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Quantum Theory of the Continuous X-Ray Spectrum. Part I

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§1. INTRODUCTION AND STATEMENT OF THE FUNDAMENTAL PROBLEM

IT is the purpose of this article to give a review of the present quantum theory of the production of the continuous x-ray spectrum in such a way that the main results and formulae will be in a form readily available to the experimentalist in order to facilitate an experimental check of the theory and perhaps to suggest further experimental research. In Part I the framework of the non-relativistic theory will be developed along the lines of the development due to A. Sommerfeld[1] and O. Scherzer.[2] Henceforth these papers will be referred to as reference 1 and reference 2, respectively. Formulae showing the intensity distribution of the radiation in wave-length and in spacial direction, its polarization properties, etc., will be given for radiation which is not too hard. In this connection it has been found possible to extend the range of validity of certain of the final expressions given in the two papers mentioned above. This is of considerable importance since the range of the existing experimental results did not coincide completely with the range adequately covered by the formulae given. Actual comparison with experimental results will be reserved for Part II where the corresponding relativistic formulae will be given. Then it will be possible to present the predictions of the theory for high velocity as well as for low primary electrons, and to give an estimate of the error made in neglecting relativistic and retardation effects. As a matter of fact, the non-relativistic theory should not be applied to cases where the initial velocity is more than 10 kv if reasonable accuracy is desired. Nevertheless there is a group of phenomena such as electron scattering, soft x-rays produced by relatively low speed electrons and by protons, to which this theory can be applied.

[1] A. Sommerfeld, Ann. d. Physik **11**, 257 (1931).
[2] O. Scherzer, Ann. d. Physik **13**, 137 (1932).

It has long been agreed that the continuous radiation spectrum is produced whenever a moving charged particle is caused to change its direction of motion or is in some way retarded by interaction with matter. It has been the aim of all theories of radiation to give an accurate description of this process, hence the difference between the theories lies in the mode of description. It was characteristic of the classical theory, in which the acceleration of the charged particle was responsible for the production of the electromagnetic radiation, that it gave an account of the details of the phenomenon at every instant of time. The quantum theoretical treatment, in its present stage of development, is not able to furnish such a fine grained analysis of the phenomena, inasmuch as it is not possible to follow the course of events with certainty. Rather, starting from a certain initial situation, such as an electron approaching a nucleus, it is only possible to find the probability of a certain result having occurred within a prescribed time interval with no further details. It may turn out that as a result of future refinements in quantum mechanics which appear necessary in order to account for recent nuclear phenomena, it will be possible to describe physical phenomena on a smaller scale and to give a knowledge of more details than at present. However that may be, we shall now take up the quantum mechanical description of the production of the continuous radiation spectrum as far as it has been developed.

The fundamental quantum mechanical problem which forms the basis for all the results that the present quantum theory can yield in regard to the continuous x-ray spectrum is the following: Given a nucleus with positive charge Ze located at the origin of a set of cartesian coordinates, and an electron initially, i.e., at time t_0, at a great distance away and having a certain specified spin orientation S_1 approaching the nucleus along the z-axis in the positive direction with the velocity v_1. The ultimate result that an experimenter could hope to determine would be that after a certain length of time his instruments would indicate that the electron, again at a great distance from the nucleus, was travelling away from it in a direction located within the solid angular region between ω and $\omega+d\omega$ with a velocity somewhere between v_2 and v_2+dv_2 and having a spin orientation S_2 and in addition a photon of frequency ν between ν and $\nu+d\nu$ also travelling away from the nucleus in a direction within a second solid angular region between Ω and $\Omega+d\Omega$ and having certain prescribed polarization characteristics. Therefore, given the initial situation stated above, the probability that the electron will be scattered into the angular domain between ω and $\omega+d\omega$ with a final velocity between v_2 and v_2+dv_2 and having the spin orientation S_2 and simultaneously therewith a photon will be ejected in the angular domain between Ω and $\Omega+d\Omega$ having a frequency between ν and $\nu+d\nu$ and certain prescribed polarization characteristics must be computed by quantum mechanical methods.

