Screening and Relativistic Effects on Beta-Spectra

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The effect of screening by atomic electrons on the form of allowed beta-ray spectra of the Fermi theory is calculated approximately, with the assumption of a screened potential based on the Thomas-Fermi model of the atom. The apparent deviation from theory caused by neglecting screening is given for the beta-emitters S^{35}, Cu^{64}, and RaE. Another smaller source of error in interpreting experimental results is the use of the non-relativistic approximation to the Coulomb correction factor. These effects cannot be neglected in an accurate analysis of data for Cu and heavier elements.

I. INTRODUCTION

RECENT measurements by Cook and Langer[1–4] of the beta-ray spectra of Cu^{64}, Cu^{61}, N^{13}, and S^{35} have been interpreted as indicating a discrepancy between the Fermi theory and experimental fact. However, the results of Albert and Wu for S^{35} [5] and Cu^{64} [6] suggest that much of the discrepancy is due to scattering in the source and the source-backing when these are of the thickness used by Cook and Langer. The fact that for Cu^{64} the positron curve of Cook and Langer deviates much more in the Kurie plot from the Fermi allowed curve than does their electron curve is consistent with this explanation, since comparable numbers of positrons and electrons scattered into the low energy region would show up as a greater discrepancy in the Kurie plot of the positrons (because there are so few positrons at low energies).

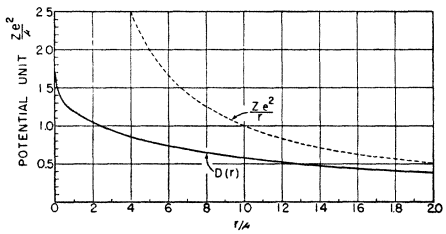

FIG. 1. Difference between Coulomb and screened Coulomb potentials.

Since the actual deviations may be small, it seems worth while to consider some small refinements of the Fermi theory which, though implicit in the theory itself, have hitherto not been considered in the interpretation of experimental data. One such refinement is the modification of the Coulomb correction factor to include the effect of screening by atomic electrons; this effect is calculated approximately below. Another improvement is the use, in analyzing data, of a better approximation to the Coulomb correction factor than has been used by many investigators. (The exact expression for the Coulomb factor contains complex Γ-functions which are not readily evaluated.)

II. THE SCREENING CORRECTION

To evaluate screening effects accurately, the screened wave functions would have to be calculated exactly. However, to make such a calculation for arbitrary atomic number Z, one would have to use an approximate screened potential, such as that provided by the Thomas-Fermi model of the atom.*

The effect of a pure Coulomb field on an allowed beta-spectrum was given by Fermi[7] in his first paper on beta-decay, and is expressed by a factor[8] $F(Z, W)$ which multiplies the spectrum

[1] C. S. Cook and L. M. Langer, Phys. Rev. **73**, 601 (1948).
[2] C. S. Cook and L. M. Langer, Phys. Rev. **74**, 227 (1948).
[3] C. S. Cook, L. M. Langer, H. C. Price, and M. B. Sampson, Phys. Rev. **74**, 502 (1948).
[4] C. S. Cook, L. M. Langer, and H. C. Price, Phys. Rev. **74**, 548 (1948).
[5] R. D. Albert and C. S. Wu, Phys. Rev. **74**, 847 (1948).
[6] Private communication. We are indebted to C. S. Wu and R. D. Albert for informing us of their results on the β-ray spectra of Cu^{64}.

* *Note added in proof:* Professor Lawrence M. Langer has kindly called our attention to an article by M. E. Rose [Phys. Rev. **49**, 727 (1936)] in which the effect of screening was estimated. Rose's results do not agree well with ours, although they are of the same order of magnitude.
[7] E. Fermi, Zeits. f. Physik **88**, 161 (1934).
[8] We use here the notation of Konopinski, Rev. Mod. Phys. **15**, 210 (1943).

obtained when the Coulomb field is ignored. Here W is the total energy of the electron. $F(Z, W)$ is unity for $Z=0$; otherwise it increases the number of low energy electrons and decreases the number of low energy positrons. $F(Z, W)$ is equal to the square of the ratio of the values of the S wave functions of the electron in the nucleus with and without the Coulomb potential (since in an allowed transition the radial wave function of the electron is replaced in the matrix element by its value at the origin). It is assumed here that both wave functions are normalized in the same way at large distances from the nucleus. In calculating the effect of screening it is necessary only to correct the value of the wave function at the origin.

