

expression (1).<sup>19</sup> The resulting values of  $\lambda$  for the  $S,T$  and  $V,T$  admixtures are

$$\lambda_{S,T} = -0.93 \pm 0.09,$$

$$\lambda_{V,T} = +0.96 \pm 0.04.$$

These quantities are indistinguishable from the case of a pure Fermi transition, which would yield values of either  $-1$  for the scalar invariant or  $+1$  for the vector invariant. The  $A^{35}$  mirror transition is, therefore, considerably more favorable for a recoil experiment than was previously indicated by the values,  $\lambda_{S,T} = -0.36$  and  $\lambda_{V,T} = 0.68$ , calculated from the old  $ft$  value of 3400 seconds. An experimental measurement of  $\lambda$  for  $A^{35}$ , however, would have to be corrected for the weak

<sup>19</sup> This method of predicting the angular correlation coefficient was suggested by D. C. Peaslee.

lower beta groups before the results could be compared with the above predictions.

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## Radiative Capture of Orbital Electrons

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A theory is developed of the continuous radiation spectrum which accompanies nuclear capture of atomic electrons. It is shown that quantitative predictions of the spectrum intensities must take into account the influence of the electrostatic field of the nucleus on the radiation process. This is accomplished by evaluating and making use of a particularly simple form of the Green's function for electron propagation in a Coulomb field. In a first approximation which treats the atomic electrons nonrelativistically, the spectra radiated by electrons captured from  $S$ -states are shown at all energies to have the form  $x(1-x)^2$ , where  $x = E/E_{\max}$ . Radiative capture of electrons from  $P$ -states is shown to produce a spectrum which becomes extremely intense at low energies, where it merges continuously with the characteristic x-ray spectrum. Certain relativistic corrections to the  $S$ -state radiative capture probabilities are evaluated and shown to bring about an energy-dependent reduction of the intensities of the corresponding spectra. Functions are tabulated from which the spectra for allowed capture from various orbital states of any element may be determined. The calculated spectra are found to be in satisfactory agreement with those observed experimentally. In particular, the unexpectedly high intensities found at low  $\gamma$ -ray energies are explained by the radiatively induced capture of electrons from  $P$  states.

### 1. INTRODUCTION

ALTHOUGH capture of orbital electrons is one of the more common forms of nuclear decay, the indirect nature of the methods by which it has been detected has limited its usefulness as a source of nuclear data. In particular the usual observation of the process by means of the subsequently emitted x-rays or Auger electrons has contributed only a knowledge of decay lifetimes. The efficient analysis of nuclear  $\gamma$  radiation, which has recently become practicable, makes possible a much more direct means for studying orbital capture. This method takes advantage of the radiation which is emitted in a certain fraction of the decay processes as a result of sudden acceleration of charge and magnetic moment. Although such radiation is weak in intensity,

an emitted photon shares the large energy which is released by the capture, an energy which would otherwise be carried off entirely by the neutrino. The continuous  $\gamma$ -ray spectra which result bear an analogy to the electron spectra of  $\beta$  decay. They may be expected to furnish corresponding information on energy releases and changes of spin and parity.

An early calculation of the radiation to be anticipated in  $K$  capture was made by Morrison and Schiff.<sup>1</sup> They predicted that the intensity distribution would have the form  $x(1-x)^2$ , where  $x$  is the ratio of the  $\gamma$ -ray energy to the energy released in the reaction. The observed spectra show a considerably larger number of low-energy  $\gamma$  rays than this form predicts. In particular, in every element for which the spectrum is known down to energies approaching the characteristic x-ray region,

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<sup>1</sup> P. Morrison and L. I. Schiff, Phys. Rev. 58, 24 (1940).

there is an unanticipated rapid increase of intensity with decreasing photon energy. For certain of the heavier elements, e.g., Cs<sup>131</sup>, the steep rise of intensity dominates the spectrum shape entirely, obliterating the expected maximum at  $E = \frac{1}{3}E_{\text{max}}$ . In a previous note<sup>2</sup> we have indicated that this behavior is caused by the radiative capture of electrons from states of unit orbital angular momentum. We have also outlined a mathematical technique with which the spectra may be accurately determined by simple analytic means. The present paper, and another that follows, will be devoted to explaining, by this means, the detailed shape of the spectrum for allowed transitions, and to furnishing quantitative predictions of its intensity.

An allowed capture process accompanied by radiation may be pictured as taking place in two stages: an electron emits a photon during a virtual transition to a state from which it is subsequently captured by the nucleus. Since an electron may be captured from any  $S$  state, and since all intermediate  $S$  states lead to equivalent decay processes, the amplitudes for the transitions they define add coherently. The virtual transitions to  $S$  states already occupied in the atom are forbidden by the exclusion principle, but equal transition amplitudes will be shown to arise from processes in which capture of the obstructing electron precedes the radiative transition. Consequently, the matrix element for radiative capture is a summation of amplitudes for transitions through all  $S$  states.

If the compound process is one which leaves vacant an initially occupied  $S$  state, the radiation is emitted during a transition between two spherically symmetric states of the system. The radiation must therefore be caused by a reorientation of the electron spin. This is the process considered by Morrison and Schiff in the calculation of the spectrum noted earlier. They employed free-particle wave functions for the intermediate states and neglected the momentum of the electron in its initial bound state. Because the process takes place in a region in which the Coulomb field is most intense, these assumptions prove quantitatively unreliable, except for very energetic  $\gamma$  rays radiated in the fields of the lightest nuclei. By avoiding these assumptions, we shall, in the present work, provide a theory of much wider applicability. The possibility of a more accurate theory is afforded by the observation that the summation over intermediate states in a Coulomb field, required to find the matrix element, may be expressed exactly in closed form. Performing the intermediate state summation will be shown equivalent to finding the amplitude that an electron which has emitted a virtual photon of a particular energy and at a given point succeed in reaching the nucleus. The latter amplitude, or Green's function, satisfies a simple inhomogeneous form of the Schrödinger equation. The

<sup>2</sup> R. J. Glauber and P. C. Martin, Phys. Rev. **95**, 572 (1954).

$\gamma$ -ray spectrum may be obtained directly from this function.

Electrons initially in  $P$  states may undergo radiative capture by making electric dipole transitions to the intermediate  $S$  states from which they are captured. Although these processes are overlooked when the initial electron momentum is neglected, simple considerations indicate that their contribution dominates the low-energy portion of the  $\gamma$ -ray spectrum. In particular, the process in which the capture of a  $1S$  electron is followed by a radiative  $2P$  to  $1S$  transition differs from the usual course of  $K$  capture followed by the radiation of a characteristic  $K$ -series x ray only by relaxing the requirement of energy conservation in the intermediate state. The continuous photon spectrum becomes extremely intense in the neighborhood of the characteristic x-ray line and, indeed, in its immediate region represents no more than the wing of the line. On the other hand, the  $P$ -state intensity remains appreciable for photon energies considerably greater than the characteristic x-ray energy. At these latter energies, as we shall see, no single type of virtual transition contributes a dominant portion of the intensity.

The sections which follow are devoted to formulation of the transition probability for radiative capture, to a discussion of the Green's function, and to calculation of the spectra radiated in electron capture from various orbital states. To simplify the discussion, nonrelativistic bound-state wave functions will be used, in most of this paper. In Sec. 9, however, the treatment of relativistic corrections to the  $S$ -state spectrum is begun by showing the influence of spin-orbit coupling. To remove the approximations made in the present paper, which may be inaccurate for the heavy elements, a fully relativistic treatment of the  $S$ -state spectrum will be given in a subsequent paper. That treatment is separated from the present one since a major part of the problem encountered is the more general one of developing simplified techniques for performing calculations with the solutions of the Dirac equation in a Coulomb field. The influence of the screening field generated by the atomic electrons will also be discussed in that paper in keeping with the desire for greater accuracy.

## 2. TRANSITION AMPLITUDE FOR RADIATIVE CAPTURE

Since the problem of radiative capture involves electrons in bound states, it is convenient to employ a representation in which the electron field operator  $\psi(x)$  satisfies a Dirac equation<sup>3</sup> containing the nuclear

<sup>3</sup> We employ units in which  $c=1$ ,  $\hbar=1$ . Points of space-time are represented by  $x_\mu = (\mathbf{r}, it)$ . The anticommuting matrices  $\gamma_\mu$  have normalization  $\gamma_\mu^2 = -1$  and we define  $\bar{\psi} = \psi^* \gamma_0$  where  $\gamma_0 = -i\gamma_4$ .

Coulomb field<sup>4</sup>  $A_\mu^{(e)} = (0, 0, 0, iZe/r)$ ,

$$\left[ \gamma_\mu \left( \frac{1}{i} \frac{\partial}{\partial x_\mu} + eA_\mu^{(e)} \right) + m \right] \psi(x) = 0. \quad (2.1)$$

Our interest in the interaction of the electron field with the radiation field  $A_\mu(x)$  is limited to processes in which a single photon is emitted. Hence we need only employ the part of the interaction Hamiltonian,

$$H^{(R)}(x) = e\bar{\psi}(x)\gamma_\mu A_\mu^{(+)}(x)\psi(x), \quad (2.2)$$

where  $A_\mu^{(+)}$  is the portion of the field operator which describes photon creation. Likewise our concern with the coupling of the electron field to the nucleon and neutrino fields is limited to processes in which an electron is captured. Hence we need only employ the corresponding terms of the general  $\beta$ -decay interaction,

$$H^{(C)}(x) = \sum_{s,\lambda} c^{(s)} (\bar{\phi}_n(x) T_\lambda^{(s)} \phi_p(x)) (\bar{\chi}(x) T_\lambda^{(s)} \psi(x)). \quad (2.3)$$

This expression, an arbitrary linear combination with coefficients  $c^{(s)}$  of the  $\beta$ -coupling operators,  $T_\lambda^{(s)}$ , allows for all possible interaction mixtures. The functions  $\bar{\phi}_n$ ,  $\phi_p$ , and  $\chi$  are operators for the neutron, proton, and neutrino fields, respectively.

The probabilities of processes involving both photon emission and electron capture may be found from the second-order term of the scattering matrix,<sup>5</sup>

$$S_2 = - \int_{-\infty}^{\infty} d^4x_1 \int_{-\infty}^{\infty} d^4x_2 (H^{(R)}(x_1), H^{(C)}(x_2))_+. \quad (2.4)$$

Here  $(\ )_+$  denotes a time-ordered product which places the operator evaluated at the earlier time on the right. On introducing the function  $\epsilon(t) = t/|t|$ , the product may be written as

$$\begin{aligned} (H^{(R)}(x_1), H^{(C)}(x_2))_+ \\ = \frac{1}{2} \{ H^{(R)}(x_1) H^{(C)}(x_2) + H^{(C)}(x_2) H^{(R)}(x_1) \} \\ + \frac{1}{2} [ H^{(R)}(x_1), H^{(C)}(x_2) ] \epsilon(t_1 - t_2). \end{aligned} \quad (2.5)$$

This expression, substituted in (2.4), effects the separation of processes whose intermediate states are respectively real and virtual. For the terms in curly brackets, the time integrations indicated in (2.4) may be factored and separately performed. This procedure imposes separate conditions of energy conservation on both the capture and radiative steps of the processes described. For an atom initially in its ground state, the terms in curly brackets describe the electron capture processes which are followed by radiation of the characteristic x-rays. The continuous spectrum of photons accompanying electron capture, however, comes from processes in which the intermediate state cannot, in

general, conserve energy. Such processes are represented by the commutator term of (2.5), and we define a part of the transition matrix,  $S_2'$ , which describes these alone:

$$S_2' = -\frac{1}{2} \int_{-\infty}^{\infty} d^4x_1 \int_{-\infty}^{\infty} d^4x_2 [H^{(R)}(x_1), H^{(C)}(x_2)] \times \epsilon(t_1 - t_2). \quad (2.6)$$

To show explicitly the influence of the exclusion principle when more than one electron is present, we express the electron field  $\psi(x)$  and its conjugate  $\bar{\psi}(x)$  as sums of the various stationary state wave functions of Eq. (2.1) multiplied by the annihilation and creation operators for these states.

$$\begin{aligned} \psi(x) &= \sum_{\alpha} a_{\alpha} \psi_{\alpha}(\mathbf{r}) \exp[-iE_{\alpha}t], \\ \bar{\psi}(x) &= \sum_{\alpha} a_{\alpha}^{\dagger} \bar{\psi}_{\alpha}(\mathbf{r}) \exp[iE_{\alpha}t]. \end{aligned} \quad (2.7)$$

The explicit separation of the time dependence will aid in the evaluation of  $S_2'$ .

For a process in which a photon of propagation vector  $\mathbf{k}$  is emitted, the operator  $H^{(R)}$  may be written in the form<sup>6</sup>

$$\left[ \int H^{(R)}(x) d\mathbf{r} \right]_{\mathbf{k}} = \sum_{\alpha, \beta} H^{(R)}_{\beta\alpha}(\mathbf{k}) a_{\beta}^{\dagger} a_{\alpha} \times \exp[i(E_{\beta} - E_{\alpha} + k)t]. \quad (2.8)$$

This operator allows a wide variety of electronic transitions to accompany photon emission. An analogous operator may be introduced for the process in which a neutrino of momentum  $\mathbf{p}$  is emitted<sup>7</sup> and an electron captured. Assuming the nucleus simultaneously undergoes a transition from its initial state  $i$  to its final state  $f$ , changing its energy by an amount  $\Delta E$ , we may write

$$\left[ \int H^{(C)}(x) d\mathbf{r} \right]_{\mathbf{p}, f, i} = \sum_{\gamma} H_{\gamma}^{(C)}(\mathbf{p}) a_{\gamma} \times \exp[i(p - E_{\gamma} + \Delta E)t]. \quad (2.9)$$

This form permits electron capture from any occupied state.