While, to the writer's knowledge, no experiment to determine both the scattering of the electron and the emission of the corresponding photon has been performed, so that the above probability cannot be checked directly, nevertheless, as soon as this probability is known any quantity which has been measured can be found from it. For example such a quantity would be the spacial distribution of the photons having a given frequency and arising from an initial beam of electrons of a given velocity regardless of their polarization characteristics and without regard to the type of scattered electron which produced them. The theoretical distribution will be found by integrating the above probability over all the spacial directions, energies and spins of the scattered electron and over all the degrees of polarization of the emitted photons, and spin orientation of the initial electrons. Another example is afforded by experiments on the scattering of electrons. In these experiments the spacial distribution of the scattered electrons having a certain energy is measured without regard to the photons emitted during the scattering process. Again the theoretical distribution is found from the above probability function by integrating over all the spacial directions, frequencies, and directions of polarization of the emitted photons. It should be noticed that this method of treatment takes into account the effect of radiative forces on the scattered electrons in so far as this is possible in the quantum theory in its present form.

The above-mentioned fundamental probability function will be computed for the non-relativistic case. This means that effects of electron spin are not taken into account and the applications must be restricted to initial electron velocities which are not too high.

§2. Remarks on the Theory of the Radiation Process

The fundamental probability function described in the preceding section can be computed from certain of the formulae of the Dirac[3, 4] radiation theory. Since there are many good expositions of this theory,[5, 6] the necessary basic formulae will not be developed here. We shall rather confine our attention to certain aspects of the mathematical treatment which clearly indicate why greater simplicity in the calculation has been achieved by Sommerfeld and Scherzer over those carried out by Sugiura[7] and Gaunt,[8] and thereby making the physical interpretation easier to understand.

If we have a material system composed of atoms and electrons which is not influenced or coupled with a radiation field, then quantum mechanics has taught us that information regarding the system must be sought in a suitable wave equation,

$$[H^{\text{mat}}-\hbar\omega(n,\xi)]u(n,\xi|q)=0. \tag{1}$$

The characteristic values of the parameter $\omega(n,\xi)$ give the allowed energy levels and the corresponding solutions $u(n,\xi)$ represent the stationary states of the system. When the parameter $\omega(n,\xi)$ takes on discrete values they will be differentiated from each other by the integral number n but if $\omega(n,\xi)$ takes on all values in a certain range, values in this range will be designated by the value of the variable ξ. It is often convenient to specify discrete values of ω by more integers than the single one n but for the present we will think of n as a shortened notation for all of these integral numbers. Similar remarks hold for ξ. $u(n,\xi|q)$ denotes the stationary solution of Eq. (1) corresponding to the parameter $\omega(n,\xi)$. All of the space variables are denoted by the one variable q and $\hbar=h/2\pi$.

When the material system is acted upon by a radiation field then the wave equation (1) is replaced by the equation

$$[H^{\text{mat}}+H^{\text{rad}}+V-\hbar\omega(n,\xi)-\hbar\nu(m)]\psi=0, \tag{2}$$

where H^{mat} and H^{rad} are the Hamiltonian operators for the material system and radiation field, respectively, and $\hbar\nu_m$ is one of the characteristic energies of the radiation field. V is the coupling energy between the material system and the radiation field. It is customary to seek approximate solutions of Eq. (2) by considering that the coupling term V is a small perturbation and that at time $t=0$ the coupling term is suddenly switched on, the material system and radiation field being in known states at that time. That is, the values of n, ξ are known and also the number N_m of light quanta having the angular frequency ν_m. After not too long a time t has elapsed the solution of Eq. (2) is given approximately by

$$\psi=\sum(n')\int A(n'\xi'|t)u(n'\xi'|q)d\xi', \tag{3}$$

where the sum is taken over all the integers n' necessary to specify all the states and the integral over all the continuous parameters ξ'. The coefficients $A(n'\xi'|t)$ are different depending on the initial state of the entire system. For the case considered here, we shall suppose that the material system is in some state specified by n, ξ but that $N_m=0$ for all m, i.e., no photons are present in the radiation field, at time $t=0$, then

$$A(n'\xi'|t)\cong\frac{\hbar^{\frac{1}{2}}}{Q^{\frac{1}{2}}\nu_m^{\frac{1}{2}}}(n\xi|\mathbf{P}_m|n'\xi')\frac{1-e^{i[\omega(n'\xi')-\omega(n,\xi)+\nu_m]t}}{\hbar[\omega(n',\xi')-\omega(n,\xi)+\nu_m]} \tag{4}$$

