Electron-Ion Interaction and the Fermi Surfaces of the Alkali Metals

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In the paper[1] to which this note is an addendum, the experimentally observed distortions of the Fermi surfaces of the alkali metals were analyzed by the augmented-plane-wave (APW) phase-shift method. We found that a set of phase shifts $\eta_l(E_F)$ can be obtained for each of the alkali metals such that, for any assumed value of the Fermi-energy parameter E_F, the surface of constant energy $E(\vec{k}) = E_F$ is consistent with the experimental Fermi-surface data. We have recently obtained a second set of phase shifts for sodium which also is consistent with the experimental data. In Table I this alternative set of phase shifts is given for values of E_F in the range 0.20–0.24 Ry.

While the experimental data are consistent with either of the two sets of phase shifts, theoretical considerations suggest that the set given here is the correct one. The present set leads to a predominantly p-like character for the state on the Fermi surface along ΓN, whereas the earlier set implies that this state is s-like. p-like character is consistent with the many first-principles band-structure calculations which indicate that in sodium the p-like state N_1' lies below the s-like state N_1. Moreover, the small positive d-wave phase shift which follows from the present interpretation of the data is perhaps more reasonable than the smaller d-wave phase shift of uncertain sign reported earlier.

That two distinct sets of phase shifts should exist, each consistent with the shape of the Fermi surface of sodium, is not surprising, since the distortions of the Fermi surface of sodium depend principally on the magnitude of the band gap at N, and are independent of the ordering of the levels N_1 and N_1'. Nevertheless, in our earlier calculations we failed to find the second set of phase shifts. A renewed search was stimulated and greatly assisted by the recent calculations of Inoue, Asano, and Yamashita.[2] These authors have constructed self-consistent potentials for all of the alkali metals, and have derived the sets of phase shifts appropriate to their Fermi energies. With the single exception of sodium, their results are in satisfactory agreement with the empirical phase shifts presented in Ref. 1. Their results for sodium, set out in the last row of Table I, are quite close to the alternative set of phase shifts presented here.

Meyer and Young[3] have compared the phase shifts deduced from their neutral pseudoatom model of the alkali metals, with our empirical phase shifts. They found generally satisfactory agreement, but a sizable discrepancy for sodium. This discrepancy also is eliminated if one adopts the alternative set of phase shifts presented here.

The author is indebted to Dr. S. T. Inoue for a valuable discussion, and to Dr. Inoue, Dr. Asano, and Dr. Yamashita for sending him their results prior to publication.

TABLE I. Partial-wave phase shifts derived from an alternative fit to the experimental Fermi-surface distortions of sodium (Ref. 1), and a comparison with the results of Inoue, Asano, and Yamashita (Ref. 2). E_F is the assumed value of the Fermi-energy parameter (Ry). η_3 is set equal to 0.0002 rad, as calculated by Inoue *et al.* $\mathfrak{F}(\eta_l)$ is the Friedel sum of the phase shifts.

	Phase Shifts (rad)				
E_F	η_0	η_1	η_2	η_3	$\mathfrak{F}(\eta_l)$
0.20	0.0650 ± 0.0103	0.0766 ± 0.0013	0.0088 ± 0.0009	0.0002	0.2165
0.21	0.0131 ± 0.0103	0.0651 ± 0.0013	0.0086 ± 0.0009	0.0002	0.1608
0.22	−0.0440 ± 0.0103	0.0533 ± 0.0013	0.0089 ± 0.0009	0.0002	0.1030
0.23	−0.1019 ± 0.0103	0.0411 ± 0.0013	0.0094 ± 0.0009	0.0002	0.0442
0.24	−0.1598 ± 0.0103	0.0284 ± 0.0013	0.0099 ± 0.0009	0.0002	−0.0150
0.2381 [a]	−0.1763	0.0195	0.0078	0.0002	

[a]Phase shifts derived by Inoue *et al.* from a Heine-Hedin-type crystal potential.

[1]M. J. G. Lee, Phys. Rev. 178, 953 (1969).
[2]S. T. Inoue, S. Asano, and J. Yamashita, J. Phys. Soc. Japan (to be published).
[3]A. Meyer and W. H. Young, Phys. Rev. Letters 23, 973 (1969).