With the use of these expressions, the corresponding matrix element of  $S_2'$  becomes

$$(S_2')_{\mathbf{k}, \mathbf{p}, f, i} = - \sum_{\alpha\beta\gamma} H_{\beta\alpha}^{(R)}(\mathbf{k}) H_{\gamma}^{(C)}(\mathbf{p}) [a_{\beta}^{\dagger} a_{\alpha} a_{\gamma}] \mathcal{G}, \quad (2.10)$$

where

$$\begin{aligned} \mathcal{G} &= \frac{1}{2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \exp[i(E_{\beta} - E_{\alpha} + k)t_1] \\ &\quad \times \exp[i(p - E_{\gamma} + \Delta E)t_2] \epsilon(t_1 - t_2) dt_1 dt_2. \end{aligned} \quad (2.11)$$

The time integrations may be performed immediately<sup>8</sup>

<sup>6</sup> Spin and polarization indices will later be indicated explicitly.

<sup>7</sup> The neutrino mass is assumed to vanish.

<sup>8</sup> Making the usual assumptions of adiabatic decoupling as  $t \rightarrow \pm\infty$ .

<sup>4</sup> See, for example, W. H. Furry, Phys. Rev. **81**, 115 (1951). The screening effects of the electrons are neglected for the present.

<sup>5</sup> F. J. Dyson, Phys. Rev. **75**, 486 (1949).

to yield

$$g = 2\pi i \delta(p+k+\Delta E - E_\gamma + E_\beta - E_\alpha)(E_\beta - E_\alpha + k)^{-1}, \quad (2.12)$$

the first factor of which represents over-all energy conservation.

The expression (2.10) involving the electron creation and annihilation operators may be reduced, in view of the anticommutation properties of these operators, in the following manner:

$$\begin{aligned} [a^\dagger_{\beta\alpha} a_\alpha, a_\gamma] &= a^\dagger_{\beta\alpha} a_\alpha a_\gamma - a_\gamma a^\dagger_{\beta\alpha} a_\alpha \\ &= -(a^\dagger_{\beta\alpha} a_\gamma + a_\gamma a^\dagger_{\beta\alpha}) a_\alpha \\ &= -\delta_{\beta\gamma} a_\alpha. \end{aligned} \quad (2.13)$$

This condition, that the state  $\gamma$  from which capture takes place be the same as the final state  $\beta$  of the radiative transition, is a direct consequence of the restriction to virtual intermediate states.

Substituting (2.12) and (2.13) in the expression for the transition operator, we obtain

$$(S_2')_{\mathbf{k}, \mathbf{p}, f, i, \alpha} = 2\pi i \sum_{\alpha\beta} \delta(p+k+\Delta E - E_\alpha) \times \frac{H_{\beta\alpha}^{(R)}(\mathbf{k}) H_\beta^{(C)}(\mathbf{p})}{E_\beta - E_\alpha + k} a_\alpha. \quad (2.14)$$

This operator accounts for radiative capture of an electron from any occupied state. It is especially to be noted that the summation over states  $\beta$  is unrestricted by the possible occupation of these states by other electrons. Although certain radiative transitions which would be followed by capture are indeed forbidden when the intermediate state is occupied, the absence of these terms in the summation is precisely compensated for by the occurrence of processes in which the capture of the obstructing electron precedes the radiative transition. The matrix element for radiative capture from any state may thus be computed as if all other states were unoccupied.

We begin the evaluation of the matrix elements describing radiative capture from occupied electron states by explicitly exhibiting the quantities  $H_{\beta\alpha}^{(R)}(\mathbf{k})$  and  $H_\beta^{(C)}(\mathbf{p})$ , which occur in (2.14). The first of these is

$$H_{\beta\alpha}^{(R)}(\mathbf{k}) = e(2\pi/k)^{\frac{1}{2}} \int \bar{\psi}_\beta(\mathbf{r}) \mathbf{e}_\mu \gamma_\mu e^{-i\mathbf{k}\cdot\mathbf{r}} \psi_\alpha(\mathbf{r}) d\mathbf{r}, \quad (2.15)$$

where  $\mathbf{e}_\mu$  is the polarization vector of the emitted photon. In considering allowed transitions the capture matrix element is given by<sup>9</sup>

$$H_\beta^{(C)}(\mathbf{p}) = \sum c^{(s)}(T_\lambda^{(s)})_{f,i} (\bar{\chi}_\beta(0) T_\lambda^{(s)} \psi_\beta(0)), \quad (2.16)$$

where  $(T_\lambda^{(s)})_{f,i}$  is the matrix element of the operator  $T_\lambda^{(s)}$  taken between the initial and final nuclear states, and  $\bar{\chi}_\beta(0)$  is the neutrino wave function evaluated at

<sup>9</sup> This form assumes the use of nonrelativistic representations of the electron bound state wave functions.

the origin. It is convenient, until the final stages of calculation, to abbreviate the summation over the different forms of coupling of the spinor fields. This is done by introducing the symbol  $N_{f,i}$ ,

$$N_{f,i} = \sum_{s,\lambda} c^{(s)}(T_\lambda^{(s)})_{f,i} T_\lambda^{(s)}, \quad (2.17)$$

for the weighted sum of Dirac matrices occurring in the expression (2.16). We designate a matrix element of the transition operator (2.14) for radiative capture of an electron from the state  $\alpha$  by

$$(S_2')_{\mathbf{k}, \mathbf{p}, f, i, \alpha} = 2\pi i \delta(p+k+\Delta E - E_\alpha) M_\alpha(\mathbf{k}, \mathbf{p}), \quad (2.18)$$

where the amplitude  $M_\alpha(\mathbf{k}, \mathbf{p})$  is given by

$$M_\alpha(\mathbf{k}, \mathbf{p}) = e(2\pi/k)^{\frac{1}{2}} (\bar{\chi}_\beta(0) N_{f,i} \psi_\beta(0)) \int \bar{\psi}_\beta(\mathbf{r}) \mathbf{e}_\mu \gamma_\mu e^{-i\mathbf{k}\cdot\mathbf{r}} \psi_\alpha(\mathbf{r}) d\mathbf{r} \times \sum_\beta \frac{1}{E_\beta - E_\alpha + k}. \quad (2.19)$$

The summation over intermediate electron states in (2.19) extends over the bound states of the Coulomb field and those of the continuum as well. The evaluation of the individual radiation matrix elements followed by the summation indicated would present a task of formidable proportions. An alternative procedure proves far simpler. We first carry out the summation over intermediate states and then perform the spatial integration. This is possible because the summation

$$\sum_\beta \frac{\psi_\beta(\mathbf{r}) \bar{\psi}_\beta(\mathbf{r}')}{E_\beta - E}, \quad (2.20)$$

which is the Green's function  $G_E(\mathbf{r}, \mathbf{r}')$  for the wave equation of the electron in a Coulomb field, occurs in a particularly simple form in Eq. (2.19).

The equations satisfied by  $G_E(\mathbf{r}, \mathbf{r}')$  are

$$(H - E)G_E(\mathbf{r}, \mathbf{r}')\gamma_0 = \delta(\mathbf{r} - \mathbf{r}'), \quad (2.21)$$

and its adjoint

$$G_E(\mathbf{r}, \mathbf{r}')\gamma_0(H - E) = \delta(\mathbf{r} - \mathbf{r}'), \quad (2.22)$$

where  $H$  is the Dirac Hamiltonian of an electron in a Coulomb field. Written more explicitly, these equations become

$$[-i\boldsymbol{\gamma}\cdot\nabla - \gamma_0(E + eA_0^{(e)}) + m]G_E(\mathbf{r}, \mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}'), \quad (2.23)$$

$$G_E(\mathbf{r}, \mathbf{r}') [i\boldsymbol{\gamma}\cdot\nabla' - \gamma_0(E + eA_0^{(e)}) + m] = \delta(\mathbf{r} - \mathbf{r}'), \quad (2.24)$$

where in the second relation  $\nabla'$  is understood to operate on the function  $G_E(\mathbf{r}, \mathbf{r}')$  which precedes it. The property which renders the use of the Green's function particularly convenient is the simple form it assumes when one of its arguments, as in (2.19), is the center of the spherically symmetric electric field. The occurrence of this symmetrical form of the Coulomb Green's function

of course reflects the fact that electron capture takes place only at the position of the nucleus.

The matrix element for radiative capture written in terms of the Green's function reduces to

$$M_\alpha(\mathbf{k}, \mathbf{p}) = e(2\pi/k)^{\frac{1}{2}} \int (\bar{\chi}_p(0) N_{f_i} G_{E\alpha-k}(0, \mathbf{r}) \times \mathbf{e}_\mu \gamma_\mu e^{-i\mathbf{k} \cdot \mathbf{r}} \psi_\alpha(\mathbf{r})) d\mathbf{r}. \quad (2.25)$$

If the electron initially in the state  $\psi_\alpha(\mathbf{r})$  is pictured as emitting the photon while at the point  $\mathbf{r}$ , it is evident that the Green's function  $G_{E\alpha-k}(0, \mathbf{r})$  represents the amplitude for its subsequent arrival at the nucleus. According to this picture the electron moves with an energy  $E_\alpha - k$  during the brief interval between the radiation and capture processes. For  $\gamma$ -ray energies which are less than<sup>10</sup>  $\sim 2m$ , a restriction imposed by the energy releases of most  $K$ -capture reactions, the energy  $E_\alpha - k$  will lie between the limits  $m$  and  $-m$ . The Green's function consequently cannot represent a freely propagating wave. Instead, as we shall see, it is a rapidly decreasing function of the distance from the nucleus with a range that depends on the energy of the emitted photon.

For purposes of calculation, it is convenient to express the Green's function  $G_E(\mathbf{r}, \mathbf{r}')$  in terms of an analogous Green's function for the second-order form of the Dirac equation. The latter function, which we shall refer to as the second-order Green's function  $\mathcal{G}_E(\mathbf{r}, \mathbf{r}')$ , is defined to satisfy the equation

$$[-i\boldsymbol{\gamma} \cdot \nabla - \gamma_0(E + eA_0^{(e)}) + m][i\boldsymbol{\gamma} \cdot \nabla + \gamma_0(E + eA_0^{(e)}) + m]\mathcal{G}_E(\mathbf{r}, \mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}'), \quad \text{or}^{11}$$

$$[\nabla^2 + (E + eA_0^{(e)})^2 - m^2 - ie\boldsymbol{\alpha} \cdot \nabla A_0^{(e)}]\mathcal{G}_E(\mathbf{r}, \mathbf{r}') = -\delta(\mathbf{r} - \mathbf{r}'), \quad (2.26)$$

together with its adjoint

$$\mathcal{G}_E(\mathbf{r}, \mathbf{r}')[\nabla'^2 + (E + eA_0^{(e)})^2 - m^2 - ie\boldsymbol{\alpha} \cdot \nabla' A_0^{(e)}] = -\delta(\mathbf{r} - \mathbf{r}'), \quad (2.27)$$

in which  $\nabla'^2$  operates to the left. The function  $G_E(\mathbf{r}, \mathbf{r}')$  which satisfies (2.23) and (2.24) may now be written in terms of the second order Green's function as

$$G_E(\mathbf{r}, \mathbf{r}') = [i\boldsymbol{\gamma} \cdot \nabla + \gamma_0(E + eA_0^{(e)}) + m]\mathcal{G}_E(\mathbf{r}, \mathbf{r}') \quad (2.28)$$

$$= \mathcal{G}_E(\mathbf{r}, \mathbf{r}')[-i\boldsymbol{\gamma} \cdot \nabla' + \gamma_0(E + eA_0^{(e)}) + m]. \quad (2.29)$$

The matrix element for radiative capture (2.25) may be expressed in terms of the second-order Green's function by substituting in it the expression (2.29) for

<sup>10</sup> More exactly, the condition is that  $k$  be less than  $2m$  minus the binding energy of the electron in the state  $\alpha$ . The availability of larger energies implies that real positron emission competes with  $K$  capture.

<sup>11</sup> The Dirac matrices  $\alpha_j$  ( $j=1, 2, 3$ ) and  $\beta$  are expressed in terms of the  $\gamma_\mu$  by the relation  $\alpha_j = \gamma_0 \gamma_j$ ,  $\beta = \gamma_0$ .

$G_E(\mathbf{r}, \mathbf{r}')$ . Upon performing an integration by parts, we then obtain

$$M_\alpha(\mathbf{k}, \mathbf{p}) = e(2\pi/k)^{\frac{1}{2}} \int (\bar{\chi}_p(0) N_{f_i} \mathcal{G}_{E\alpha-k}(0, \mathbf{r}) [i\boldsymbol{\gamma} \cdot \nabla + \gamma_0(E_\alpha - k + eA_0^{(e)}) + m] \mathbf{e}_\mu \gamma_\mu e^{-i\mathbf{k} \cdot \mathbf{r}} \psi_\alpha(\mathbf{r})) d\mathbf{r}.$$

Because  $\psi_\alpha(\mathbf{r})$  satisfies the stationary state wave equation this expression reduces to<sup>12</sup>

$$M_\alpha(\mathbf{k}, \mathbf{p}) = e(2\pi/k)^{\frac{1}{2}} \int (\bar{\chi}_p(0) N_{f_i} \mathcal{G}_{E\alpha-k}(0, \mathbf{r}) e^{-i\mathbf{k} \cdot \mathbf{r}} \times [-2i\mathbf{e} \cdot \nabla + ie_\mu \sigma_{\mu\nu} k_\nu] \psi_\alpha(\mathbf{r})) d\mathbf{r}. \quad (2.30)$$

The two operators  $\mathbf{e} \cdot \nabla$  and  $e_\mu \sigma_{\mu\nu} k_\nu$  are, respectively, of odd and even parity under spatial inversion and so play their principal roles in basically different types of transitions.

