

ment of extensive air showers^{6,7}.

The lateral distribution of electrons in extensive air showers produced by primaries with the energy of $(1-2) \times 10^{15}$ ev does not conform with the functions calculated by Nishimura and Kamata for the distribution of electrons in the electron-photon cascade for any value of the parameter s , including $s = 1.2$.

¹Vavilov, Evstigneev, and Nikol'skii, *J. Exptl. Theoret. Phys. (U.S.S.R.)* **32**, 1319 (1957), *Soviet Phys. JETP* **5**, in press (1957).

²K. Greisen, *Progress in Cosmic Ray Physics*, v. III, Amsterdam 1956.

³Dobrovolskii, Nikol'skii, Tukish, and Iakovlev, *J. Exptl. Theoret. Phys. (U.S.S.R.)* **31**, 939 (1956), *Soviet Phys. JETP* **4**, 799 (1957).

⁴Dovzhenko, Nelepo, and Nikol'skii, *J. Exptl. Theoret. Phys. (U.S.S.R.)* **32**, 463 (1957), *Soviet Phys. JETP* **5**, 391 (1957).

⁵I. Nishimura and K. Kamata, *Progr. Theor. Phys.* **6**, 628 (1951).

⁶I. L. Rozental', *J. Exptl. Theoret. Phys. (U.S.S.R.)* **22**, 92 (1952).

⁷G. B. Khristiansen, *The Oxford Conference on Extensive Air Showers*, s. 11, Harwell, 1956.

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On Quasiclassical Single-Electron Wave Functions

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FOR THE PURPOSE OF evaluating the matrix elements for various interactions between matter and a radiation field it is necessary to have good nonrelativistic wave functions of the radiating electron. Hydrogen-like functions or Slater functions are ordinarily used in calculations. However, the results obtained by using these functions are not accurate because they do not take into account the influence of all other electrons of an atom on the radiating electron, or do so insufficiently.

We have constructed approximate wave functions

for an electron in bound states which allow for the electrostatic screening effect of the atomic electrons on the radiating electron. The calculations were based on a combination of the Fermi-Thomas statistical method of obtaining the effective electrostatic field which acts on an individual electron in an atom with a generalized quasiclassical method of calculating wave functions in a given potential field.

The effective electrostatic field acting on a radiating electron in a heavy atom can be described by the Thomas-Fermi potential corrected at small and large distances from the nucleus, as follows:

$$U(r) = \begin{cases} -Z(1 - \alpha r) / r, & r \leq 1/Z; \\ -\frac{1}{r} - \frac{(Z-1)}{r} \varphi_0\left(\frac{r}{\mu}\right); & 1/Z \leq r \leq r_0, \\ -1/r; & r \geq r_0, \end{cases} \quad (1)$$

where r_0 is the boundary radius of a $(Z-1)$ -fold ionized atom in the Thomas-Fermi statistical model and the constant α is determined from the continuity of the potential at $r = 1/Z$ [all quantities in Eq. (1) are measured in atomic units].

Since $U(r)$ is a centrally symmetrical field the angular dependence of the eigenfunctions ψ is exactly the same as in the case of the hydrogen atom. The problem is therefore reduced to the calculation of the radial functions $R_{nl}(r)$ from the equation

$$d^2 x_{nl}(r) / dr^2 + \{2[\epsilon_{nl} - U(r)] - l(l+1)/r^2\} x_{nl}(r) = 0, \\ x_{nl}(r) = r R_{nl}(r), \quad (2)$$

where $U(r)$ is taken from (1).

The solutions of (2) are obtained quasiclassically in the generalized form first indicated by Fock and by Petrashen'¹ and later by other authors². Using the Fock-Petrashen' method the desired solutions of (2) can be represented approximately as

$$x_{nl}(r) = A (S')^{-1/2} \varphi [S(r)], \quad (3)$$

where $\varphi(S)$ is the solution of the radial Schroedinger equation with a Coulomb potential:

$$\varphi(S) = S R_{nl}^{\text{hydr}}(S),$$

and $S = S(r)$, which we shall call the screening function, is determined from the equation

$$\int_{r_1}^r \sqrt{2[\epsilon_{nl} - U(r)] - \frac{l(l+1)}{r^2}} dr \\ = \int_{S_1}^S \sqrt{-\frac{Z^2}{n^2} + \frac{2Z}{S} - \frac{l(l+1)}{S^2}} dS. \quad (4)$$