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[3] P. A. M. Dirac, Proc. Roy. Soc. **A114**, 243 (1927).
[4] P. A. M. Dirac, Proc. Roy. Soc. **A114**, 710 (1927).
[5] See for instance E. Fermi, Rev. Mod. Phys. **4**, 87 (1932).
[6] A. Landé, Handb. d. Physik **20**, 406 (1928).
[7] Y. Sugiura, Scientific papers, Institute of Phys. and Chem. Research of Tokio.
[8] A. Gaunt, Roy. Soc. Phil. Trans. **A229**, 163 (1930).

and

$$(n\xi|\mathbf{P}_m|n'\xi')=-i\hbar\int u(n\xi|q)\{\sum_{k=1}^{N}e^{-i(\kappa_m\cdot r_k)}(e_k/m_k)(\mathbf{P}_m\cdot\text{grad}_k)\}u^*(n'\xi',q)dq_1, \tag{5}$$

where the sum is taken over all the charged particles of the system, e_k is the charge of the particle and m_k its mass. Q is the volume of the radiation space, κ_m is a vector of magnitude ν/c in the direction of propagation of the photon of angular frequency ν_m, $\mathbf{P}_m$ is a unit vector in the direction of the electric vector of the component of radiation having the frequency ν_m and $\mathbf{r}_k$ is the radius vector of the kth particle. The three quantities $\nu(m)$, $\mathbf{P}_m$, and κ_m fully specify the state of the emitted light quantum. The $|A(n'\xi'|t)|^2$ is to be interpreted as the probability that after a time t has elapsed the material system has made a transition from the state n, ξ to n', ξ' and a photon has been emitted in the direction κ_m with frequency $\nu(m)$ and polarization $\mathbf{P}_m$.

In the case of one electron and a fixed nucleus Eq. (5) becomes

$$(n\xi|\mathbf{P}_m|n'\xi'\nu(m))=-(ei\hbar/m)\int u(n\xi|q)e^{-i(\kappa_m\cdot r)}(\mathbf{P}_m\cdot\text{grad})u^*(n'\xi'|q)dq. \tag{6}$$

Also since this calculation is non-relativistic the initial velocity of the electron cannot be too great and since $\hbar\nu_m$ is nearly equal to the difference between the initial energy and final energy, we shall treat ν_m/c as sufficiently small so that the retardation factor $e^{-i(\kappa_m\cdot r)}$ may be considered to be a very slowly varying function over the domain where most of the contribution to the integral takes place. By neglecting this term Eq. (6) becomes,

$$(n\xi|\mathbf{P}_m|n'\xi')=(e\hbar/mi)\cdot\int u(n\xi|q)\mathbf{P}_m\ \text{grad}\ u^*(n'\xi',|q)dq. \tag{7}$$

It can readily be shown (Appendix A) that

$$(\hbar/mi)\int u(n\xi|q)[\mathbf{P}_m\cdot\text{grad}\ u^*(n'\xi'|q)]dq=[\omega(n\xi)-\omega(n'\xi')]\int(\mathbf{P}_m\cdot\mathbf{r})u(n\xi|q)u^*(n'\xi'|q)dq$$
$$=[\omega(n\xi)-\omega(n'\xi')](n\xi|\mathbf{P}_m\cdot\mathbf{r}|n'\xi'). \tag{8}$$

The problem has now been reduced to the calculation of the matrix elements $(n\xi|x|n'\xi')$, $(n\xi|y|n'\xi')$ and $(n\xi|z|n'\xi')$ in terms of which one can compute the probability that the emitted photon will have any prescribed polarization. The above matrix elements involve only the solutions of the wave equation (1) for the material system which represent its initial and final states. These two solutions must also belong to a complete orthonormal* set of solutions of Eq. (1). The problem, therefore, is that of finding solutions of Eq. (1) which have the property that at a great distance away from the nucleus they represent a nearly plane wave travelling toward the nucleus along any direction, or a nearly plane wave travelling away from the nucleus in an arbitrary direction. It is clear at the outset that none of the solutions belonging to the usual orthonormal set found by solving Eq. (1) for the hydrogen atom with nuclear charge Ze in polar coordinates, represent the states which are required here. It requires an infinite series of such solutions to represent a plane wave, consequently if this set of solutions were used the functions $u(n\xi|q)$ occurring in Eq. (8) would have to be expressed in terms of an infinite series of such solutions which makes the evaluation of the relevant matrix elements difficult and very complicated. This method has, however, been used by Gaunt[8] but the mathematical treatment is quite complicated. Similar remarks apply to the work of Sugiura,[7] who used another orthonormal set, but the mathematical work is formidable. An ortho-

