such effects could be sought.[7] Some of these are listed in Table I. For those which are semiconductors, one arrives at conclusions similar to the conclusions of the previous discussion. With others, one would expect an anisotropic photoconductivity or extrinsic semiconductivity to tend toward isotropicity in the presence of a spiral dislocation. This "short-circuiting" of the anisotropicity might also be observed for diffusion, ionic conduction, and the like.

Note added in proof.—Many spiral dislocations have large Burgers' vectors, corresponding to axial displacement of many lattice distances. For such dislocations one has a set of interleaved helicoids rather than a single one (like a screw with a multiple thread) and similar considerations apply.

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[7] CdI_2 seems like a particularly favorable case to investigate, as dislocations of the type contemplated have been much studied, e.g., A. J. Forty, reference 4, and Phil. Mag. **43**, 72 and 377 (1952). Spiral dislocations in beryl and CdI_2 are reported by B. J. Applebe and H. F. Kay, Phil. Mag. **44**, 105 (1953). For a general survey (with much information on SiC) and many references see A. R. Verma, *Crystal Growth and Dislocations* (Academic Press, Inc., New York, 1953).

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Comparison of Various Approximate Exchange Potentials

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A modification of Slater's simplification of the Hartree-Fock equations is proposed, in which an averaged exchange potential is defined for each set of states having a common angular momentum. For a germanium atom we have calculated the approximate exchange potentials according to Slater's averaging procedures and according to our own, and have compared these with the usual Hartree-Fock exchange potentials.

SLATER[1] has recently shown how the Hartree-Fock equations can be approximated by a set of Schrödinger-type equations each containing the same "averaged" exchange potential. The Hartree-Fock equations as modified by Slater are more easily solved than are the original Hartree-Fock equations. It is natural to ask: is it possible to obtain approximate exchange potentials for the individual states better than the one represented by Slater's single averaged exchange potential and at the same time retain most of the simplicity and convenience of Slater's formulation?

That the exchange potentials of the states having a common angular momentum should bear a greater resemblance to each other than to the exchange potentials corresponding to states having other l was suggested to the authors by Herring.[2] Accordingly, we have defined an averaged exchange potential for each set of electronic states having a common l. Each of these averaged exchange potentials is formed from the Hartree-Fock exchange potentials belonging to the occupied states having a particular value of l.

With a view to comparing the various approximate exchange potentials, we calculated the Hartree-Fock, the Slater averaged, the s, p, and d averaged, and the free-electron exchange potentials for a germanium atom. Each of these potentials was computed from an orthonormalized set of radial wave functions $Q_{nl}(r)$ derived from the self-consistent wave functions $P_{nl}(r)$ obtained by Hartree and Hartree for the $(4s)^2(4p)^2$ state of the germanium atom.[3]

We made no attempt to determine self-consistent eigensolutions or potentials using any of the various exchange potential approximations.[4] Each of the potentials we did evaluate may be regarded as the starting potential in the first cycle of a self-consistent iteration procedure. Although a comparison of the potentials corresponding to self-consistent solutions would be more significant, we feel that some insight on the relative merits and special features of the various approximate exchange potentials may be gained by placing our potentials side by side.

The exact Hartree-Fock and the Slater averaged exchange potentials appearing in the wave equation for

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[1] J. C. Slater, Phys. Rev. **81**, 385 (1951).

[2] C. Herring (private communication); see also H. B. Huntington, Phys. Rev. **61**, 325 (1942).

[3] W. Hartree and D. R. Hartree, Phys. Rev. **59**, 306 (1941). We will express the orthonormalized wave function corresponding to state nlm in the form $\psi_{nlm}(\mathbf{r})=r^{-1}Q_{nl}(r)Y_l^m(\theta,\phi)$, where $\mathbf{r}=r,\theta,\phi$, and the $Y_l^m(\theta,\phi)$ are normalized spherical harmonics.