Our attention in the sections that follow will be devoted chiefly to methods of evaluating the matrix element (2.30). For the present we merely note the way in which a knowledge of the matrix element as a function of the photon and neutrino momenta determines the photon spectrum. In particular, the total probability per unit time  $w_\alpha$  for radiative capture of an electron from the state  $\alpha$  may be found in the familiar way by summing the squared absolute values of the appropriate matrix elements (2.30) of the transition operator. We thereby obtain

$$w_\alpha = (2\pi)^{-5} \sum_{s, \mathbf{e}, f} \int |M_\alpha(\mathbf{k}, \mathbf{p})|^2 \times \delta(p + k + \Delta E - E_\alpha) d\mathbf{p} d\mathbf{k}, \quad (2.31)$$

where the summation is over the spin variable  $s$ , of the emergent neutrino, the polarization  $\mathbf{e}$  of the photon, and the magnetic quantum numbers of the final nuclear states, labelled by  $f$ . This expression should, of course, be averaged over the orientations of the initial nuclear states  $i$ , an operation which is assumed implicitly hereafter.

The integration over the momentum directions of the emitted quanta in (2.31) is simplified by the fact that we are in general interested in summing all of the transition probabilities for the electrons which fill an atomic subshell, that is, all of the electrons with a given principal quantum number and a given orbital angular momentum. Since completed subshells are spherically symmetric, the only angular dependence of the resulting photon-neutrino emission probability is on the angle between  $\mathbf{k}$  and  $\mathbf{p}$ . Labeling the subshells explicitly with the indices  $n$  and  $l$  and the states within them with their orbital and spin magnetic quantum numbers  $m$  and  $s$ , we may write the transition rate for a full

<sup>12</sup> The relativistic spin operator is defined as  $\sigma_{\mu\nu} = \frac{1}{2}i[\gamma_\mu, \gamma_\nu]$ .

subshell as

$$\begin{aligned}
 w_{nl} &= \sum w_{nlms} \\
 &= (2\pi^3)^{-1} \sum_{s,p} \sum_{m,s} \int \langle |M_{nlms}(\mathbf{k}, \mathbf{p})|^2 \rangle_p \\
 &\quad \times \delta(p+k-k_{\max}) p^2 dp k^2 dk. \quad (2.32)
 \end{aligned}$$

Here the symbol  $k_{\max} = E_{nl} - \Delta E$  has been introduced for the maximum photon energy available, along with the brackets  $\langle \rangle_p$  indicating a function of the neutrino momentum averaged over the directions of  $\mathbf{p}$  with  $p = |\mathbf{p}|$  fixed. Performing the integration over the magnitude of the neutrino momentum in (2.32), we have

$$\begin{aligned}
 w_{nl} &= (2\pi^3)^{-1} \sum_{s,p} \sum_{m,sf} \int \langle |M_{nlms}(\mathbf{k}, \mathbf{p})|^2 \rangle_{k_{\max}-k} \\
 &\quad \times k^2 (k_{\max} - k)^2 dk, \quad (2.33)
 \end{aligned}$$

an expression whose integrand represents the energy spectrum of the radiated photons.

### 3. APPROXIMATIONS

The atomic system in which radiative capture occurs furnishes a natural scale for the energies of the emitted  $\gamma$  rays. It will be convenient for later purposes to distinguish between three energy regions which may be expressed, using the fine-structure constant  $\alpha = e^2 = 1/137$ , as

$$k < \frac{1}{2}(Z\alpha)^2 m, \quad (\text{I})$$

$$\frac{1}{2}(Z\alpha)^2 m < k < Z\alpha m, \quad (\text{II})$$

$$Z\alpha m < k. \quad (\text{III})$$

The first, or low-energy, region is one in which the photon energy is less than the binding energy of a  $K$ -shell electron. The second region extends from this level to the energy at which the momentum of the emitted photon equals the average momentum of a  $K$  electron, and the third includes all higher energies. The behavior of the spectrum, it will later be shown, may be approximated by somewhat different means in all three regions.

In the present paper we shall carry the analysis of the internal bremsstrahlung spectrum as far as possible using nonrelativistic approximations to the atomic electron wave functions. This procedure, we shall show, yields the spectral intensity distributions in general to a relative accuracy of order  $Z\alpha$ . Slightly more detailed representations of the wave functions, however, prove necessary to correct for certain relativistic effects in the low-energy portions of the  $S$ -state spectra, and these are introduced in Sec. 9. Since corrections of order  $Z\alpha$  and higher may be noticeable in the heavier elements, the problem has been examined further by methods based on the exact relativistic wave functions. These rather more elaborate calculations will be presented in a subsequent paper.

While, for the present, we shall make certain non-relativistic approximations in treating the atomic electrons, it must be emphasized that the appearance of a neutrino in the capture process limits the extent of the consequent simplifications. Since the neutrino is presumed massless, the four components of its spinor wave function are in general of the same magnitude. We must, therefore, preserve the four-component spinor form of the wave functions and be careful only to discard terms of order  $Z\alpha$ . To this accuracy, the space and spin dependence of the initial electron wave functions may be factorized by writing

$$\psi_\alpha(\mathbf{r}) = u_\alpha \varphi_\alpha(\mathbf{r}), \quad (3.1)$$

where the  $\varphi_\alpha$  are the usual nonrelativistic atomic orbital functions and  $u$  is a normalized spinor eigenfunction of the operator  $\beta$  corresponding to the positive eigenvalue unity,  $\beta u = u$ .

Corresponding to the above reduction of the wave functions, a considerable simplification may be made in the form of the Green's function. The relativistic Green's functions defined earlier must be expressed, in general, as four-by-four matrix functions of position coordinates. A particular advantage of using the second order form of the Green's function is that if the term  $\alpha \cdot \nabla A_0^{(e)}$  in the differential Eqs. (2.26) and (2.27) may be neglected, the function may be approximated as a unit matrix in its spin-energy dependence. The terms containing  $\alpha \cdot \nabla A_0^{(e)}$  in these equations are responsible along with the  $(eA_0^{(e)})^2$  terms, for the effects of fine structure in atomic systems. Since effects of this order have already been neglected in the wave functions, it will be consistent to drop these terms. At a later point where somewhat higher accuracy is desired (Sec. IX) the effect of retaining them will be estimated by means of a simple transformation applied to the approximate Green's function.

On neglecting the fine-structure terms in the differential equations defining it, the second-order Green's function may be written in the form

$$\mathcal{G}_E(\mathbf{r}, \mathbf{r}') = \mathcal{G}_E'(\mathbf{r}, \mathbf{r}') I,$$

where  $I$  is the unit matrix and  $\mathcal{G}_E'(\mathbf{r}, \mathbf{r}')$  is a scalar Green's function. The particular function  $\mathcal{G}_E'(0, \mathbf{r}')$  required for the evaluation of the matrix element (2.30) is seen to satisfy a reduced form of Eq. (2.27),

$$(\nabla'^2 + E^2 - m^2 + 2eEA_0^{(e)}(\mathbf{r}')) \mathcal{G}_E'(0, \mathbf{r}') = -\delta(\mathbf{r}'). \quad (3.2)$$

The approximations noted simplify the calculation of the transition probability by allowing the factorization of the quantities to be summed over spin states and to be integrated spatially. Before discussing the Green's function further, it will be useful to illustrate the spin summation. For this purpose we begin by considering radiative capture from  $S$  states.

#### 4. S-STATE SPECTRA, PRELIMINARY CALCULATIONS

In a nonrelativistic approximation, all orbital wave functions except those of  $S$  states vanish at the nucleus. This implies that electron capture takes place only from intermediate  $S$  states. An equivalent statement is that the Green's function  $\mathcal{G}_{E'}(0, \mathbf{r})$  is spherically symmetric and hence expressible as a superposition of  $S$ -state wave functions.

In discussing the radiative capture of electrons which are initially in  $S$  states, it becomes possible to simplify considerably the form of the matrix element (2.30). In particular, since the radiative transition takes place between spherically symmetric states, the matrix element of  $\exp[-i\mathbf{k}\cdot\mathbf{r}]\mathbf{e}\cdot\nabla$  is found to vanish, a fact which expresses the forbiddenness of electric radiation in zero-to-zero transitions. The operator  $\mathbf{e}_{\mu\sigma\nu}k_\nu$ , on the other hand, contributes magnetic transitions which are clearly permitted. With the neutrino wave function at the nucleus designated by

$$\chi_{\mathbf{p}}(0) = v_{\mathbf{p}}, \quad (4.1)$$

where  $v_{\mathbf{p}}$  is a normalized spinor, and with the approximate forms introduced for the wave functions and Green's function, the matrix element for radiative capture of an  $nS$  electron may be written in the form

$$M_{nS}(\mathbf{k}, \mathbf{p}) = ie(2\pi/k)^{\frac{1}{2}}(\bar{v}_{\mathbf{p}}N_{fi}\mathbf{e}_{\mu\sigma\nu}k_\nu u_{nS})\mathcal{G}(k), \quad (4.2)$$

where  $\mathcal{G}(k)$  represents the integral

$$\mathcal{G}(k) = \int \mathcal{G}_{En_s-k}(0, \mathbf{r})e^{-i\mathbf{k}\cdot\mathbf{r}}\varphi_{nS}(\mathbf{r})d\mathbf{r}. \quad (4.3)$$

The squared absolute values of these matrix elements must be summed rather than averaged over the initial electron spins since both spin states of the  $S$  shell are occupied. They must further be summed over the spin states of the emitted neutrino. These calculations are performed in the familiar way by introducing the positive energy projection operators  $\frac{1}{2}(1+\beta)$  and  $(2p)^{-1}(p+\alpha\cdot\mathbf{p})$  for the electron and neutrino respectively, and extending the summations over all states. When averaged over directions of the neutrino momentum, the result is

$$\sum_{s_{\nu}, s} \langle |M_{nS}(\mathbf{k}, \mathbf{p})|^2 \rangle_p = (\pi e^2/2k) \text{Tr}\{\mathbf{e}_{\rho\sigma\nu}k_\lambda^* N_{fi}^\dagger N_{fi} \mathbf{e}_{\mu\sigma\nu}k_\nu (1+\beta)\} \mathcal{G}^2,$$

which, with use of the relation  $\mathbf{e}_{\mu\sigma\nu}k_\nu = i(e_{\mu\nu}\gamma_\mu)(\gamma_\nu k_\nu)$  and its adjoint, reduces to

$$\sum_{s_{\nu}, s} \langle |M_{nS}(\mathbf{k}, \mathbf{p})|^2 \rangle_p = \pi e^2 \text{Tr}\{N_{fi}^\dagger N_{fi}(k+\alpha\cdot\mathbf{k})\} \mathcal{G}^2. \quad (4.4)$$

The matrix product  $N_{fi}^\dagger N_{fi}$ , when averaged over the initial nuclear magnetic quantum numbers and summed over the final ones, becomes invariant under the unitary transformations expressing rotation. Since the trace as

a whole is invariant, the contribution of the  $\alpha\cdot\mathbf{k}$  term must vanish. By making use of (2.33), and noting that the photon polarization sum introduces a factor of two, we may write the total transition rate for radiative capture from the  $nS$  shell as

$$w_{nS} = \frac{e^2}{\pi^2} \sum_f \text{Tr}\{N_{if}^\dagger N_{fi}\} \int \mathcal{G}^2(k) k^3 (k_{\text{max}} - k)^2 dk. \quad (4.5)$$

For purposes of comparison, the rate of ordinary electron capture without radiation from the  $1S$  shell may be computed by the same methods. The result is

$$w_K = \frac{1}{4\pi} \sum_f \text{Tr}\{N_{if}^\dagger N_{fi}(1+\beta)\} \varphi_{1S}^2(0) (k_{\text{max}})_{1S}^2, \quad (4.6)$$

where  $\varphi_{1S}(0)$  is the central value of the  $1S$  wave function. The matrix  $\beta$  occurring in the trace in (4.6) gives rise to interference terms when the factors  $N_{fi}$  are written as the linear combinations of coupling matrices (2.17) which they represent. These are the familiar Fierz terms which would yield interference between the scalar and vector couplings, and between the tensor and axial vector forms, if both members of either pair occurred in the beta-decay interaction. Searches for the effects of these terms on the shapes of  $\beta$ -decay spectra<sup>13</sup> and on ratios of electron capture to positron emission<sup>14</sup> have furnished uniformly negative results. Any  $T$ - $A$  interference has been shown to represent an effect of less than 2%, while  $S$ - $V$  interference is less than ~10%. If we assume the interference terms to vanish, the trace occurring in (4.6) becomes the same as that in (4.5). The ratio of the transition rate for radiative capture from the  $nS$  shell to that of ordinary  $K$  capture may then be written as

$$\frac{w_{nS}}{w_K} = \frac{4e^2}{\pi \varphi_{1S}^2(0) (k_{\text{max}})_{1S}^2} \int \mathcal{G}^2(k) k^3 (k_{\text{max}} - k)^2 dk. \quad (4.7)$$

#### 5. S-STATE SPECTRA, HIGH-ENERGY FORMS

Before undertaking the more general solution of the problem it is instructive to perform a simple approximate calculation of the  $S$ -state spectrum shape at high energies. This may be done by means of the assumptions introduced by Morrison and Schiff. These authors simplified the problem by neglecting the initial momentum of the captured electron and neglecting the influence of the Coulomb field on the electron in the intermediate states. Only when the recoil momentum of the electron after photon emission greatly exceeds its initial momentum, will the first of these assumptions be valid. The second may be characterized as a Born approximation treatment of the intermediate states, which requires for its validity  $Z\alpha/v \ll 1$ , where  $v$  is the approximate recoil velocity of the electron following

<sup>13</sup> J. P. Davidson and D. C. Peaslee, Phys. Rev. **91**, 1232 (1953).