The numerical values of the screening function for the Thomas-Fermi[9] model have been given by Bush and Caldwell.[10] Figure 1 shows the difference $D(r)$ between the Coulomb potential Ze^2/r and the screened potential $V(r)$, plotted as a function of the distance from the nucleus. The unit of length, $\mu=0.885a_0/Z^{\frac{1}{3}}$, and the unit of energy, Ze^2/μ, are the natural units associated with the Thomas-Fermi model. (a_0 is the Bohr radius.) For $r<\mu$ (i.e., over most of the atom), the difference between screened and unscreened potentials is remarkably constant, compared with the potentials themselves. In the region $r>\mu$, and for electron kinetic energies greater than 10 kev, the WKB method is valid for both screened and unscreened potentials. For the approximate calculation below it is specifically assumed that the difference $D(r)$ is constant (equal to D_0) up to some value of r (equal to r_0) beyond which the WKB method is valid.

How this assumption is applied can be understood by considering Fig. 2 for the case of electron emission. In Fig. 2 the solid curve represents the assumed potential, and the dashed curve represents a Coulomb potential shifted upward by a constant D_0. Let us define the following quantities relating to the electron wave function:

$B_f \equiv$ value at the origin for a free electron;
$B_a \equiv$ value at the origin for the assumed potential;
$B_s \equiv$ value at the origin for the shifted potential;
$A_f(\infty) \equiv$ amplitude at infinity for a free electron;
$A_a(\infty) \equiv$ amplitude at infinity for the assumed potential;

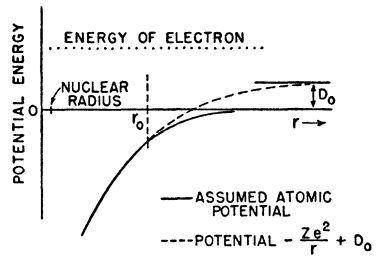

FIG. 2. Potentials used in making the approximation (for electrons).

$A_s(\infty) \equiv$ amplitude at infinity for the shifted potential;
$A_a(r_0) \equiv$ amplitude at $r=r_0$ for the assumed potential;
$A_s(r_0) \equiv$ amplitude at $r=r_0$ for the shifted potential.

Normalization in a large sphere requires

$$A_f(\infty)=A_a(\infty)=A_s(\infty). \quad (1)$$

Furthermore, since the assumed potential and the shifted potential are identical for $r<r_0$,

$$B_a/A_a(r_0)=B_s/A_s(r_0). \quad (2)$$

From these relations it follows that

$$(B_a/B_f)^2=(B_s/B_f)^2(A_s(\infty)/A_s(r_0))^2 \times(A_a(r_0)/A_a(\infty))^2. \quad (3)$$

The quantity $(B_a/B_f)^2$ is the correction factor for the screened potential; denote it by $F_c^-(Z, W)$. The term $(B_s/B_f)^2$ is the usual Coulomb correction factor for a shifted energy, $F(Z, W-D_0)$. The quantities $(A_s(\infty)/A_s(r_0))^2$ and $(A_a(r_0)/A_a(\infty))^2$ can be found, by hypothesis, from the WKB method. Therefore, Eq. (3) reduces, for electrons, to

$$F_c^-(Z, W)=F(Z, W-D_0) \times(W-mc^2/W-mc^2-D_0)^{\frac{1}{2}}. \quad (4)$$

This formula does not contain the critical radius r_0 explicitly. However, D_0 will depend (but not sharply) on r_0/μ, for D_0 is an average of the difference $D(r)$ for $r<r_0$. Strictly speaking, r_0/μ (and therefore D_0) is a function of W and of Z. But it is a reasonable approximation, for all electron kinetic energies greater than 10 kev and all Z, to set

$$D_0=Ze^2/\mu=1.13Z^{4/3}e^2/a_0, \quad (5)$$

where the value of Z is that of the residual nucleus. For the highest possible Z, it may be significantly better to use about nine-tenths of this value for D_0.

[9] E. Fermi, Zeits. f. Physik **48**, 73, **49**, 550 (1928).
[10] V. Bush and S. H. Caldwell, Phys. Rev. **38**, 1898 (1931).

TABLE I. The screening correction.