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ERRATA

Velocity Acquired by an Electron in a Finite Electric Field in a Polar Crystal, K. K. Thornber and Richard P. Feynman [Phys. Rev. B 1, 4099 (1970)]. In Eq. (18), $|C_k|$ should be $|C_k|^2$; in Eq. (22b), $\cos(\frac{1}{2}s_0v\beta)$ should be $\cos(\frac{1}{2}sv_0\beta)$; in Eq. (24), $C=4B/A\beta^2$ rather than as given. Equation (27) should read

$$R_{\vec{k}}'' = -i\{C_{\vec{k}}^* a_{\vec{k}}^+ \vec{k}\cdot[e^{-i\vec{k}\cdot\vec{r}},\vec{p}]_+ - C_{\vec{k}} a_{\vec{k}}^- \vec{k}\cdot[e^{+i\vec{k}\cdot\vec{r}},\vec{p}]_+\}/2m\ .$$

The third from the last equality in Appendix B should read $-4\pi i[G_x'(\nu) - G_x'(-\nu)]$.

Ultrasonic Attenuation Due to Electron-Phonon Interaction in Potassium, T. M. Rice and L. J. Sham [Phys. Rev. B 1, 4546 (1970)]. We have discovered a numerical error in the evaluation of the resistivities quoted in Table I and shown in Fig. 3. The correct values of the resistivity ρ are obtained by multiplying the quoted values by a factor of $\frac{2}{3}$. The values quoted for τ_2/τ_1 are unchanged. We are grateful to Dr. J. Ekin of Cornell University for a correspondence which led to the discovery of the error.

Anomalous Electron-Phonon Transport Properties of Impure Metals. I. The Electrical Resistivity, M. J. Rice and O. Bunce [Phys. Rev. B 2, 3833 (1970)]. Dr. H. Smith has brought to our attention the following typographical errors in the published paper. The factors of $(1+\rho_{ep}^0/\rho_0)$ occurring explicitly in Eqs. (3.7) and (3.8) should be absent.

On a more serious note we should like to call the attention of the reader of our paper to the recent paper by Dr. H. Smith, [Solid State Commun. 8, 1991 (1970)]. In this paper Dr. Smith has demonstrated that the use of our ansatz (2.15) considerably overestimates the deviation from additivity of the impurity and electron-phonon resistivities in the intermediate temperature range $T\sim T_0$. In fact, Dr. Smith argues that the peaks obtained by us in the deviations from additivity in the region $T\sim T_0$ would be absent in a more rigorous calculation.

Interaction of Dislocations with Electrons and with Phonons, A. Hikata, R. A. Johnson, and C. Elbaum [Phys. Rev. B 2, 4856 (1970)]. The following corrections should be noted:

(1) On p. 4861, Eq. (8) should read $K_2=\Gamma 3\hbar/2\pi^2C^4$.

(2) On p. 4861 first column, starting with line 37 note that $\sigma=1.2\times10^{-8}$ cm, $K_2=7.2\times10^{-73}$ cgs, $\Gamma=2.7\times10^{-23}$ cm sec.

(3) On p. 4861, first column, the last line should read $g(\beta_1)^{1/2}\sim2.4\times10^{10}$ (cgs) and $\gamma(\beta_2)^{1/2}\sim0.1$.

(4) On p. 4861, second column, first paragraph (top) should read:

In order for γ and g to have physically plausible values, these results imply that β_1 and β_2 have to be of the order of 10^{-2} to 10^{-3}; we have not been able to evaluate β_1 and β_2 theoretically. Thus, in conclusion, a comparison of the present results with Leibfried's theory yields a physically plausible value of the scattering width σ. The scattering widths obtained from a comparison of the present results with the theories based on strain field scattering depend on the values chosen for β_1 and β_2.

(5) On p. 4863, second column, the last four lines should read:

However, the phonon scattering width (cross section per unit length) of dislocations deduced from the present measurements, using Leibfried's approach, is quite close to the value expected from physical arguments.

Compton Scattering and Electron Momentum Density in Beryllium, R. Currat, P. D. DeCicco, and Roy Kaplow [Phys. Rev. B 3, 243 (1971)]. We regret that, in mentioning previous positron annihilation work which has been done, we inadvertently omitted reference to the work of S. Berko [Phys. Rev. 128, 2166 (1962)].

Far-Infrared Properties of Lattice Resonant Modes. V. Second-Order Stark Effect, B. P. Clayman, R. D. Kirby, and A. J. Sievers [Phys. Rev. B 3, 1351 (1971)]. A type-setting error was introduced during the galley-correction procedure and resulted