* The term orthonormal set means a normalized and orthogonal set in accordance with the usage of M. H. Stone, *Linear Transformations in Hilbert Space.*

normal set of relatively simple solutions which do represent the states of the atomic system required here, have been found by A. Sommerfeld[1] and O. Scherzer.[2]

§3. Determination of an Appropriate Orthonormal Set of Solutions

The problem now is to find an orthonormal set of solutions of the wave equation for the hydrogen atom with nuclear charge Ze since Eq. (1) reduces to this for the special case under consideration. The way in which the appropriate wave equation for hydrogen is found is so well known that we merely write it in a familiar form, namely in polar coordinates, i.e.,

$$\nabla^2\psi+(2m/\hbar^2)[Ze^2/r+E]\psi=0.$$

It is well known that in the orthonormal set of solutions of this equation there exists none that will specify the initial state. We therefore hunt solutions in the parabolic coordinates

$$x=(\xi\eta)^{\frac{1}{2}}\cos\varphi; \qquad y=(\xi\eta)^{\frac{1}{2}}\sin\varphi; \qquad z=\tfrac{1}{2}(\xi-\eta).$$

The above equation then becomes

$$\frac{\partial}{\partial\xi}\left(\xi\frac{\partial\psi}{\partial\xi}\right)+\frac{\partial}{\partial\eta}\left(\eta\frac{\partial\psi}{\partial\eta}\right)+\frac{1}{4}\left(\frac{1}{\xi}+\frac{1}{\eta}\right)\frac{\partial^2\psi}{\partial\varphi^2}+\left(\frac{k^2}{4}(\xi+\eta)+\frac{z}{a}\right)\psi=0, \tag{9}$$

where $k^2=(2m/\hbar^2)E$ and $a=\hbar^2/me^2$ the radius of the first Bohr orbit. On account of the symmetry of the present problem the dependence on φ drops out. The resulting equation is separable so that we may write

$$\psi=f(\xi)g(\eta), \tag{10}$$

which, when substituted in Eq. (9), yields the following ordinary differential equations

$$\frac{d}{d\xi}\xi\frac{df}{d\xi}+\left(\frac{k^2}{4}\xi+\frac{z}{2a}-\lambda\right)f=0, \tag{11a}$$

$$\frac{d}{d\eta}\eta\frac{dg}{d\eta}+\left(\frac{k^2}{4}\eta+\frac{z}{2a}+\lambda\right)g=0. \tag{11b}$$

Each of these equations is of the form

$$\frac{d}{du}u\frac{dF}{du}+\left(n+\tfrac{1}{2}-\frac{u}{4}\right)F=0, \tag{12}$$

where in Eq. (11a)

$$u=-ik\xi; \qquad n=(i/k)(Z/2a-\lambda)-\tfrac{1}{2}=n_1 \tag{13}$$

and in Eq. (11b) the following substitutions were made

$$u=ik\eta; \qquad n=-(i/k)(Z/2a+\lambda)-\tfrac{1}{2}=n_2. \tag{14}$$

Then on writing $F=e^{-u/2}L_n(u)$ Eqs. (11a) and (11b) reduce to the well-known Laguerre differential equation

$$ud^2L_n/du^2+(1-u)dL_n/du+nL_n=0. \tag{15}$$

Since we are interested in solutions with positive energy, k will be positive and continuous for the interval $0\leq k<\infty$. This makes n continuous and purely imaginary so that the solution L_n is no longer the simple Laguerre polynomial. The properties of these functions are well known so that we need not discuss them in detail here (see for instance reference 1, page 270).