Element	Z	D_0 (kev)
S^{35}	17	1.3
Cu^{64} (electrons)	30	2.8
Cu^{64} (positrons)	28	2.7
RaE	84	11.2

(a) S^{35}

$T=W-mc$ (kev)	$\frac{F(Z, W-D_0)}{F(Z, W)}$	$\left(\frac{T}{T-D_0}\right)^{\frac{1}{2}}$	$\frac{F_c^-(Z, W)}{F(Z, W)}$	$\left(\frac{F_c^-(Z, W)}{F(Z, W)}\right)^{\frac{1}{2}}$
10	1.007	1.072	1.080	1.039
12	1.006	1.058	1.064	1.032
15	1.004	1.048	1.050	1.025
20	1.002	1.036	1.038	1.019
25	1.001	1.028	1.029	1.014
40	1.000	1.019	1.019	1.009
100	1.000	1.006	1.006	1.003

(b) Cu^{64} (electrons)

10	1.172	1.180	1.382	1.177
12	1.137	1.142	1.298	1.140
15	1.102	1.108	1.222	1.105
20	1.073	1.078	1.159	1.075
25	1.054	1.063	1.120	1.059
30	1.048	1.052	1.100	1.049
40	1.037	1.037	1.075	1.037
50	1.032	1.030	1.062	1.031
70	1.018	1.022	1.040	1.020
100	1.016	1.014	1.030	1.015
200	1.003	1.007	1.010	1.005

(c) RaE

20	1.418	1.430	2.05	1.425
50	1.112	1.135	1.255	1.120
100	1.048	1.062	1.113	1.055
150	1.025	1.042	1.067	1.033
200	1.018	1.030	1.048	1.024
500	1.006	1.012	1.018	1.009

(d) Cu^{64} (positrons)

	$\frac{F(Z, W+D_0)}{F(Z, W)}$	$\left(\frac{T}{T+D_0}\right)^{\frac{1}{2}}$	$\frac{F^+(Z, W)}{F(Z, W)}$	$\left(\frac{F^+(Z, W)}{F(Z, W)}\right)^{\frac{1}{2}}$
10	1.858	0.890	1.654	1.285
12	1.605	0.904	1.449	1.205
15	1.408	0.921	1.295	1.138
20	1.225	0.940	1.151	1.073
25	1.152	0.953	1.099	1.049
30	1.113	0.960	1.068	1.033
40	1.070	0.969	1.038	1.019
50	1.042	0.976	1.010	1.009
70	1.030	0.982	1.012	1.006
100	1.013	0.986	0.999	0.999
200	1.002	0.993	0.995	0.997

A similar analysis for the case of positron emission gives the result

$$F_c^+(Z, W)=F(Z, W+D_0)\times(W-mc^2/W-mc^2+D_0)^{\frac{1}{2}}, \quad (6)$$

where, as usual, Z in $F(Z, W)$ is negative for positrons.

The screening correction increases the numbers of both electrons and positrons, at low energies, over the values for a pure Coulomb field. The increase was to be expected for positrons, since the screening reduces the amount of barrier through which the positron must pass. Any intuitive feeling that the correction should be opposite for electrons is not borne out. Indeed, it seems that the increase of electrons can be understood physically, as follows. That a pure Coulomb field gives more low energy electrons than the free case is in contradiction to the WKB method (wave function small in regions of large kinetic energy), and is a result of the fact that the Coulomb potential dies off too rapidly with increasing r near the nucleus. But the screened Coulomb potential dies off more rapidly, and therefore the contradiction with the WKB method is accentuated.

The only non-relativistic part of the calculation was in the application of the WKB method. Since the potential is small in the region where the WKB method was applied, the non-relativistic WKB formula should be good for electron energies less than about 100 kev. Above this energy the screening correction is small, as shown by the calculations in Section IV. But before examining numerical values we consider the accuracy of various approximations to $F(Z, W)$.

