIII, we obtain for Li, $k_t(1) = -200$ dyn/cm and $k_t(2) = 153$ dyn/cm; for Na, $k_t(1) = -142$ dyn/cm and $k_t(2) = 104$ dyn/cm; and for K, $k_t(1) = -109$ dyn/cm and $k_t(2) = 29$ dyn/cm. This says that values of $dV(r)/dr$ evaluated at the first and second neighbor are of opposite sign which suggests that $V(r)$ goes through a minimum in the region between the first and second neighbors. As we have seen earlier such behavior is observed if one includes the exchange and correlation corrections to the ion-electron-ion $G(q)$ function. It may be interesting to carry out directly a full detailed calculation of phonon spectra in the q space, particularly for the noncubic metals like Be, Mg, Cd, and In, where no detailed careful force-constant analysis exists.

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†NDEA Predoctoral Fellow.

‡Alfred P. Sloan Fellow.

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