The approximate energy eigenvalues ε_{nl} are obtained from

$$\int_{r_1}^{r_2} \sqrt{2[\varepsilon_{nl} - U(r)] - \frac{l(l+1)}{r^2}} dr = \pi [n - \sqrt{l(l+1)}].$$

(for states with $l \neq 0$) and

$$\int_0^{r_1} \sqrt{2[\varepsilon_{n0} - U(r)]} dr = n\pi$$

(for s states), where r_1 , r_2 and S_1 , S_2 are the roots of the integrands.

Energy values have been calculated for Ag and In atoms in $1s$, $2s$, $2p$, $3s$, $3p$, $3d$ and $4p$ states and Gd in $3p$, $3d$, $4p$ and $4d$ states. These energies (in Rydbergs) are given in Table 1.

TABLE 1.

Atom	1s	2s	2p	3s	3p	3d	4p	4d
Ag	1791.2	260.5	241.7	50.0	42.6	29.4	5.9	—
In	1956.4	289.9	268.4	57.2	48.7	34.6	7.2	—
Gd	—	—	—	—	108.6	87.1	20.4	12.2

Our calculated energy levels are in quite satisfactory agreement with experiment³; the discrepancies do not exceed 6 to 7% except for the outermost electronic shells. For such shells the statistical method of describing the electrostatic field is no longer valid.

The single-electron wave functions obtained by the Fock-Petrashen' method are continuous over the entire field under consideration, so that they can be used for calculation of the matrix elements. But the screening function $S(r)$, as seen from Eq. (4), cannot be represented in exact analytic form; therefore the matrix elements based on the approximate single-electron functions (3) can only be calculated numerically. In order to avoid numerical integration and represent the approximate radial functions (3) in analytic form the screening function must be suitably approximated. Numerical calculations of the screening functions for several of the above states showed that they can be approximately represented by logarithmic functions of the form $a \ln(1 + br)$, where a and b are such that

$$a \ln(1 + br_2) = S_2, \quad (dS/dr)_{r=r_2} = ab / (1 + br_2)$$

The screening function is very well approximated by $S(r) = a \ln(1 + br)$ in the spatial region which is most important for calculation of the matrix elements. This approximation of the screening functions also permits a relatively easy calculation of the normalization constants A in the approximate wave functions (3).

The approximate radial functions (3) are finally of the form (the $3p$ state of indium being used as an example):

$$R_{31} = \frac{1,887 \cdot 10^3}{a_0^{1/2}} \left\{ \left[\ln \left(\frac{0,789}{a_0} r + 1 \right) \right]^2 r \left(\frac{0,789}{a_0} r + 1 \right)^{17.76} \right\} \left[1 - 9,13 \ln \left(\frac{0,789}{a_0} r + 1 \right) \right].$$

Our approximate radial functions (3) have been used to calculate the relative intensities of the K -series lines of silver and indium X-ray spectra. The intensities are listed in Table 2 (with the intensity of K_{α_1} taken as 100) and compared with the available experimental values^{4,5}.

TABLE 2.

Transition	Line	Ag			In		
		Calculated intensity	Experimental values		Calculated intensity	Experimental values	
			Meyer ⁴	Williams ⁵		Meyer ⁴	Williams ⁵
$K \rightarrow L_{II}$	K_{α_2}	50	51.7	49.9	50	51.8	49.9
$K \rightarrow L_{III}$	K_{α_1}	100	100	100	100	100	100
$K \rightarrow M_{II+III}$	$K_{\beta_1+\beta_2}$	27.2	24	29	24.7	21.7	29.6
$K \rightarrow N_{II+III}$	K_{β_2}	5.14	4.22	6.17	4.48	3.65	6.47

A comparison of our results with the theoretical calculations of others who used hydrogen-like wave functions shows that our quasiclassical radial functions give much better agreement with experimental lines as calculated by the use of hydrogen-like functions are 50: 100: 34: 12 for all atoms, which does not agree with experiment.

In conclusion I must express my gratitude to B. T. Geilikman, who directed this work.