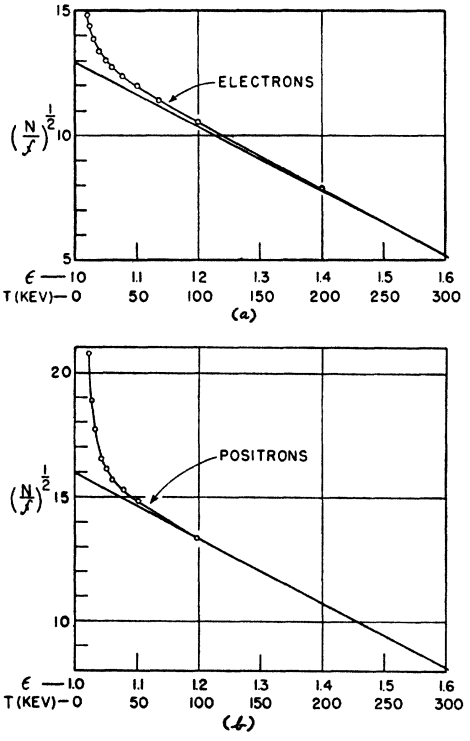

FIG. 3. The effect of screening on the electron and positron spectra of Cu^{64}. The straight lines are the results expected if the Fermi ansatz is correct; the curved lines are the results which will be obtained if the Fermi ansatz is correct but the screening is not considered. The ordinate represents, in arbitrary units, $(N/f)^{\frac{1}{2}}$, where N is the number of particles per unit momentum range and $f=\eta^2(\epsilon-\epsilon_0)^2F(Z, \epsilon)$.

TABLE II. The relativistic correction.

T (kev)	$Z=17$ $\gamma=0.110$ $s=-0.006$	29 0.212 −0.022	84 0.613 −0.209	Cu (ratio of correction at ϵ to correction at ϵ_0)
10	1.009	1.017	0.954	1.032
25	1.007	1.013	0.944	1.028
50	1.005	1.009	0.923	1.024
100	1.002	1.004	0.905	1.019
200	1.000	0.997	0.868	1.012
300	0.998	0.993	0.839	1.007
400	0.997	0.988	0.817	1.003
500	0.095	0.983	0.795	1.000
750	0.993	0.979	0.757	
1000	0.992	0.974	0.725	
1250	0.991	0.971	0.703	

TABLE III. Total effect of screening and relativistic corrections for Cu^{64}

T (kev)	Correction (positron)	Correction (electron)
10	1.317	1.209
12	1.236	1.171
15	1.168	1.135
20	1.102	1.104
25	1.077	1.087
30	1.059	1.076
40	1.044	1.062
50	1.033	1.055
70	1.028	1.042
100	1.018	1.034
200	1.009	1.017
400	1.001	1.003

III. APPROXIMATIONS TO THE COULOMB CORRECTION FACTOR

There seems to be no uniform practice for the approximation to be used for the Coulomb correction factor. Fermi in his original paper deduced that the number of electrons per unit momentum range is proportional to

$$f(\epsilon)=\eta^2(\epsilon_0-\epsilon)^2F(Z,\epsilon), \tag{7}$$

where $F(Z,\epsilon)$, the Coulomb correction factor, is given exactly by

$$F(Z,\epsilon)=\eta^{2s}e^{\pi\delta}|\Gamma(1+s+i\delta)|^2. \tag{8}$$

Here ϵ is the total electron energy in units of the rest energy mc^2, η is the electron momentum in units of mc, Z is the charge of the residual nucleus, and

$$s=(1-\gamma^2)^{\frac{1}{2}}-1, \tag{9}$$

$$\delta=\gamma\epsilon/\eta, \tag{10}$$

$$\gamma=Z\alpha=Z/137. \tag{11}$$

Because these are no adequate tables of the complex Γ-function, it is necessary to approximate the expression in Eq. (8). For $Z=82.2$, Fermi gave the approximation

$$F(82.2,\eta)\approx 1/\eta+0.355. \tag{12}$$

Subsequently, Kurie, Richardson, and Paxton[11] gave the approximation

$$F(Z,\epsilon)\approx 2\pi\delta/1-\exp(-2\pi\delta)\equiv F_N(Z,\epsilon), \tag{13}$$

and remarked that it was good up to $Z=29$ (which was certainly correct for experimental accuracies attainable at the time). This formula can be derived exactly using the non-relativistic Coulomb wave functions,[12] and may therefore be called the non-relativistic approximation. Calculations carried out in Section IV show that for the recent investigations below 200 kev, with high transmission spectrometers having the accuracy claimed, the non-relativistic approximation is sufficiently accurate only for very low Z.