<sup>14</sup> R. Sherr and R. H. Miller, Phys. Rev. **93**, 1076 (1954).

photon emission. It is evident that both conditions restrict the treatment to photons in the high-energy region,  $k \gg Z\alpha m$ .

Ignoring the Coulomb field in the intermediate states amounts to setting  $A_0^{(e)} = 0$  and using the free-particle Green's function solution to (2.27) or (3.2). The second-order free-particle Green's function may be written in the familiar scalar form

$$\begin{aligned} \mathcal{G}_E^{(0)}(0, \mathbf{r}) &= \frac{1}{(2\pi)^3} \int \frac{e^{i\mathbf{q}\cdot\mathbf{r}}}{q^2 - E^2 + m^2} d\mathbf{q} \\ &= e^{-\mu r} / 4\pi r, \end{aligned} \quad (5.1)$$

where  $\mu = (m^2 - E^2)^{1/2}$ . The initial momentum of the electron is neglected by approximating its wave function as a constant. Since capture takes place from the immediate neighborhood of the nucleus the constant is chosen as the value of the wave function at the center. These replacements greatly simplify evaluation of the integral  $\mathcal{J}(k)$  given by (4.3). With the electron energy  $E_{nS}$  approximated by  $m$ , we find

$$\begin{aligned} \mathcal{J}(k) &= \int \mathcal{G}_{m-k}^{(0)}(0, \mathbf{r}) e^{-i\mathbf{k}\cdot\mathbf{r}} d\mathbf{r} \varphi_{nS}(0) \\ &= \varphi_{nS}(0) / 2mk. \end{aligned} \quad (5.3)$$

Substitution of this result in (4.7) indicates immediately an intensity distribution of the form  $x(1-x)^2$ , where  $x = k/k_{\max}$ .

An important consequence of ignoring the initial electron momentum is to forbid the radiative capture of electrons from states of nonvanishing angular momentum. This is immediately seen on re-examining the general expression for the matrix element (2.30). Electric radiations proceed via the operator  $-i\mathbf{e}\cdot\nabla = \mathbf{e}\cdot\mathbf{p}$ , which is assumed negligible when applied to the initial state. Magnetic contributions are not present either since the wave functions for  $l \neq 0$  vanish at the origin.

While these arguments show that states of nonvanishing orbital angular momentum cannot contribute appreciably to the  $\gamma$ -ray intensity for  $k \gg Z\alpha m$ , the spectra observed experimentally show strong deviations from the form  $x(1-x)^2$  at lower energies. To account at all for the possibility of capture from other states as a means of explaining these deviations, it is necessary to remove the approximation of neglecting the initial electron momentum. This is quite easy to do and furnishes, together with our later results, separate measures of the accuracy of the two approximations underlying (5.3). The integration of  $\mathcal{J}(k)$  remains elementary when the full expression for an  $S$ -state wave function is substituted along with the free-particle Green's function. Neglecting terms of order  $(Z\alpha)^2$  and

higher, we find for the  $1S$  state, for example,

$$\mathcal{J}(k) = \frac{\varphi_{1S}(0)}{2mk + 2Z\alpha\mu}, \quad (5.4)$$

where  $\mu = [m^2 - (m-k)^2]^{1/2}$ . Accounting correctly for the initial electron momentum therefore reduces the  $1S$ -state spectral intensity by a factor  $[1 + Z\alpha(\mu/k)]^2$ . This expression is a decreasing function of energy, taking on the values  $\sim [1 + (2Z\alpha)^{1/2}]^2$  for  $k = Z\alpha m$ ,  $(1 + Z\alpha)^2$  for  $k = m$ , and unity for  $k = 2m$ . For  $\text{Fe}^{55}$ , for example, the  $1S$  state intensity is reduced by a factor 2.6 at 100 keV and, even at the upper limit of the spectrum (220 keV), by a factor of 1.7. The effects of the initial electron momentum are hardly negligible for any save the most energetic capture processes. We shall show nevertheless that the result (5.3) obtained by neglecting these effects along with those of the Coulomb field is essentially correct.

The intensity reduction brought about by accounting for the initial electron momentum is easily explained. The Green's function (5.2) entering the matrix element has a range  $\mu^{-1} = [m^2 - (m-k)^2]^{-1/2}$  so that electrons which emit virtual photons within this distance from the nucleus may undergo capture. The  $1S$  wave function decreases exponentially and may be considerably overestimated, within this range, by its value at the nucleus. While removing this approximation reduces the  $S$ -state intensities, taking proper account of the Coulomb field in the intermediate states may be seen to have the opposite effect. The probability amplitude for an electron reaching the nucleus following emission of a photon is enhanced by the electrostatic field. That is to say, the Green's function evaluated in a Coulomb field will be found to exceed the free-particle function (5.2). It will be proved presently that this effect largely counterbalances the reduction due to the initial momentum. To show this, we first solve for the Green's function in a Coulomb field.

## 6. COULOMB GREEN'S FUNCTION

We seek the spherically symmetric solution to Eq. (3.2), which, with the Coulomb field inserted, becomes

$$[\nabla^2 - m^2 + E^2 + 2E(Ze^2/r)] \mathcal{G}_E'(0, \mathbf{r}) = -\delta(\mathbf{r}). \quad (6.1)$$

On introducing the parameters

$$\mu = (m^2 - E^2)^{1/2}, \quad \eta = Ze^2 E / \mu = Z\alpha E / \mu, \quad (6.2)$$

together with the dimensionless variable

$$x = 2\mu r, \quad (6.3)$$

the homogeneous form of the differential equation (6.1), obtained by omitting the delta function on the right, may be written as

$$\left[ \frac{d^2}{dx^2} - \frac{1}{4} + \frac{\eta}{x} \right] x \mathcal{G}_E' \left( 0, \frac{x}{2\mu} \right) = 0. \quad (6.4)$$



In the energy interval  $|E| < m$ , to which our interest will be principally confined, this homogeneous form of the equation is analogous to the radial wave equation for bound states in a Coulomb field. Since, however, the energy is a fixed parameter, not equal in general to any of the bound state energies, it follows that the solutions for  $\mathcal{G}_{E'}$  must be irregular either at infinity, at the origin, or both. The only solution of (6.4) which remains regular at infinity is the Whittaker function<sup>15</sup>  $x\mathcal{G}_{E'} \sim W_{\eta, \frac{1}{2}}$ , which decreases exponentially with increasing  $x$ . Since  $W_{\eta, \frac{1}{2}}$  remains finite at the origin,

$$W_{\eta, \frac{1}{2}} = 1/\Gamma(1-\eta), \quad (6.5)$$

$\mathcal{G}_{E'}$  will be singular there as  $1/x$ , or  $r^{-1}$ . With this solution of the homogeneous equation, solving the inhomogeneous equation (6.1) becomes simply a matter of adjusting the normalization. By integrating both sides of (6.1) over the volume of an infinitesimal sphere described about the origin, the condition that the solution satisfy the inhomogeneous equation may be stated as the boundary condition,

$$\lim_{r \rightarrow 0} 4\pi r^2 \frac{d}{dr} \mathcal{G}_{E'}(0, r) = -1. \quad (6.6)$$

The properly normalized solution is therefore

$$\mathcal{G}_{E'}(0, r) = \Gamma(1-\eta) W_{\eta, \frac{1}{2}}(2\mu r) / 4\pi r. \quad (6.7)$$

It may be seen from the behavior of the gamma function in (6.7) that the Green's function becomes infinite for positive integer values of the parameter  $\eta$ . This occurs at the energies  $E_n = m[1 + (Z\alpha/n)^2]^{-\frac{1}{2}}$  where  $n = 1, 2, 3, \dots$ , that is, apart from fine structure corrections which have been partially omitted, just at the energies of the bound  $S$  states. That this is the behavior required of the Green's function may be seen by noting that for  $E$  near  $m$  the wave Eq. (6.1) is nonrelativistic in form. The Green's function which solves it may then be written as the familiar expansion in orbital eigenfunctions,<sup>16</sup>

$$\mathcal{G}_{E'}(0, r) = \frac{1}{2m} \sum_n \frac{\varphi_{nS}(0) \varphi_{nS}(r)}{E_{nS} - E}, \quad (m-E) \ll m, \quad (6.8)$$

which has poles at the bound state energies noted.

It is convenient for computational purposes to introduce an integral representation of the Whittaker function. This may be done by means of the contour integral<sup>16</sup>

$$\Gamma(1-\eta) W_{\eta, \frac{1}{2}}(x) = \frac{e^{-x/2}}{e^{-2\pi i \eta} - 1} \int_{\infty}^{(0+)} e^{-t} \left( \frac{t+x}{t} \right)^{\eta} dt, \quad (6.9)$$

<sup>15</sup> E. T. Whittaker and G. N. Watson, *A Course of Modern Analysis* (The Macmillan Company, New York, 1943), p. 337.

<sup>16</sup> Similar eigenfunction expansions of the Green's function may be made at all energies, but since the wave Eq. (6.1) is still partially relativistic in form the eigenfunctions used must correspond to an effective charge  $Z' = (E/m)Z$ . In particular for  $E=0$ , a case which arises with photons of energy near  $k=m$ , the Green's function assumes the free-particle form.

where the path of integration encloses a cut extending from 0 to  $\infty$  and encircles the origin in the positive sense. In the work that follows we shall be chiefly interested in values of the parameter  $\eta$  lying between zero and one. In particular for  $\eta < 1$  the contour integral may be reduced to the real integral

$$\Gamma(1-\eta) W_{\eta, \frac{1}{2}}(x) = e^{-x/2} \int_0^{\infty} t^{-\eta} (t+x)^{\eta} e^{-t} dt, \quad (6.10)$$

with the aid of which the Green's function may be written as

$$\mathcal{G}_{E'}(0, r) = \frac{e^{-\mu r}}{4\pi r} \int_0^{\infty} \left( 1 + \frac{2\mu r}{t} \right)^{\eta} e^{-t} dt. \quad (6.11)$$

The latter expression shows explicitly that the Green's function in a Coulomb field,  $\mathcal{G}_{E'}(0, r)$ , exceeds the free-particle function (5.2) for  $\eta \geq 0$ . By changing the variable of integration in (6.11) to  $s = t/2\mu r$ , we secure the form

$$\mathcal{G}_{E'}(0, r) = (\mu/2\pi) e^{-\mu r} \int_0^{\infty} e^{-2\mu r s} s^{-\eta} (1+s)^{\eta} ds, \quad (6.12)$$

which is a convenient one where further integration with respect to  $r$  is required.

## 7. S-STATE SPECTRA, GENERAL METHODS

The most important step, as we have noted, in finding the spectra radiated by electrons captured from  $S$ -states is the evaluation of the integral

$$\mathcal{J}(k) = \int \mathcal{G}_{E_{nS-k}}(0, \mathbf{r}) e^{-i\mathbf{k} \cdot \mathbf{r}} \varphi_{nS}(\mathbf{r}) d\mathbf{r}. \quad (7.1)$$

We shall now show that for these particular states this may be done to an accuracy of order  $Z\alpha$  simply by making use of certain general properties of the Green's function. The arguments we employ are different in each of the three regions of photon energy noted earlier.

For photon energies  $k < Z\alpha m$ , that is, in both the low-energy and intermediate regions, the Green's function may be represented as the eigenfunction expansion (6.8) so that  $\mathcal{J}(k)$  becomes

$$\mathcal{J}(k) = \frac{1}{2m} \sum_{n'} \frac{\varphi_{n'S}(0)}{E_{n'S} - E_{nS} + k} \int \varphi_{n'S}(r) \times e^{-i\mathbf{k} \cdot \mathbf{r}} \varphi_{nS}(r) d\mathbf{r}. \quad (7.2)$$

Photons in the low-energy region  $k < \frac{1}{2}(Z\alpha)^2 m$  have wavelengths at least  $(Z\alpha)^{-1}$  times larger than the atomic system. For these we may therefore drop the retardation factor  $\exp[-i\mathbf{k} \cdot \mathbf{r}]$ . The integrals then all vanish for  $n' \neq n$ , showing that the radiative process is a simple spin flip, and we find

$$\mathcal{J}(k) = \varphi_{nS}(0) / 2mk. \quad (7.3)$$

In the intermediate energy region,  $\frac{1}{2}(Z\alpha)^2 m < k < Z\alpha m$ , retardation is not negligible and many terms of the summation (7.2) may be expected to contribute. Here insight may be gained by considering the overall form (6.11) for the Green's function  $\mathcal{G}_{E_{nS}-k'}(0, r)$ . In particular it is to be noted that the function decreases rapidly with a range

$$\mu^{-1} = [m^2 - (E_{nS} - k)^2]^{-\frac{1}{2}} \quad (7.4)$$

$$\approx [2mk - k^2 + (Z\alpha/n)^2 m(m-k)]^{-\frac{1}{2}}, \quad (7.5)$$

which is of the order of atomic dimensions for  $k \sim (Z\alpha)^2 m$  and roughly  $(2Z\alpha)^{-\frac{1}{2}} m^{-1}$  for  $k = Z\alpha m$ . Throughout this interval the range of the Green's function remains much smaller than the photon wavelength so that the retardation factor may again be omitted. Since the wave function and Green's function are spherically symmetric, the error thereby incurred is of the order of  $k^2/\mu^2$  which does not exceed  $Z\alpha$  for  $k \sim Z\alpha m$ . Once the omission of the retardation factor is justified, it is convenient to return to the summation (7.2) for  $g(k)$ , in which we again find that the only contribution comes from the term  $n' = n$ . The value of the integral is once again  $g(k) = \varphi_{nS}(0)/2mk$ . It is interesting to note that the foregoing argument traces an almost circular path. The summation (7.2) consists of many terms in which retardation is by no means negligible, but in the summation as a whole we have shown that retardation is negligible. When the retardation factor is dropped, the summation reduces to a single term. The many orbital transitions possible interfere to produce the same radiation as a simple spin-flip with no change of orbital state.