[4] A self-consistent solution for the Cu^+ ion has been obtained by Pratt using the free-electron approximation for the exchange potential; see G. W. Pratt, Jr., Phys. Rev. **88**, 1217 (1952).

$\psi_{nlm}(\mathbf{r}_1)$ may be written as

$$V_{HF;\,nlm}{}^{\mathrm{exch}}(\mathbf{r}_1)=\frac{\sum_{n'l'm'}\int\psi_{nlm}{}^*(\mathbf{r}_1)\psi_{n'l'm'}{}^*(\mathbf{r}_2)(2/\mathbf{r}_{12})\psi_{n'l'm'}(\mathbf{r}_1)\psi_{nlm}(\mathbf{r}_2)d\mathbf{r}_2}{\psi_{nlm}{}^*(\mathbf{r}_1)\psi_{nlm}(\mathbf{r}_1)},\tag{1}$$

and

$$V_{\mathrm{Slater}}{}^{\mathrm{exch}}(\mathbf{r}_1)=\frac{\sum_{n'l'm'}\sum_{n''l''m''}\int\psi_{n'l'm'}{}^*(\mathbf{r}_1)\psi_{n''l''m''}{}^*(\mathbf{r}_2)(2/\mathbf{r}_{12})\psi_{n''l''m''}(\mathbf{r}_1)\psi_{n'l'm'}(\mathbf{r}_2)d\mathbf{r}_2}{\sum_{n'l'm'}\psi_{n'l'm'}{}^*(\mathbf{r}_1)\psi_{n'l'm'}(\mathbf{r}_1)},\tag{2}$$

for all nlm [see reference 1, Eqs. (4) and (7), respectively].[5] In (1), the summation is restricted to all occupied states $n'l'm'$ having the same spin as the state nlm. In (2), the summations in both numerator and denominator are carried over all occupied states having the same spin as the state under consideration.

The averaged exchange potential constructed by us for the states having angular momentum l may be derived from (2) by requiring that $l'=l$ in both numerator and denominator.

The free-electron exchange potential [see reference 1, Eq. (10)] is given by

$$V_{\mathrm{f.e.}}{}^{\mathrm{exch}}(\mathbf{r}_1)=6\left[\frac{3}{4\pi}\sum_{n'l'm'}\psi_{n'l'm'}{}^*(\mathbf{r}_1)\psi_{n'l'm'}(\mathbf{r}_1)\right]^{\frac{1}{3}},\tag{3}$$

for all nlm. The summation is confined to states having the same spin as the state being considered. Throughout this paper, distances will be measured in Bohr units, potentials, in rydbergs.

In our study of the germanium atom, we chose to deal with the $^5S\ (4s)^1(4p)^3$ (valence) state. The spin of each of the four valence electrons is "up." We evaluated the exchange potentials for electrons having both upward and downward spin. In Table I we list selected values of the electronic Coulomb potential $V_{\mathrm{elec}}{}^{\mathrm{coul}}(r)$, the net Coulomb potential [defined as $64/r-V_{\mathrm{elec}}{}^{\mathrm{coul}}(r)$], the free electron exchange potential $V_{\mathrm{f.e.}}{}^{\mathrm{exch}}(r)$, and the various averaged exchange potentials.

The following features of Table I should be noted: (a) The $V_l{}^{\mathrm{exch}}(r)$, $l=0$, 1, 2, differ from each other at all values of r. The different behavior is significant only at moderately large values of r, where the exchange potentials have magnitudes comparable with the

TABLE I. Coulomb and approximate exchange potentials for germanium atom in $^5S\ (4s)^1(4p)^3$ state. The exchange potentials for electrons of spin up and down are shown at the left and right, respectively, of the appropriate columns. (The four valence electrons are all assigned upward spin.) The entries directly below the exchange potential column headings are the arithmetic means. The radial distance r is measured in Bohr units, the various potentials, in rydbergs.