A better approximation, especially for large Z, was given by Bethe and Bacher.[13] In our notation it is

$$F(Z,\epsilon)\approx F_N(Z,\epsilon)\eta^{2s}(\delta^2+\tfrac{1}{4})^s = F_N(Z,\epsilon)[\epsilon^2(1+4\gamma^2)-1]^s. \tag{14}$$

The only approximation made in obtaining (14) from (8) is in setting

$$\left[\frac{1+s^2/\delta^2}{1+\dfrac{\sin^2\pi s}{\sinh^2\pi\delta}}\right]^{\frac{1}{2}}\left|\frac{\Gamma(1+s+i\delta)}{\Gamma(1-s+i\delta)}\right|=(\delta^2+\tfrac{1}{4})^s. \tag{15}$$

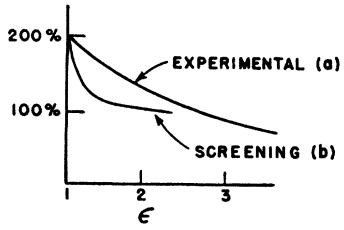

FIG. 4. The RaE spectrum, as experimentally obtained and as given by the screening correction. The curves give (a) the ratio of the number of particles found to the number predicted by Fermi theory without considering screening and (b) the ratio of the number of particles expected using screening to the number expected neglecting it.

[11] F. N. D. Kurie, J. R. Richardson, and H. C. Paxton, Phys. Rev. 49, 368 (1936).

[12] See Mott and Massey, *Theory of Atomic Collisions* (Oxford University Press, New York, 1933).

[13] H. A. Bethe and R. F. Bacher, Rev. Mod. Phys. 8, 194 (1936).

By direct calculation, this approximation seems to be accurate to about 1 percent for Z as large as 84, and to about 0.25 percent for Cu and lighter emitters. (In addition, the percentage error in this approximation depends only slowly on the energy ϵ.)

IV. THE EFFECT ON EXPERIMENTAL RESULTS

Screening Correction

Table I summarizes the calculation of the effect of screening by extranuclear electrons on the S^{35} electron, Cu^{64} positron and electron, and RaE electron spectra. The quantity $F_c^{\pm}(Z, W)/F(Z, W)$ is the ratio of the actual number of particles emitted to the number to be expected for an allowed spectrum without considering screening. The square root of this quantity, also tabulated, is the number by which the uncorrected ordinates of the Fermi[14] plot must be divided to obtain a straight line if the spectrum is of the Fermi allowed type.

For S^{35} the screening correction is extremely small even for low energies, being about 2.5 percent in the Fermi plot at 15 kev. This is in agreement with the results of Albert and Wu,[5] who found a straight line for the Fermi plot; when the screening correction is applied, their result is still a straight line within experimental error. At 10 kev the effect is approximately 4 percent and should be noticeable as a rise.

For Cu^{64} different results are obtained for positrons and electrons. Figure 3 shows what is to be expected. If the straight lines are the results expected on the Fermi model, neglecting screening, for allowed transitions, the curved lines show the effect which screening will have. Because the two parts of the correction (effective shift of energy of the emitted particle and WKB correction) are in opposite direction for positrons but in the same direction for electrons, the electron curve should depart from linearity in the Fermi plot at higher energies than the positron curve. (The energies of departure are 150 as opposed to 50 kev, if a 1 percent deviation is taken as the criterion for departure.) In fact, in the region of 200 kev the positron curve may fall below linearity by a fraction of a percent. However, the positron curve should rise much more rapidly as the energy decreases and the first part of the correction comes to predominate, until at 10 kev the electron curve should be 18 percent and the positron curve 29 percent above the expected values. This means that the actual numbers of positrons and electrons at this energy will exceed the expected numbers by 65 percent and 38 percent, respectively.

Cook and Langer[1] have reported deviations of the experimental electron and positron spectra of Cu^{64} from the shapes predicted by the Fermi theory. These deviations occur at low energies and are generally in the same direction as the screening correction. However, the screening correction is too small to account for the major part of the deviations found by Cook and Langer. Furthermore, their electron curve deviates at a lower energy than their positron curve.

RaE is the only known beta-emitter with a spectrum differing radically from the allowed shape. It is interesting to see if the difference[15] can be explained by the screening. The energy shift, rising as $Z^{4/3}$, is very much larger for RaE than for the light emitters. Hence the deviation from linearity in the Fermi plot begins at a much higher energy, being 1 percent at 500 kev and increasing with decreasing energy until at 20 kev it is 43 percent. This means that there are 2.05 times as many electrons at this energy as would be expected neglecting screening.