¹V. A. Fock, Dokl. Akad. Nauk SSSR 3, 147 (1934). M. I. Petrashen', Uch. Zap. LGU, Ser. Fiz., 7, 59 (1949); Dokl. Akad. Nauk SSSR 50, 147 (1945).

²S. C. Miller and R. H. Good, Phys. Rev. 91, 174 (1953); S. C. Miller, Phys. Rev. 94, 1345 (1954).

³E. Vainshtein and M. Kakhana, *Tables for X-Ray Spectroscopy*, Acad. Sci. U.S.S.R., 1953.

⁴H. T. Meyer, *Wissenschaftliche Veroeffentlichungen aus dem Siemens-Konzern* 7, 108 (1929).

⁵J. H. Williams, Phys. Rev. 7, 661 (1930) [sic].

Translated by I. Emin

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Magnetic Properties of Oxides of Manganese at Temperatures from 20 to 300° K

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IN CONNECTION with the anomaly in the magnetic properties of manganese carbonate below 31° K, discovered by the authors¹, it was deemed of interest to study the magnetic properties of oxides of manganese at low temperatures. These were the most probable impurities in the preparations studied. The magnetic properties of manganese monoxide (MnO) and of manganese dioxide (MnO₂) have been studied in detail by a number of authors². Both compounds become antiferromagnetic at temperatures 122° K (MnO) and 84° K (MnO₂).

Measurements of the magnetic susceptibility of Mn₂O₃ and Mn₃O₄ were carried out on natural samples of these compounds in the temperature range 20 to 300° K. The measurements were made on the same samples of hausmannite (Mn₃O₄) and of braun-

ite (Mn₂O₃) for which a physico-chemical analysis had earlier been made by Rode³. In Rode's judgment, the composition of these samples was quite close to stoichiometric.

The results of the measurements of the magnetic susceptibility of hausmannite (Mn₃O₄), in the temperature range 43 to 300° K, are presented in Fig. 1 as a plot of $1/\chi$ vs. T (curve 1). Below 42.5° K, hausmannite exhibits characteristic ferromagnetic properties. In Fig. 2 is drawn a curve showing the dependence of the magnetic moment M on the field H for 20.4° K. Hausmannite has the structure of a spinel elongated in the [001] direction⁴. Therefore it is natural to suppose that hausmannite, like the ferrites, is antiferromagnetic with an uncompensated moment. The ordering temperature is $T_C = 42.5^\circ\text{K}$.

The temperature dependence of the inverse magnetic susceptibility in the paramagnetic range agrees qualitatively with the formula proposed by Néel⁵ for such substances,

$$1/\chi = \frac{T}{C_{\text{mol}}} + \frac{1}{\chi_0} - \frac{s}{(T - \theta)}. \quad (1)$$

Curve 2 of Fig. 1 corresponds to formula (1) with the following values of the constants:

$$C_{\text{mol}} = C(\text{Mn}^{2+}) + 2C(\text{Mn}^{3+}) = 10,4;$$

$$1/\chi_0 = 91,3; s = 3480, \theta = 31,1.$$

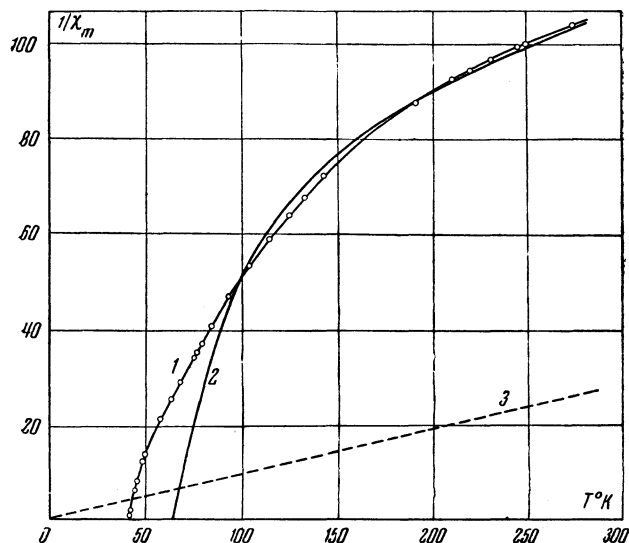


FIG. 1. Temperature dependence of the inverse magnetic susceptibility (molar) of hausmannite (Mn₃O₄). 1—experimental curve; 2—Néel's formula; 3—Curie's law.