r	$V_{\mathrm{f.e.}}{}^{\mathrm{exch}}(r)$	$V_{\mathrm{Slater}}{}^{\mathrm{exch}}(r)$	$V_{l=0}{}^{\mathrm{exch}}(r)$	$V_{l=1}{}^{\mathrm{exch}}(r)$	$V_{l=2}{}^{\mathrm{exch}}(r)$	$V_{\mathrm{net}}{}^{\mathrm{Coul}}(r)$	$V_{\mathrm{elec}}{}^{\mathrm{Coul}}(r)$
0.01	67.30	62.61	62.66	45.38	36.40	6099.64	300.36
0.02	54.52	55.85	56.13	37.48	29.64	2913.52	286.48
0.05	30.67	35.21	38.52	23.19	17.65	1034.58	245.42
0.10	19.54	19.36	24.26	17.97	12.10	435.35	204.65
0.20	12.59	13.79	14.89	14.02	7.584	161.73	158.27
0.40	6.852 7.015 6.689	6.126	7.076	7.100	5.070	49.24	110.76
0.60	5.417 5.527 5.307	5.420	6.263	5.903	4.733	20.29	86.38
0.80	3.861 3.867 3.855	4.303	5.140	4.768	3.753	10.17	69.83
1.00	2.831 2.921 2.741	3.273 3.257 3.290	4.006 3.822 4.190	3.780 3.754 3.806	2.881 2.888 2.874	5.96	58.04
1.20	2.340 2.716 1.963	2.495 2.454 2.535	2.950 2.397 3.503	2.976 2.843 3.108	2.268 2.295 2.241	3.86	49.47
1.40	2.091 2.746 1.436	1.862 1.724 1.999	2.336 1.643 3.029	2.292 1.944 2.639	1.855 1.907 1.803	2.65	43.06
1.60	1.905 2.743 1.066	1.560 1.497 1.622	2.050 1.400 2.700	1.866 1.406 2.325	1.574 1.653 1.495	1.89	38.11
2.00	1.593 2.575 0.612	1.175 1.188 1.163	1.786 1.258 2.313	1.535 1.092 1.978	1.242 1.371 1.113	1.01	30.99
2.40	1.330 2.297 0.363	0.976 1.045 0.908	1.631 1.180 2.082	1.449 0.966 1.932	1.065 1.241 0.889	0.57	26.10

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[5] The Hartree-Fock radial wave equations may be readily constructed with the aid of the information contained in D. R. Hartree and W. Hartree, Proc. Roy. Soc. (London) **A156**, 45 (1936). The Hartree-Fock and the Slater averaged exchange potentials appropriate to the radial wave equations for the $Q_{nl}(r)$ may be determined by writing the forms analogous to Eqs. (1) and (2), respectively.

TABLE II. Comparison of Hartree-Fock and various averaged exchange potentials. $U_{nl}^{HF}(r)$ is defined as $[Q_{nl}(r)]^2$ multiplied by the Hartree-Fock exchange potential appropriate to state nl [see Eq. (1)]. Similarly, $U_{nl}^{\mathrm{Slater}}(r)$ is defined as $[Q_{nl}(r)]^2 V_{\mathrm{Slater}}^{\mathrm{exch}}(r)$, and $U_{nl}^{(l)}(r)$ as $[Q_{nl}(r)]^2 V_l^{\mathrm{exch}}(r)$. In all cases, we have listed the exchange potentials appropriate to electron states with upward spin, i.e., with the same spin as the four valence electrons. In the case of germanium, $U_{3d}^{HF}(r)$ is identical to $U_{3d}^{(l=2)}(r)$.