Comparison with experimental data[15] (Fig. 4) shows that the correction is adequate to explain the deviation from the allowed spectrum at very low energy, but falls off much too rapidly with increasing energy to explain fully the forbidden shape of the RaE spectrum.

Relativistic Correction

Using Bethe's approximation, Eq. (14), Table II gives the square root of the correction factor for various values of Z, by which the ordinates of the Kurie plot must again be divided if the non-relativistic approximation has been used, to obtain a straight line, if the Fermi theory is correct.

The final column gives the ratio of the correction factor to its value at the endpoint of the

[14] The terms "Fermi plot" and "Kurie plot" are used here interchangeably. Strictly, the first is the relativistic and the second the non-relativistic form.

[15] E. J. Konopinski, Rev. Mod. Phys. **4**, 229 (1943).

Cu^{64} electron spectrum taken approximately at 500 kev. The positron endpoint is somewhat higher, which would tend to increase the numbers in the last column by about 0.1 percent for positron emission. For the electrons of this isotope $Z=30$, for the positrons $Z=28$; 29 is taken as a good approximation for both. The above tables show, as expected, that the non-relativistic approximation is best for low Z and low energy, relativistic effects being more important for electrons of higher energy in stronger Coulomb fields.

For S^{35} the relativity correction is negligible because of (a) the smallness of its magnitude everywhere, (b) the shortness of the spectrum, with $\epsilon_0 \sim 1.3$, so that the correction over the entire spectrum varies by only about 0.8 percent.

For Cu^{64} the total effect of the screening and relativity corrections is given in Table III. Again the numbers refer to the division of the ordinates in the Kurie plot—this time to correct for both screening and relativistic effects.

Figure 5 shows the results which are to be expected if both screening and relativity effects are neglected for Cu^{64} positrons and electrons. The Kurie plot for electrons should begin to deviate from linearity at about 250 kev, and for positrons at about 180 kev. In particular, the relativity correction affects the region from 50 to 250 kev. The deviations from linearity might not be noticed until lower energies are reached because of a possible tendency, in the case of a correction which extends over so much of the spectrum, to draw the straight line at a somewhat larger angle with the energy axis. With decreasing energy, the positron curve should rise more gradually at first, then more rapidly than the electron curve until at 10 kev there should be a 32 percent positron and 21 percent electron excess in the Kurie plot.

The investigators of RaE[16–18] seem to have used Fermi's approximation (Eq. (12)) of the relativistic formula, which differs by about 10 percent at 10 kev, 5 percent at 25 kev, and 1 percent at 200 kev from the approximation of Bethe. This discrepancy does not go very far toward explaining the forbidden nature of the RaE spectrum.

In calculating the effect of the screening, the non-relativistic term $\{[F_N(Z, W-D_0)/F_N(Z, W)]\}^{\frac{1}{2}}$ was actually used instead of the corresponding relativistic term $\{[F(Z, W-D_0)/F(Z, W)]\}^{\frac{1}{2}}$. Calculation shows that for the worst case (RaE) they differ at 200 kev only by 0.3 percent, which is about 10 percent of the effect of the energy shift. Furthermore, the non-relativistic WKB method was used. This leads to an error (in the opposite direction from that just mentioned) which is largest for large D_0 and largest relative to the entire screening correction for high energies. As an example, a rough calculation indicates that it amounts to about 0.7 percent in the Kurie plot for RaE at 200 kev. Since the entire method used in calculating the screening correction is probably not accurate to better