For still higher photon energies,  $k \sim m$ , retardation must be taken into account. But the Coulomb Green's function may be adequately approximated by the free-particle Green's function. The latter, as we have noted, is accurate to order  $Z\alpha/v$  (where  $v$  is the electron recoil velocity), and this is of order  $Z\alpha$  for  $k \sim m$ . Since the error of neglecting the initial electron momentum in this region is again of order  $Z\alpha$ , we may use the calculation of Sec. 5 which led to the result (5.3), the same expression we have found in the two regions of lower energy.

Since the result (7.3) for  $g(k)$  is now established to order  $Z\alpha$  over the entire energy range, the total transition rate for radiative capture from the  $nS$  shell may be written, using (4.5) as

$$w_{nS} = (e/2\pi m)^2 \varphi_{nS}^2(0) \sum_f \text{Tr}\{N_{if}^\dagger N_{fi}\} \times \int k(k_{\max} - k)^2 dk. \quad (7.6)$$

If the Fierz interference terms in the  $K$ -capture probability (4.6) are neglected, the ratio of radiative to

ordinary  $K$  capture is then

$$\frac{w_{nS}}{w_K} = \frac{\alpha}{\pi m^2 (k_{\max})_{1S}^2} \left( \frac{\varphi_{nS}(0)}{\varphi_{1S}(0)} \right)^2 \int k(k_{\max} - k)^2 dk \quad (7.7)$$

$$= \frac{\alpha k_{\max}^2}{12\pi m^2} \left( \frac{k_{\max} \varphi_{nS}(0)}{(k_{\max})_{1S} \varphi_{1S}(0)} \right)^2, \quad (7.8)$$

where  $k_{\max}$ , of course, varies slightly with the binding energy of the state. That this more accurate spectrum preserves at all energies the high-energy form derived in Sec. 5 shows explicitly the compensation of the two approximations discussed there.

It may be noted that the role played by positrons in radiative capture process is included implicitly in the foregoing calculation. One of the paths by which the reaction takes place is the virtual emission of a positron followed by single-quantum annihilation with an orbital electron. It is the possibility of positron emission which explains the behavior of the range of the Green's function with increasing photon energy. This parameter, as we have seen, represents the distance from the nucleus at which virtual photon emission may occur if it is to be associated with a capture process. From (7.5), the range may be seen to correspond to the atomic radius for low-energy photons, the electron Compton wavelength for  $k \sim m$ , and to increase without limit as the photon energy approaches the threshold for real positron emission  $k = m + E_{nS}$ .

That electron-positron annihilation accounts for part of the result (7.6) may be seen by resolving the operator  $\mathbf{e}_\mu \sigma_{\mu\nu} k_\nu$  contained in the matrix element (4.2) as follows:

$$\mathbf{e}_\mu \sigma_{\mu\nu} k_\nu = \boldsymbol{\sigma} \cdot (\mathbf{e} \times \mathbf{k}) + i(\mathbf{e} \cdot \boldsymbol{\alpha})k. \quad (7.9)$$

The term  $\boldsymbol{\sigma} \cdot (\mathbf{e} \times \mathbf{k})$  leads to the usual positive energy magnetic transitions, while the term  $i(\mathbf{e} \cdot \boldsymbol{\alpha})k$ , being an odd Dirac matrix, leads to annihilation. Since the four components of the spinor wave function of the emitted neutrino are in general of equal magnitude, the effect of annihilation is equal to that of the positive-energy transitions. Intermediate states containing positrons contribute half of the intensity (7.6). It is remarkable that positrons play a part even in the emission of low-energy photons, and some interest attaches to following the effect in closer detail. This is done in Sec. 9 where more detailed representations of the wave functions and Green's function are introduced, and the consequent corrections to the  $S$ -state intensities at low energies are discussed.

## 8. P-STATE SPECTRA

The present section will be devoted to calculating the  $\gamma$ -ray spectra radiated by electrons captured from  $P$  states. Such spectra will be shown to make up a large part of the observed intensity. This is in marked contrast to the result based on the approximations of

Morrison and Schiff<sup>1</sup> (Sec. 5) which showed a vanishing contribution from  $P$  states. The latter result, as we shall see, correctly indicates that the  $P$ -state intensity is weak at high energies. At low and intermediate energies, however, ( $k < Z\alpha m$ ) the  $P$ -state spectra are characteristically quite intense. In a large part of this range they dominate the  $S$ -state spectra completely.

The matrix element for radiative capture from the  $nP$  state is given by Eq. (2.30) with substitution of the appropriate wave function and energy. It is seen to contain as a factor the integral

$$\int \mathcal{G}_{E_{nP}-k'}(0, \mathbf{r}) e^{-i\mathbf{k}\cdot\mathbf{r}} [-2i\mathbf{e}\cdot\nabla + i\mathbf{e}_{\mu\sigma_{\mu\nu}}k_{\nu}] \varphi_{nP}(\mathbf{r}) d\mathbf{r}. \quad (8.1)$$

Since the Green's function is spherically symmetric, the orbital angular momentum of the electron changes by one unit in a radiative transition from a  $P$  state. The amplitude furnished by the  $\mathbf{e}_{\mu\sigma_{\mu\nu}}k_{\nu}$  term would vanish by orthogonality were it not for the retardation factor. As a consequence, for photon energies which are not too high, the  $P$ -state intensity is furnished almost entirely by the  $\mathbf{e}\cdot\nabla$  term. An order-of-magnitude estimate using the range of the Green's function,  $\mu^{-1}$ , and the general form of the  $P$ -state wave functions shows that the contribution of the  $\mathbf{e}_{\mu\sigma_{\mu\nu}}k_{\nu}$  term is smaller than that of  $\mathbf{e}\cdot\nabla$  by a factor  $k^2/\mu^2 \sim k/2m$ , and may consequently be neglected for  $k < Z\alpha m$ . At higher energies these terms may become comparable in magnitude, but both are insignificantly small.

Since almost all of the  $P$ -state radiation lies in the range  $0 < k < Z\alpha m$ , we may restrict our consideration to this region and retain only the  $\mathbf{e}\cdot\nabla$  term of (8.1). We may furthermore neglect the retardation factor in the integrand since the error in so doing is again of order  $k^2/\mu^2$ , which is less than  $Z\alpha$ . The matrix element then becomes

$$M_{nP}(\mathbf{k}, \mathbf{p}) = -2ie(2\pi/k)^{\frac{1}{2}} (\bar{v} N_{fi} u) \times \int \mathcal{G}_{E_{nP}-k'}(0, \mathbf{r}) \mathbf{e}\cdot\nabla \varphi_{nP}(\mathbf{r}) d\mathbf{r}. \quad (8.2)$$

To illustrate the further calculations it becomes convenient to specialize to the case of the  $2P$  states. An orthonormal set of  $2P$  wave functions may be written as the three components of the vector  $(32\pi a^5)^{-\frac{1}{2}} \mathbf{r} \exp[-r/2a]$ , where  $a = (Z\alpha m)^{-1}$  is the Bohr radius divided by  $Z$ . If, for a given photon polarization  $\mathbf{e}$ , one of the states is taken to be the component

$$\varphi_{2P}(r) = (32\pi a^5)^{-\frac{1}{2}} (\mathbf{e}\cdot\mathbf{r}) \exp[-r/2a], \quad (8.3)$$

it is immediately clear that the remaining two orthogonal states yield vanishing matrix elements. The integral required for the wave function (8.3) may be

written as

$$\int \mathcal{G}_{E_{2P}-k'}(0, \mathbf{r}) \mathbf{e}\cdot\nabla \varphi_{2P}(\mathbf{r}) d\mathbf{r} = (2\pi a)^{-\frac{1}{2}} Q_{2P}(k), \quad (8.4)$$

where  $Q_{2P}(k)$  is the dimensionless integral

$$Q_{2P}(k) = \frac{1}{4a^2} \int \mathcal{G}_{E_{2P}-k'}(0, r) [1 - (r/6a)] e^{-r/2a} dr. \quad (8.5)$$

An analogous integral  $Q_{nP}(k)$  may be defined for capture from each of the higher  $P$  states by using the appropriate wave functions in (8.4).

To find the total probability of radiative capture the matrix elements are again substituted in the expression (2.33). The required summations over initial and final spins are carried out as in Sec. 4. The expression which results for the transition rate from the  $nP$  state is

$$w_{nP} = \frac{e^2}{\pi^3 a} \sum_f \text{Tr}\{N_{if}^\dagger N_{fi} (1 + \beta)\} \times \int Q_{nP}^2(k) k (k_{\max} - k)^2 dk. \quad (8.6)$$

The trace occurring here is the same as that in the rate of ordinary  $K$  capture (4.6) since the radiation interaction employed for  $P$  states involves no Dirac matrices.<sup>17</sup> The ratio of  $nP$ -state radiative capture to ordinary capture is therefore

$$\frac{w_{nP}}{w_K} = \frac{4}{\pi Z^2 \alpha m^2 (k_{\max})_{1S}^2} \int Q_{nP}^2(k) k (k_{\max} - k)^2 dk, \quad (8.7)$$

where the value  $(\pi a^3)^{-1} = (Z\alpha m)^3/\pi$  has been substituted for  $\varphi_{1S}^2(0)$ .

To evaluate the integral  $Q_{2P}(k)$ , explicit use must be made of the representations of the Green's function developed in Sec. 6. The energy parameter of the required Green's function is  $E = E_{2P} - k$ , in which the bound state energy  $E_{2P}$  may be written, neglecting fine structure, as  $m - \frac{1}{8}(Z\alpha)^2 m$ . Since consideration is being restricted to the region  $k < Z\alpha m$ , the parameters  $\mu$  and  $\eta$  defined by (6.2) may be approximated as

$$\mu = [2mk + \frac{1}{4}(Z\alpha)^2 m^2]^{\frac{1}{2}}, \quad (8.8)$$

and

$$\eta = Z\alpha m/\mu = 1/\mu a. \quad (8.9)$$

The inverse range parameter  $\mu$  assumes the value  $1/2a$  for  $k=0$  and is an increasing function of  $k$ . The parameter  $\eta$  thus decreases from the value 2 at  $k=0$ , and tends toward zero for large  $k$ . As we have noted in Sec. 6, the Green's function has a pole, and the

<sup>17</sup> It is of some interest to note that the  $P$ -state intensities contain the same Fierz interference terms as the  $K$ -capture probability, while these are absent from the  $S$ -state intensity (4.5). Failure of these terms to vanish would cause a relative readjustment of the  $S$  and  $P$  state intensities.

integral  $Q_{2P}(k)$  therefore becomes infinite, at the energy corresponding to  $\eta=1$ . This behavior is seen more directly by using the representation (6.8) of the Green's function as a superposition of  $S$ -state wave functions. With the energy  $E$  given by  $E_{2P}-k$  the denominator of the term contributed by the  $1S$  state has a pole at the photon energy  $k=E_{2P}-E_{1S}\approx\frac{3}{8}(Z\alpha)^2m$ , which corresponds to  $\eta=1$ . The energy at which this resonant behavior occurs is that of the characteristic  $K$ -series x-ray which ordinarily follows capture from the  $K$  shell. The inner bremsstrahlung which takes place in capture from  $P$  states is, as we shall presently show, very closely related to the characteristic x-radiation, and, in fact, inseparable from it although extending to much higher energies.