r	U_{1s}^{HF}	U_{1s}^{Slater}	$U_{1s}^{(0)}$	U_{2s}^{HF}	U_{2s}^{Slater}	$U_{2s}^{(0)}$	U_{3s}^{HF}	U_{3s}^{Slater}	$U_{3s}^{(0)}$
0.01	428.7	419.3	419.6	29.71	37.28	37.31	3.863	5.237	5.241
0.02	812.1	791.9	796.0	50.93	64.01	64.34	6.507	8.935	8.981
0.05	518.2	471.3	515.7	9.580	10.69	11.70	0.9712	1.207	1.321
0.10	62.67	44.56	55.81	32.12	29.36	36.78	3.853	4.709	5.898
0.20	0.7535	0.2812	0.3035	75.55	69.61	75.15	3.597	4.045	4.367
0.40				5.162	3.507	4.039	6.488	6.476	7.458
0.60				0.2259	0.1101	0.1270	11.86	10.26	11.83
0.80				0.0109	0.0021	0.0025	5.773	4.838	5.783
1.00							1.945	1.521	1.785
1.20							0.5684	0.4007	0.3915
1.40							0.1584	0.0900	0.0496
1.60							0.0431	0.0233	0.0218
2.00							0.0034	0.0015	0.0016

r	U_{2p}^{HF}	U_{2p}^{Slater}	$U_{2p}^{(1)}$	U_{3p}^{HF}	U_{3p}^{Slater}	$U_{3p}^{(1)}$	$U_{3d}^{HF}=U_{3d}^{(2)}$	U_{3d}^{Slater}
0.01	0.2727	0.3773	0.2734	0.0379	0.0511	0.0370		
0.02	2.665	3.972	2.666	0.3604	0.5341	0.3585		
0.05	26.24	39.18	25.80	2.916	5.071	3.340	0.0314	0.0157
0.10	75.84	79.96	74.23	6.463	8.636	8.017	0.4442	0.2774
0.20	57.79	56.70	57.66	0.9620	1.067	1.085	3.931	2.161
0.40	3.172	2.264	2.622	7.373	6.792	7.865	6.895	5.707
0.60	0.1478	0.0765	0.0833	10.07	9.266	10.09	6.561	5.728
0.80	0.0094	0.0022	0.0025	5.246	4.740	5.252	3.877	3.379
1.00				1.994	1.715	1.976	1.936	1.718
1.20				0.6936	0.5415	0.6273	0.8982	0.8403
1.40				0.2337	0.1473	0.1662	0.3818	0.4222
1.60				0.0775	0.0462	0.0434	0.1939	0.2140
2.00				0.0091	0.0044	0.0040	0.0502	0.0580

net Coulomb potential. (b) $V_{\mathrm{Slater}}^{\mathrm{exch}}(r)$ resembles $V_{l=0}^{\mathrm{exch}}(r)$ at small r, as expected. (c) $V_{\mathrm{f.e.}}^{\mathrm{exch}}(r)$ approximates $V_{\mathrm{Slater}}^{\mathrm{exch}}(r)$ remarkably well at small and intermediate values of r.

In Table II we have listed selected values of the various exchange potentials (for states having spin up) multiplied by $[Q_{nl}(r)]^2$, $nl = 1s \cdots 3d$.

An inspection of Table II reveals that the Hartree-Fock exchange potentials are approximated more closely by the $V_l^{\mathrm{exch}}(r)$ than by $V_{\mathrm{Slater}}^{\mathrm{exch}}(r)$ for most of the core states over most of the range of r.

As expected, the results indicate that our modification of Slater's treatment of the Hartree-Fock equations yields better approximate exchange potentials for the core states than Slater's single averaged exchange potential. The fact that the free electron exchange potential resembles $V_{\mathrm{Slater}}^{\mathrm{exch}}(r)$ so well (see Table I) bears out Slater's view[1] that the exchange potential depends more upon the local charge density than upon the detailed nature of the wave functions of the occupied states.[6]

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[6] A comparison of Slater's averaged exchange potential and the free-electron exchange potential has recently been made by H. J. Juretschke, Phys. Rev. **92**, 1140 (1953) for the case of the surface region of a free-electron metal.