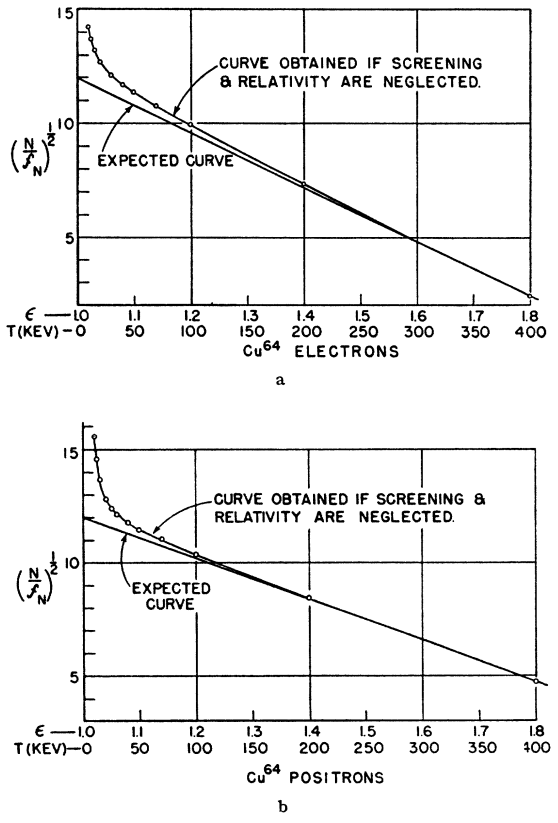

FIG. 5. The effect of neglecting screening and relativistic corrections on the positron and electron spectra of Cu^{64}. The curves are to be interpreted as those of Fig. 3, except that $f_N=\eta^2(\epsilon-\epsilon_0)^2F_N(Z, \epsilon)$.

[16] G. J. Neary, Proc Roy. Soc. **175A**, 71 (1940).
[17] A. Flammersfeld, Zeits f. Physik **112**, 727 (1939).
[18] L. M. Langer and M. D. Whitaker, Phys. Rev. **51**, 713 (1937).

than about 10 percent of the correction itself, these effects are of minor importance.

We would like to express our appreciation to Professors W. W. Havens, Jr. and L. J. Rainwater for their encouragement and for numerous helpful discussions concerning this paper.

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Rotational Absorption Spectrum of OCS*

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Extended measurements in the microwave rotational spectrum of carbonyl sulfide (OCS) are presented and correlated with the data obtained by other investigators. Precision measurements of rotational transitions for $J_{1\to2}$, $J_{2\to3}$, $J_{3\to4}$, $J_{4\to5}$ allow the evaluation of precise reciprocal moments of inertia in the ground vibrational state, and the centrifugal distortion coefficient. From frequencies observed for $O^{16}C^{12}S^{32}$, $O^{16}C^{13}S^{32}$, and $O^{16}C^{12}S^{34}$, internuclear distances have been calculated. Equilibrium moments of inertia and internuclear distances cannot as yet be given, since thus far only one of the three vibrational-rotational interaction coefficients (α_2) has been reported. Theoretical considerations involving such equilibrium data are discussed. Data on l-doubling in $O^{16}C^{12}S^{32}$, $O^{16}C^{13}S^{32}$, and $O^{16}C^{14}S^{32}$ are presented. The Stark effect of carbonylsulfide has been measured in $O^{16}C^{12}S^{32}$ and $O^{16}C^{13}S^{32}$. These measurements lead to the evaluation of the dipole moment and indicate the effect of isotopic changes on the dipole moment.

CARBONYL sulfide (OCS) is known to be a linear molecule. In this paper we have attempted to correlate existing information regarding the structure of this molecule which may be deduced from the rotational absorption spectrum, and to give extended measurements in order to allow a unified presentation. We wish to point out that several other investigators have been instrumental in obtaining much of the experimental and theoretical data considered below.

I. GENERAL THEORY

The rotational contribution to the energy levels of an unperturbed linear rotor in any vibrational state can be shown to be[1]

$$W=[J(J+1)-l^2]hcB_v - [J(J+1)-l^2]^2hcD_v, \quad (1)$$

where W is in ergs, J = total orbital angular momentum quantum number, l = quantum number of angular momentum parallel to figure axis due to a degenerate bending vibration, h = Planck's constant, c = speed of light, B_v = "reciprocal moment of inertia" in cm^{-1}, and D_v = centrifugal distortion coefficient in cm^{-1}.

Thus, from the Bohr frequency condition and the selection rule $\Delta J=+1$, rotational transitions are induced in a molecule with an electric dipole moment by radiation with frequencies in cycles/sec. given by

$$\nu_{J\to J+1}=2cB_v(J+1) - 4cD_v[(J+1)^3-l^2(J+1)]. \quad (2)$$

The "reciprocal moment of inertia" of the molecule in any vibrational state is related to the moment of inertia with the atoms in the minima of the vibrational potentials through the relation[1]

$$B_v=B_e-\sum_i \alpha_i[v_i+(d_i/2)] \quad (3)$$

where $B_e=(h/8\pi^2I_ec)$ cm^{-1}, I_e = equilibrium mo-

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[1] G. Herzberg, *Infra-Red and Raman Spectra of Polyatomic Molecules* (D. Van Nostrand Company, Inc., New York, 1945), p. 370–371.