All experimental measurements of the photon spectrum are made at energies above the characteristic x-ray region and hence correspond to  $\eta$  in the interval  $0<\eta<1$ . The integral representation (6.11) may thus be used for the Green's function in evaluating  $Q_{2P}(k)$  as given by (8.5). The spatial integrations required to find  $Q_{2P}(k)$  then become simply those of powers of  $r$  multiplying a decreasing exponential and may be carried out directly, so that we are left the parametric integral

$$Q_{2P}(k)=\eta^2\int_0^\infty\left(\frac{1+s}{s}\right)^\eta\frac{1+2s}{(1+2s+\frac{1}{2}\eta)^4}ds. \quad (8.10)$$

With the substitutions

$$v=s/(1+s), \quad \lambda=(2-\eta)/(2+\eta),$$

the integral becomes

$$Q_{2P}(k)=\frac{\eta^2}{(1+\frac{1}{2}\eta)^4}\int_0^1\frac{v^{-\eta}(1-v^2)}{(1+\lambda v)^4}dv. \quad (8.11)$$

The integrand of this expression may be expanded in partial fractions and each of the resulting integrals expressed in terms of the function

$$K(\rho)=\rho\int_0^1\frac{x^{-\eta}}{1+\rho x}dx \quad (8.12)$$

$$=\rho^\eta\int_0^\rho\frac{y^{-\eta}}{1+y}dy \quad (8.13)$$

and its derivatives by means of the identities

$$\begin{aligned} \int_0^1\frac{v^{-\eta}}{(1+\lambda v)^{1+p}}dv &= \frac{(-1)^p}{p!}\frac{d^p}{d\zeta^p}\int_0^1\frac{v^{-\eta}}{\zeta+\lambda v}dv\Bigg|_{\zeta=1} \\ &= \frac{(-1)^p}{\lambda p!}\frac{d^p}{d\zeta^p}K(\lambda/\zeta)\Bigg|_{\zeta=1} \\ &= \frac{1}{p!\lambda^{p+1}}\left(\rho^2\frac{d}{d\rho}\right)^p K(\rho)\Bigg|_{\rho=\lambda}. \end{aligned} \quad (8.14)$$

In this way, after algebraic reduction we find

$$Q_{2P}(k)=\frac{\eta^2}{4(1-\frac{1}{4}\eta^2)^2}\times[1+\frac{2}{3}\eta-(7/12)\eta^2+(4/3)\eta^2K(\lambda)]. \quad (8.15)$$

The integral  $K(\lambda)$  defined by (8.12) cannot be evaluated in closed form, but may be represented by rapidly converging series expansions. Performing the integration of (8.12) by parts, we obtain

$$K(\lambda)=\log(1+\lambda)+\eta\int_0^1x^{-\eta-1}\log(1+\lambda x)dx. \quad (8.16)$$

Substitution of the power series expansion of  $\log(1+\lambda x)$  provides the series for  $K(\lambda)$ ,

$$K(\lambda)=\log(1+\lambda)-\eta\sum_{j=1}^\infty\frac{(-\lambda)^j}{j(j-\eta)}, \quad (8.17)$$

which is seen to converge as  $j^{-2}$ . It is possible, by performing a second integration by parts before expanding, to obtain an alternating series which converges as  $j^{-3}$ . Since  $\lambda$  is small, however, the convergence of (8.17) is already conveniently rapid. Numerical values of  $Q_{2P}(k)$  for several photon energies, expressed in units of the  $1S$ -state binding energy  $\frac{1}{2}(Z\alpha)^2m$ , are given in Table I.

The calculations for radiative capture from the  $3P$  states proceed in an entirely analogous way. Once again only one of the three oriented substates can radiate photons of a given polarization. The integral  $Q_{3P}(k)$  which corresponds to  $Q_{2P}(k)$  is defined by

$$\int\mathcal{G}_{E_{3P}-k'}(0,\mathbf{r})\mathbf{e}\cdot\nabla\varphi_{3P}(\mathbf{r})d\mathbf{r}=(2\pi a)^{-\frac{1}{2}}Q_{3P}(k). \quad (8.18)$$

With the substitution of the appropriate wave function,  $Q_{3P}(k)$  assumes the form

$$Q_{3P}(k)=(2/81a^2)\int\mathcal{G}_{E_{3P}-k'}(0,\mathbf{r})[6-2(r/a)+\frac{1}{3}(r/a)^2]e^{-r/3a}d\mathbf{r}. \quad (8.19)$$

The inverse range parameter of the Green's function is

$$\mu=[2mk+\frac{1}{9}(Z\alpha)^2m^2]^{\frac{1}{2}}, \quad (8.20)$$

TABLE I. The integral  $Q_{2P}(k)$ , defined by (8.4), with corresponding values of the parameter  $\eta$ . The photon energy  $k$  is given in units of  $\frac{1}{2}(Z\alpha)^2m$ , the  $1S$ -state binding energy.

$k$	$\eta$	$Q_{2P}(k)$
1.79	0.7	0.340
2.53	0.6	0.192
3.75	0.5	0.109
4.92	0.440	0.0769
6.00	0.4	0.0594
8.75	0.333	0.0378
12.50	0.280	0.0248

TABLE II. The integral  $Q_{3P}(k)$  and the parameter  $\eta$  for several values of the photon energy  $k$ , measured in units of  $\frac{1}{2}(Z\alpha)^2m$ .

$k$	$\eta$	$Q_{3P}(k)$
1.67	0.75	0.246
2.67	0.6	0.0992
3.51	0.525	0.0648
4.83	0.45	0.038
7.0	0.375	0.022
11.0	0.3	0.010

and  $\eta = (\mu a)^{-1}$  lies in the interval  $0 < \eta < 3$ . The Green's function consequently has two poles at finite photon energies corresponding to  $\eta = 2$  and 1. These are at the frequencies of the  $3P-2S$  and  $3P-1S$  characteristic x-rays, respectively. At energies above the latter of these, the integral representation (6.12) may again be used for the Green's function, and the same succession of integrations and transformations carried out as for the  $2P$  case. In this way we find

$$Q_{3P}(k) = \frac{4}{27} \frac{\eta^2}{(1 - \frac{1}{3}\eta)^3} \left\{ (1 - \frac{1}{3}\eta) [1 + \eta - 2(\frac{1}{3}\eta)^2 - 8(\frac{1}{3}\eta)^3] \right. \\ \left. + (4/3)\eta^2(1 - \frac{1}{3}\eta^2)K(\nu) \right\}, \quad (8.21)$$

where

$$\nu = (3 - \eta)/(3 + \eta),$$

and the function  $K$  is given by (8.12) or (8.17). Values of  $Q_{3P}(k)$  are given in Table II. A rough comparison of the intensities of  $3P$  and  $2P$  radiation may be made from the high-energy behavior of  $Q_{3P}$  and  $Q_{2P}$ . For small values of  $\eta$  we find the intensity ratio  $(Q_{3P}/Q_{2P})^2 = (16/27)^2 = 0.35$ , a figure which will be subject to considerable reduction when the effects of screening are accounted for.

The foregoing calculations establish the intensities of the  $P$ -state spectra for photon energies lying above the characteristic x-ray resonances. For energies lying between or below these resonances, the integrals  $Q(k)$  may be evaluated by employing the more general contour integral representation (6.9) for the Green's function. The detailed intensity distributions are, however, of little experimental interest in this region, so we confine the discussion to some qualitative properties of the spectra at low energies. To find the form of  $Q_{nP}(k)$  as  $k$  approaches zero, it is convenient to use the summation (6.8) to represent the Green's function, so that we have

$$(2\pi a)^{-\frac{1}{2}} Q_{nP}(k) = \frac{1}{2m} \sum_{n'} \frac{\varphi_{n'S}(0)}{E_{n'S} - E_{nP} + k} \\ \times \int \varphi_{n'S}(\mathbf{r}) \mathbf{e} \cdot \nabla \varphi_{nP}(\mathbf{r}) d\mathbf{r}. \quad (8.22)$$

The gradient operator may be written as  $\nabla = i\mathbf{p} = m[\mathbf{r}, H]$ , where  $H$  is the electron Hamiltonian. On inserting this expression and taking the limit of  $Q$  as

$k \rightarrow 0$ , we find

$$(2\pi a)^{-\frac{1}{2}} Q_{nP}(0) = -\frac{1}{2} \sum'_{n'} \int \varphi_{n'S}(0) \varphi_{n'S}(\mathbf{r}) \mathbf{e} \cdot \mathbf{r} \varphi_{nP}(\mathbf{r}) d\mathbf{r}.$$

The primed summation indicates that the term  $n' = n$  is to be omitted from the sum, as a consequence of the degeneracy of the  $nS$  and  $nP$  states. The sum may then be written as

$$(2\pi a)^{-\frac{1}{2}} Q_{nP}(0) = -\frac{1}{2} \int \delta(\mathbf{r}) \mathbf{e} \cdot \mathbf{r} \varphi_{nP}(\mathbf{r}) d\mathbf{r} \\ + \frac{1}{2} \varphi_{nS}(0) \int \varphi_{nS}(\mathbf{r}) \mathbf{e} \cdot \mathbf{r} \varphi_{nP}(\mathbf{r}) d\mathbf{r},$$

where the first term on the right clearly vanishes, so that we have

$$Q_{nP}(0) = \frac{1}{2} (2\pi a)^{\frac{1}{2}} \varphi_{nS}(0) \int \varphi_{nS} \mathbf{e} \cdot \mathbf{r} \varphi_{nP} d\mathbf{r}. \quad (8.23)$$

In particular we find  $Q_{2P}(0) = -\frac{3}{4}$ . Since  $Q_{nP}(0)$  is finite, the  $P$ -state spectra may be seen from (8.7) to rise linearly at first. Their initial slope greatly exceeds that of the  $S$ -state spectra.

The calculated forms of the  $P$ -state spectra are shown in Fig. 1 for  ${}_{26}\text{Fe}^{55}$  which has a maximum photon energy of 220 kev. Since this energy is considerably greater than that of the characteristic x-rays (7 kev for the unscreened atom), the scale does not permit showing detail in the x-ray region. In particular the two peaks of the  $3P$  spectrum remain unseparated.

Some qualitative interpretations of the form of the  $P$ -state spectra will be presented in Sec. 10.

## 9. S-STATE SPECTRA, RELATIVISTIC CORRECTIONS

The calculations of the preceding sections have neglected, as a relativistic effect, the interaction of the magnetic moment of the electron with the Coulomb field surrounding the nucleus. In the present section we shall show that this interaction, although a weak one, significantly affects the low-energy behavior of the  $S$ -state spectra.

When spin-orbit coupling is accounted for, the orbital angular momentum of an electron is no longer constant. A state originally of angular momentum  $l$  has added to it an admixture of wave functions corresponding to  $l-1$  or  $l+1$ . This has the important consequence of allowing capture to take place directly from the " $P$  states" of total angular momentum  $J = \frac{1}{2}$ , since they contain a certain amount of  $S$ -state wave function which does not vanish at the nucleus. Since this relativistic admixture is an effect of order  $Z\alpha$  the corrections it introduces are in general no larger than others which have already been neglected. An exception, however, is found to occur in the low-energy parts of the  $S$ -state spectra, where the factor of  $Z\alpha$  may be partially compensated by an increased probability of radiation.

In the previous work, in which spin-orbit coupling was neglected, it was noted that radiative capture of an electron from an  $S$  state requires emission of a photon in a transition between spherically symmetric states. It followed that the radiation takes place through a reorientation of the electron spin. The matrix element for this is proportional to the frequency of the emitted photon, a fact responsible for the weakness of the  $S$ -state spectra at low energies. When spin-orbit coupling is taken into account, the radiative transition is no longer between spherically symmetric states. An electron initially in an  $S_{3/2}$  state may make a radiative transition to a  $P_{3/2}$  state by means of the electric dipole operator  $\mathbf{e} \cdot \nabla$ , and subsequently undergo direct capture. In the low-energy region  $k < \frac{1}{2}(Z\alpha)^2 m$ , the electric dipole matrix element is larger than that for magnetic dipole transitions by a factor sufficient to overcome the admixture parameter  $Z\alpha$  noted earlier. As a result, in the binding energy region, where the  $S$ -state intensities are quite weak, the spectrum forms will be shown to deviate from those given by (7.7). While the percentage corrections due to this coupling decrease with increasing photon energy, their effect remains noticeable at higher energies where the  $S$ -state intensities are much stronger.

In the preceding sections, the second-order Green's function  $\mathcal{G}_E(\mathbf{r}', \mathbf{r})$ , which is in general a four-by-four matrix function of  $\mathbf{r}'$  and  $\mathbf{r}$ , was approximated as a scalar function multiplying the unit matrix. The approximation which permitted this was the neglect of the term  $\boldsymbol{\alpha} \cdot \nabla A_0^{(e)}$  in the differential equations (2.26) and (2.27). It is this term which destroys the constancy of the orbital angular momentum and leads to the effect we wish to calculate. A convenient means of representing the second order Green's function more correctly is to express it in terms of a similarity transformation performed upon another function  $\mathcal{G}_{E'}(\mathbf{r}', \mathbf{r})$  by writing

$$\mathcal{G}_E(\mathbf{r}', \mathbf{r}) = \exp(\boldsymbol{\alpha} \cdot \mathbf{p}'/2E) \mathcal{G}_{E'}(\mathbf{r}', \mathbf{r}) \exp(-\boldsymbol{\alpha} \cdot \mathbf{p}/2E). \quad (9.1)$$

The function  $\mathcal{G}_{E'}(\mathbf{r}', \mathbf{r})$  so defined satisfies transformed differential equations in which the coupling  $\boldsymbol{\alpha} \cdot \nabla A_0^{(e)} = i\boldsymbol{\alpha} \cdot \mathbf{p} A_0^{(e)}$  is eliminated to first order. These equations, apart from the terms of order  $(Z\alpha)^2$  and higher, assume the same form as those used to define the scalar Green's function discussed earlier. To this accuracy, which is ample for the present, the function  $\mathcal{G}_{E'}$  may be identified with the Green's function of Secs. 3 to 8. In particular,  $\mathcal{G}_{E'}(0, \mathbf{r})$  satisfies (3.2) and (6.1). To corresponding accuracy, the electron wave functions can be represented as<sup>18</sup>

$$\psi_{nl}(\mathbf{r}) = \exp(-\beta \boldsymbol{\alpha} \cdot \mathbf{p}/2m) u \varphi_{nl}(\mathbf{r}), \quad (9.2)$$

where the spinor  $u$  and the orbital function  $\varphi_{nl}$  are those defined in (3.1).

Finding the matrix element for radiative capture (2.30) requires evaluating a spatial integral which may

<sup>18</sup> L. Foldy and S. Wouthuysen, Phys. Rev. 78, 29 (1950).

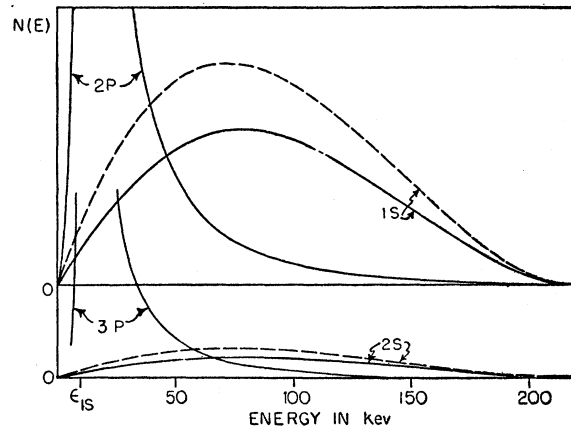


FIG. 1. Gamma-ray spectra for radiative capture from various electron shells of  $\text{Fe}^{55}$ . The dashed curves for the  $1S$  and  $2S$  spectra are the nonrelativistic forms (7.7). The solid curves beneath them are the  $1S$  and  $2S$  spectra with the relativistic modifications of Sec. 9. The characteristic x-ray region lies to the left of  $\epsilon_{1s}$ , the  $K$ -shell ionization energy.

be expressed as the limit as  $\mathbf{r}'$  approaches zero of

$$L_{nl}(\mathbf{r}') = \int \mathcal{G}_{E_{nl-k}}(\mathbf{r}', \mathbf{r}) e^{-i\mathbf{k} \cdot \mathbf{r}} [-2\mathbf{e} \cdot \nabla + \mathbf{e}_\mu \sigma_{\mu\nu} k_\nu] \psi_{nl}(\mathbf{r}) d\mathbf{r}. \quad (9.3)$$

Since the intensity corrections sought are larger than  $Z\alpha$ , it will suffice to preserve a relative accuracy of order  $Z\alpha$  in evaluating this expression. The corrections occur principally at low energies  $k < Z\alpha m$ , for which it is permissible, according to the arguments of Sec. 3, to drop the retardation factor in the integrand of (9.3). To this order we may also write  $E_{nl-k} = m$  in the correction terms, and by means of (9.1) and (9.2) reduce  $L_{nl}(\mathbf{r}')$  to the form

$$L_{nl}(\mathbf{r}') = [1 - i(2m)^{-1} \boldsymbol{\alpha} \cdot \nabla'] \int \mathcal{G}_{E_{nl-k}'}(\mathbf{r}', \mathbf{r}) \times [-2\mathbf{e} \cdot \nabla + \mathbf{e}_\mu \sigma_{\mu\nu} k_\nu] u \varphi_{nl}(\mathbf{r}) d\mathbf{r}. \quad (9.4)$$

The occurrence of the term  $\boldsymbol{\alpha} \cdot \nabla'$  operating on the Green's function in this expression requires that the dependence of the Green's function on the angle between  $\mathbf{r}$  and  $\mathbf{r}'$  be taken into account even in the limit  $\mathbf{r}' \rightarrow 0$ . While in the preceding sections it was sufficient to use the spherically symmetric form the Green's function assumes in the limit  $\mathbf{r}' \rightarrow 0$ , we must now carry out an expansion for small  $\mathbf{r}'$ . This expansion may be written in the form

$$\mathcal{G}_{E'}(\mathbf{r}', \mathbf{r}) = \mathcal{G}_E(0, r) + (\mathbf{r}' \cdot \mathbf{r}) \mathcal{G}_E^{(1)}(0, r) + \dots \quad (9.5)$$

The function  $\mathcal{G}_E^{(1)}$  which is thereby defined represents the  $P$ -wave part of the Green's function. The differential equation it satisfies may be found by separating

the equation for the Green's function,

$$[\nabla^2 + E^2 - m^2 + 2E(Ze^2/r)]\mathcal{G}_E'(\mathbf{r}', \mathbf{r}) = -\delta(\mathbf{r} - \mathbf{r}'), \quad (9.6)$$

into its partial wave components. The homogeneous form of the radial equation for  $\mathcal{G}_E^{(1)}(0, r)$  is then

$$\left[ \frac{d^2}{dr^2} - \mu^2 + \frac{2\eta\mu}{r} - \frac{2}{r^2} \right] r^2 \mathcal{G}_E^{(1)}(0, r) = 0 \quad (9.7)$$

where the parameters  $\eta$  and  $\mu$  are the ones defined by (6.2). The solution of this equation which remains regular at infinity is once again a Whittaker function,  $r^2 \mathcal{G}_E^{(1)}(0, r) \sim W_{\eta, \frac{3}{2}}(2\mu r)$ . The function  $\mathcal{G}_E^{(1)}(0, r)$  must become singular at the origin, and from (9.7) it may be seen to do so as  $r^{-3}$ . The simplest method of normalizing the solution for  $\mathcal{G}_E^{(1)}(0, r)$  so that it satisfies a suitable inhomogeneous equation is to note that the Green's function must become singular as  $1/4\pi|\mathbf{r} - \mathbf{r}'|$ , when  $\mathbf{r}$  approaches  $\mathbf{r}'$ . That is, when  $r$  becomes small, but remains larger than  $r'$ , the series (9.5) must assume the form

$$\mathcal{G}_E'(\mathbf{r}', \mathbf{r}) = \frac{1}{4\pi r} + \frac{\mathbf{r}' \cdot \mathbf{r}}{4\pi r^3} + \dots \quad (9.8)$$

The normalized function  $\mathcal{G}_E^{(1)}(0, r)$  is given by

$$\mathcal{G}_E^{(1)}(0, r) = \mu \Gamma(2 - \eta) W_{\eta, \frac{3}{2}}(2\mu r) / 4\pi r^2. \quad (9.9)$$

As in (6.12), an integral representation<sup>16</sup> may be introduced for the Whittaker function which yields

$$\mathcal{G}_E^{(1)}(0, r) = (\mu^3/\pi) e^{-\mu r} \int_0^\infty e^{-2\mu r s} s^{1-\eta} (1+s)^{1+\eta} ds, \quad (9.10)$$

a form valid for  $\eta < 2$ .

To evaluate the matrix element for capture from  $S$  states we substitute the expansion (9.5) in (9.4) and take the limit of  $L_{nS}(\mathbf{r}')$  as  $\mathbf{r}' \rightarrow 0$ :

$$\begin{aligned} L_{nS}(0) &= \mathbf{e}_\mu \sigma_{\mu\nu} k_\nu \int \mathcal{G}_{E_{nS-k}}'(0, \mathbf{r}) \varphi_{nS}(\mathbf{r}) d\mathbf{r} \\ &+ im^{-1} \int \mathcal{G}_{E_{nS-k}}^{(1)}(0, \mathbf{r}) (\boldsymbol{\alpha} \cdot \mathbf{r}) (\mathbf{e} \cdot \nabla) \varphi_{nS}(\mathbf{r}) d\mathbf{r}. \end{aligned} \quad (9.11)$$

The first of the integrals occurring in this expression is given by (7.3). The integrand of the second is easily averaged over angles, with the result that

$$\begin{aligned} L_{nS}(0) &= \mathbf{e}_\mu \sigma_{\mu\nu} k_\nu \frac{\varphi_{nS}(0)}{2mk} \\ &+ (\boldsymbol{\alpha} \cdot \mathbf{e}) \frac{i}{3m} \int \mathcal{G}_{E_{nS-k}}^{(1)}(0, \mathbf{r}) r \frac{d}{dr} \varphi_{nS}(\mathbf{r}) d\mathbf{r}. \end{aligned} \quad (9.12)$$

The sum  $\mathbf{e}_\mu \sigma_{\mu\nu} k_\nu$  may be separated into two terms, as

shown in (7.9), and the expression for  $L_{nS}(0)$  written as

$$\begin{aligned} L_{nS}(0) &= [\boldsymbol{\sigma} \cdot (\mathbf{e} \times \mathbf{k}) \\ &+ i(\mathbf{e} \cdot \boldsymbol{\alpha}) k B_{nS}(k)] \varphi_{nS}(0) / 2mk, \end{aligned} \quad (9.13)$$

where the factor  $B_{nS}(k)$  is defined by

$$B_{nS}(k) = 1 + \frac{2}{3\varphi_{nS}(0)} \int \mathcal{G}_{E_{nS-k}}^{(1)}(0, \mathbf{r}) r \frac{d}{dr} \varphi_{nS}(\mathbf{r}) d\mathbf{r}. \quad (9.14)$$

The form (9.13) for  $L_{nS}(0)$  facilitates the comparison of the present calculation of the  $S$ -state spectrum with the previous one. In particular, when  $B_{nS}(k) = 1$  the matrix element and the spectrum which follows from it become the same as those of Sec. 7. Since the range of the Green's function decreases with increasing photon energy, the expression (9.14) for  $B_{nS}(k)$  may be seen to approach unity for large  $k$ . More generally, for  $B_{nS} \neq 1$ , the spin summations of the squared matrix element are easily performed and yield a ratio of  $nS$ -radiative capture to ordinary  $K$  capture which may be expressed as

$$\begin{aligned} \frac{w_{nS}}{w_K} &= \frac{\alpha}{\pi m^2 (k_{\max})_{1S}^2} \left( \frac{\varphi_{nS}(0)}{\varphi_{1S}(0)} \right)^2 \int R_{nS}(k) \\ &\times k (k_{\max} - k)^2 dk. \end{aligned} \quad (9.15)$$

The relativistic correction factor for the energy spectrum  $R_{nS}(k)$  is given by

$$R_{nS}(k) = \frac{1}{2} [1 + B_{nS}^2(k)]. \quad (9.16)$$

In addition to the expression (9.14) for  $B_{nS}$  another useful one may be derived by using in (9.4) the identity  $\mathbf{e} \cdot \nabla = i\mathbf{e} \cdot \mathbf{p} = m[\mathbf{e} \cdot \mathbf{r}, H]$ . After some reduction, we then find

$$B_{nS}(k) = \frac{2mk}{3\varphi_{nS}(0)} \int \mathcal{G}_{E_{nS-k}}^{(1)}(0, \mathbf{r}) r^2 \varphi_{nS}(\mathbf{r}) d\mathbf{r}, \quad (9.17)$$

a form which simplifies the discussion of low-energy behavior. The Green's function  $\mathcal{G}^{(1)}$  remains finite in the limit  $k \rightarrow 0$  when its energy variable  $E_{nS}$  is that of the lowest  $S$  state,  $E_{1S}$ . Since  $B_{1S}$  then vanishes as  $k \rightarrow 0$ , the  $1S$  spectrum according to (9.16), is only half as intense, at this limit, as the form predicted earlier. For the higher  $S$  states,  $n \geq 2$ , the existence of  $P$  states which are degenerate with these causes the function  $\mathcal{G}^{(1)}$  to become singular as  $k^{-1}$  in the limit  $k \rightarrow 0$ . The values  $B_{nS}(0)$  for  $n \geq 2$  therefore do not vanish. They are most easily found by means of the technique used to evaluate  $Q_{nP}(0)$  in Eqs. (8.22)–(8.23). This yields, in particular,  $B_{2S}(0) = -\frac{3}{2}$ , so that the  $2S$  spectrum is slightly enhanced at its low-energy extreme.

To evaluate either of the integral forms (9.14) or (9.17) for  $B_{nS}(k)$ , it is convenient to express the Green's function  $\mathcal{G}_E^{(1)}(0, \mathbf{r})$  in terms of the  $S$ -state Green's function  $\mathcal{G}_E'(0, \mathbf{r})$  discussed in the earlier

TABLE III. The quantity  $B_{1S}(k)$  defined by (9.14), and the relativistic correction factor  $R_{1S}(k)$  for the intensity of the 1S spectrum. [Photon energy  $k$  in units of  $\frac{1}{2}(Z\alpha)^2m$ , the 1S-state binding energy.]

$k$	$B_{1S}(k)$	$R_{1S}(k)$
0.00	0.000	0.500
1.04	0.280	0.539
3.00	0.462	0.607
5.25	0.557	0.655
8.00	0.622	0.693
12.0	0.678	0.730
18.0	0.728	0.765
24.0	0.761	0.790

sections. For this purpose, we note a connection between the integral representations (6.12) and (9.10) which may be stated as

$$\frac{1}{2} \left( \frac{d^2}{dr^2} - \mu^2 \right) \mathcal{G}_{E'}(0, r) = \mathcal{G}_{E^{(1)}}(0, r) \quad (9.18)$$

for  $r > 0$ . Using the differential equation (6.4) for  $\mathcal{G}_{E'}$ , we then find

$$r \mathcal{G}_{E^{(1)}}(0, r) = - \left( \frac{1}{a} + \frac{d}{dr} \right) \mathcal{G}_{E'}(0, r), \quad (9.19)$$

where  $a = (Z\alpha m)^{-1}$ . Substitution of this expression in (9.14), followed by integration by parts and use of the Schrödinger equation for  $\varphi_{nS}$  yields

$$\begin{aligned} B_{nS}(k) &= 1 - \frac{2}{3a\varphi_{nS}(0)} \int \mathcal{G}_{E_{nS-k'}}(0, r) \left[ \frac{d}{dr} + \frac{2}{r} - \frac{1}{n^2 a} \right] \varphi_{nS}(r) dr \\ &= 1 + (3n^2 m a^2 k)^{-1} \\ &\quad - \frac{2}{3a\varphi_{nS}(0)} \int \mathcal{G}_{E_{nS-k'}}(0, r) \left[ \frac{d}{dr} + \frac{2}{r} \right] \varphi_{nS}(r) dr, \quad (9.20) \end{aligned}$$

where the integration of one of the terms has been carried out by using the representation (6.8) for the Green's function.

The integral remaining in (9.20) is quite similar in structure to the integral  $Q_{nP}(k)$  which occurred in the calculations of the  $P$ -state intensities. It may be evaluated by the same sequence of steps as was used in deriving (8.10)–(8.17). Hence only the results for the different states need be given.

For the 1S state, the parameter  $\eta$  is given by

$$\eta = [1 + (2k/Z^2\alpha^2 m)]^{-\frac{1}{2}}. \quad (9.21)$$

The quantity  $B_{1S}(k)$ , expressed in terms of  $\eta$ , is found to be

$$B_{1S}(k) = 1 - \frac{4}{3} \frac{\eta}{1+\eta} \left\{ 1 + \frac{\eta}{1-\eta} [2K(\xi) - 1] \right\}, \quad (9.22)$$

where

$$\xi = (1-\eta)/(1+\eta),$$

TABLE IV.  $B_{2S}(k)$  and the relativistic correction factor  $R_{2S}(k)$  for the intensity of the 2S spectrum. [ $k$  is given in units of  $\frac{1}{2}(Z\alpha)^2m$ .]

$k$	$B_{2S}(k)$	$R_{2S}(k)$
0.00	-1.500	1.63
0.75	-0.161	0.51
1.79	0.171	0.51
3.75	0.392	0.58
6.00	0.51	0.63
8.75	0.59	0.67
12.50	0.65	0.71
24.75	0.74	0.77

and the function  $K(\xi)$  is given by (8.12) and (8.17). A convenience in tabulating  $B_{1S}(k)$  is the slow variation of  $K(\xi)$  in the interval  $0 < \eta < 1$ . In particular for  $\eta < 0.7$  the function  $K(\xi)$  is approximated to accuracy better than 1% by the first two terms of its power series expansion,

$$K(\xi) = \log 2 - [1 - (\pi^2/12)]\eta. \quad (9.23)$$

Numerical values of  $B_{1S}(k)$  for several photon energies expressed in units of the 1S state binding energy are given in Table III. Although the increase of  $B_{1S}$  from the value zero for  $k=0$  is fairly rapid for energies not greatly exceeding the binding energy, its approach to the value unity at high energies is seen to be quite slow. As a result, the correction factor for the intensity distribution,  $R_{1S}(k)$ , remains noticeably less than one at energies relatively far above the characteristic x-ray region.

For the 2S state, the parameter  $\eta$  is given by

$$\eta = \left[ \frac{1}{4} + (2k/Z^2\alpha^2 m) \right]^{-\frac{1}{2}}. \quad (9.24)$$

The expression for  $B_{2S}(k)$  in terms of  $\eta$ , for  $\eta < 1$ , is found to be

$$\begin{aligned} B_{2S}(k) &= 1 - \frac{\eta}{(1-\frac{1}{4}\eta^2)} \left( \frac{4}{3} + \frac{5}{6}\eta \right) \\ &\quad - \frac{\eta^2}{(1-\frac{1}{4}\eta^2)^2} \left[ \frac{8}{3} (1-\eta^2) K(\lambda) - 3 - \eta + \frac{5}{4}\eta^2 \right], \quad (9.25) \end{aligned}$$

where

$$\lambda = (2-\eta)/(2+\eta),$$

and  $K(\lambda)$  is again the function discussed in Sec. 8. Numerical values of  $B_{2S}(k)$  at several photon energies are given in Table IV along with corresponding values of the relativistic correction factor  $R_{2S}(k)$ . For energies above the characteristic x-ray region,  $R_{2S}$  is slightly smaller than  $R_{1S}$  and increases toward the value one in a similarly slow manner.

The effect of the relativistic corrections on the  $S$ -state spectra of Fe<sup>55</sup> is shown in Fig. 1, where both the uncorrected and the corrected forms are plotted. Since the variation of  $R_{1S}(k)$  and  $R_{2S}(k)$  over the energy range of the spectrum is not large, these factors do not appreciably alter the spectrum shapes. For capture



processes whose energy releases are larger in comparison to their  $1S$ -state binding energies, the total variation of the correction factors would be larger and the consequent changes of spectrum shapes more noticeable. For the more energetic processes, however, it must be emphasized that the neglect of retardation which underlies the calculation of the present effect is correct only for energies less than or comparable with  $Z\alpha m$ . In the spectrum of  $\text{Fe}^{55}$ , this is no limitation since  $k_{\text{max}}$  is roughly  $2Z\alpha m$ . The decay of  $\text{A}^{37}$ , by contrast, has an energy release of 816 keV which corresponds to  $12Z\alpha m$ , so that it is only in the lower portion of its spectrum that the present corrections apply.

Estimates of the relativistic corrections to the  $P$ -state spectra show that these do not exceed the order  $Z\alpha$ , which is the level of accuracy maintained thus far. This accuracy will be improved and the  $S$ -state correction factors evaluated at all energies in a forthcoming paper based on a fully relativistic treatment of the problem.

## 10. RESULTS AND DISCUSSION

The preceding sections have been devoted to detailed calculations of the spectra emitted in the radiative capture of electrons from  $S$  and  $P$  states. For the states of higher orbital angular momentum, the radiative capture probabilities are decreased because of the smaller probabilities that the electrons are in the immediate neighborhood of the nucleus and the higher multipole orders of the radiation processes. The  $D$ -state spectra, for example, are much weaker than those considered here and negligible for present purposes.

The results of Secs. 7 to 9 may be summarized in a single formula for the spectrum intensities which takes account of the influence of the binding energies of the different states on the maximum energies of their spectra. If the photon energy  $k$  is measured in units of the  $1S$  state binding energy for a pure Coulomb field,  $\frac{1}{2}(Z\alpha)^2 m = Z^2 \times 13.6$  eV, the ratio of radiative capture from the state  $nl$  to ordinary  $K$  capture becomes

$$\frac{w_{nl}}{w_K} = \frac{Z^4 \alpha^5}{4\pi} \int_0^{k_{\text{max}}} I_{nl}(k) \left[ 1 - \frac{k + \epsilon_{nl} - \epsilon_{1S}}{(k_{\text{max}})_{1S}} \right]^2 dk. \quad (10.1)$$

The constants  $\epsilon_{nl}$  are the ionization potentials ( $\epsilon_{nl} > 0$ ) of the various atomic states measured in the same units as  $k$ . For the  $S$ -state spectra the function  $I_{nl}(k)$  assumes the form

$$I_{nS}(k) = k R_{nS}(k) [\varphi_{nS}(0)/\varphi_{1S}(0)]^2, \quad (10.2)$$

where the relativistic correction factor  $R_{nS}(k)$  is defined by (9.16) and given numerically for  $n=1$  and  $2$  in Tables III and IV. When screening is neglected, the required electron density ratio at the nucleus is  $\frac{1}{8}$  for  $n=2$ , and decreases as  $n^{-3}$ . The effects of screening cause it to decrease more rapidly still. The relativistic corrections of Sec. 9 do not substantially alter the

simple shape of the  $S$ -state spectra, but they bring about noticeable reductions of the absolute intensities.

For the  $P$ -state spectra, the function  $I_{nP}(k)$  assumes the form

$$I_{nP}(k) = (2/Z\alpha)^2 k Q_{nP}^2(k), \quad (10.3)$$

where the function  $Q_{nP}(k)$  is defined by (8.4) and given numerically for  $n=2$  and  $3$  in Tables I and II. The  $P$ -state intensities are found to be quite weak at high photon energies but to rise rapidly as the energy decreases, reaching precipitous heights near the characteristic x-ray region.

The singularities of the  $P$ -state spectra which occur at the characteristic x-ray frequencies show that the two types of radiation are, in fact, inseparable. This may be seen directly by noting that among the processes summed over in determining the rates of decay are those in which capture of an electron from a low-lying  $S$  state precedes the radiative transition of a  $P$  electron which refills the state. These processes, which give rise to a continuous spectrum, differ from the vastly more probable course of ordinary  $K$  or  $L$  capture, followed by the emission of characteristic x-rays, only in that the intermediate states do not conserve energy. When the photon energy is close to a characteristic x-ray frequency, however, energy is nearly conserved in the appropriate intermediate state and the processes become indistinguishable.

In the immediate neighborhoods of the x-ray frequencies, the continuous  $P$ -state spectra may be thought of as representing the wings of the characteristic lines. The expression (8.22) for  $Q_{nP}(k)$ ,

$$Q_{nP}(k) = \frac{(2\pi a)^{\frac{1}{2}}}{m} \sum_{n'} \frac{\varphi_{n'S}(0)}{E_{n'S} - E_{nP} + k} \int \varphi_{n'S} \mathbf{e} \cdot \nabla \varphi_{nP} d\mathbf{r},$$

illustrates this behavior. When  $k$  takes on a value for which one of the denominators is particularly small, the function  $Q_{nP}(k)$  assumes the form of a line shape seen at a distance from its center much larger than its intrinsic width.<sup>19</sup> While the singularities of the  $P$  spectra represent the x-ray lines, it should be noted that their intensities are only given correctly by the one-level resonance formula within small intervals (of the order of an electron binding energy) about the line centers. The general rise of the  $P$  spectra which begins at energies far above the x-ray region represents the constructive interference of a large variety of transition amplitudes.

Certain limitations should be noted on the accuracy of the foregoing calculations. In particular, no explicit consideration has thus far been given to the influence of atomic screening. While screening causes little change

<sup>19</sup> The radiative damping corrections which would remove the singularities of the  $P$ -state spectra have no numerical effect at distances from the line centers measurable by counter spectroscopy.

in the lowest  $S$  state, it will decrease the electron densities near the nucleus for states of higher  $l$  and  $n$ . Its principal effect then, will be to reduce the  $2P$  and, more especially, the  $3P$  intensities in comparison with the  $S$ -state spectrum. Secondly, the relativistic corrections, whose effect on the spectrum shape partly compensates that of screening by reducing the  $S$  intensities preferentially, have only been evaluated completely for energies up to  $k \sim Z\alpha m$ . These omissions are justified in the present work because the effect of screening and the relativistic corrections at high energies are numerically comparable, in general, with terms of order  $Z\alpha$  which have been consistently neglected in order to simplify the calculations. Attention will be given to all of these in the more exact treatment of the paper to follow.

The observations by Madansky and Rasetti<sup>20</sup> of the  $\gamma$ -ray spectrum emitted in the decay of  $\text{Fe}^{55}$  were the first in which the intensity distribution was measured over a wide enough energy range to provide a substantial test of the theory. These measurements showed an unexpected and steep rise of the intensity with decreasing  $\gamma$ -ray energy which has since been found<sup>21-24</sup> in a number of other elements including  $\text{A}^{37}$ ,  $\text{V}^{49}$ ,  $\text{Ge}^{71}$ , and  $\text{Cs}^{131}$ . The intensity distribution in each of these cases is found to be of just the type which follows from summing the spectra contributed by the various states, as given by (10.1). The relative contributions of the  $S$  and  $P$  states vary greatly in form and magnitude among these elements. Thus for  $\text{A}^{37}$ , with  $k_{\text{max}} \sim 800$  kev, the rise of the  $P$  spectrum takes place at energies much lower than the maximum of the  $S$  spectrum, leaving the features of the two spectra separately distinguishable.<sup>21</sup> For  $\text{Cs}^{131}$ , on the other hand, the large nuclear charge and low-energy release (350 kev) cause the  $P$  spectra to overwhelm the  $S$ -state contributions, and only a steeply sloping intensity curve is seen.<sup>24</sup> In both these cases, as well as in the others, the predicted

shapes are in general accord with those observed experimentally.

More detailed comparisons of the theoretical and experimental intensities would be difficult in the present context since the experimental spectra have been reported directly as curves of counting rates *versus* energy. These subject the actual intensity distributions to substantial changes due to the resolution and sensitivity of the counters used. The comparison is best carried out at present by reducing the theoretical spectrum to the form which might be detected by a particular spectrometer. The nonrelativistic forms of the spectra predicted here have already been compared with experiment in this way by Lindqvist and Wu,<sup>21</sup> using their own measurements for  $\text{A}^{37}$  and those of Madansky and Rasetti for  $\text{Fe}^{55}$ . The fit is found to be excellent at high energies and the sudden rise at low energies occurs where predicted. The intensity discrepancies of  $\sim 20\%$  which arise in the intermediate region would be removed by a slight readjustment of the relative normalizations of the  $S$  and  $P$  spectra, which is quite consistent with the level of accuracy noted earlier. Indeed, for the case of  $\text{A}^{37}$ , further calculation has shown that the discrepancies are removed by using a more fully relativistic treatment of the process and taking screening into account. The slightly altered theoretical spectrum which results has been shown in a recent letter<sup>25</sup> to agree quite well with the experimental measurements.

An interesting experimental check of the theory presented would be provided by the detection of photons of the continuous spectrum in coincidence with the characteristic x-rays. This would make it possible to separate the  $1S$  spectrum from the others which overlap it, since the x-rays which follow radiative capture from the higher states are very much softer than those which follow  $K$  capture. Intensity calibrations of the photon spectrum relative to the rate of ordinary capture are also of interest. The present theory predicts a dependence of this ratio on the nuclear charge which should be observable even at high energies.

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<sup>22</sup> R. W. Hayward and D. D. Hoppes, Phys. Rev. **99**, 659 (1955).

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