In order to test whether our solution will represent the initial state, it will be necessary to ascertain the behavior of L_n for large values of the argument. To do this it is sufficient to make use of the first

term in the asymptotic expansion of L_n. This is (see reference 1, pp. 274)

$$L_n(u) \cong e^{-i\pi n}\left[\frac{u^n}{\Gamma(n+1)} - \frac{n}{u}\frac{e^u(-u)^{-n}}{\Gamma(1-n)} + \cdots\right].$$

Using this expression and the relations (13) and (14) we have

$$f(\xi) = [A(\xi)e^{\frac{1}{2}ik\xi} + (n_1/ik\xi)A^*(\xi)e^{-\frac{1}{2}ik\xi}]e^{-i\pi n_1},$$
$$g(\eta) = [B(\eta)e^{-\frac{1}{2}ik\eta} - (n_2/ik\eta)B^*(\eta)e^{\frac{1}{2}ik\eta}]e^{-i\pi n_2},$$

where

$$A(\xi) = (k\xi)^{n_1}e^{-\frac{1}{2}n_1\pi i}/\Gamma(n_1+1) \qquad \text{and} \qquad B(\eta) = (k\eta)^{n_2}e^{\frac{1}{2}n_2\pi i}/\Gamma(n_2+1),$$

so that

$$\psi = f\cdot g = [ABe^{\frac{1}{2}ik(\xi-\eta)} - (n_2/ik\eta)AB^*e^{\frac{1}{2}ik(\xi+\eta)}]e^{-i\pi(n_1+n_2)}$$
$$+[(n_1/ik\xi)A^*Be^{-\frac{1}{2}ik(\xi+\eta)} + (n_1n_2/k^2\xi\eta)A^*B^*e^{-\frac{1}{2}ik(\xi-\eta)}]e^{-i\pi(n_1+n_2)}$$

or

$$\psi = [ABe^{ikz} - (n_2/ik\eta)AB^*e^{ikr}]e^{-i\pi(n_1+n_2)} + [(n_1/ik\xi)A^*Be^{-ikr} + (n_1n_2/k^2\xi\eta)A^*B^*e^{-ikz}]e^{-i\pi(n_1+n_2)}. \quad (16)$$

It is now evident that the first two terms on the right-hand side do indeed comprise the type of solution required. These terms represent a plane wave travelling in the positive z-direction and diverging spherical waves scattered by the nucleus and travelling away from it, whose amplitude becomes zero at an infinite distance. The third and fourth terms, taken together, represent a plane wave travelling in the negative z-direction and converging spherical waves. These terms are superfluous for the representation of the initial state and can be conveniently removed by setting n_1 equal to zero. It should be noticed that the type of solution represented by the third and fourth term can be obtained after n_1 is placed equal to zero by merely taking the complex conjugate of ψ. Setting n_1 equal to zero is allowable since this can be effected by the proper choice of the arbitrary constant λ in Eq. (13).

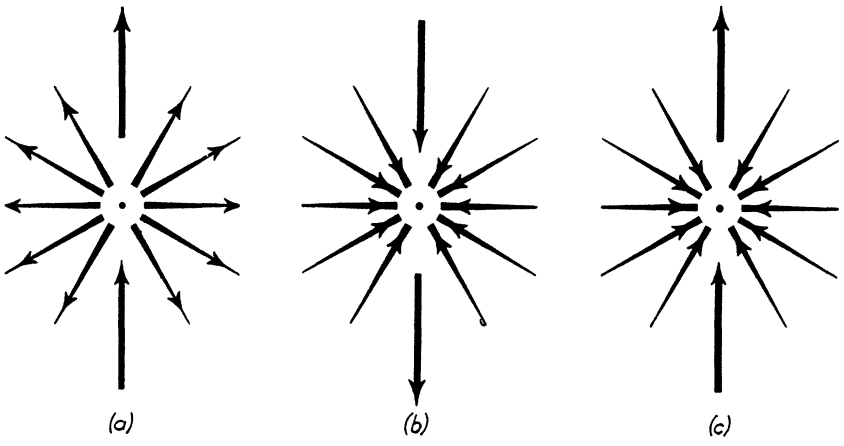

FIG. 1. Schematic representation of the asymptotic behavior of the wave functions. Tapering lines show decreasing amplitude of electron waves.

Since $L_0(u)=1$, the solution of Eq. (9) that is suitable to represent the initial state is then

$$\psi=e^{ikz}L_n(ik\eta) \qquad \text{where } \eta=z/ika. \tag{17}$$

The state represented by this solution is shown schematically in Fig. 1a. The complex conjugate of Eq. (17) represents the situation shown in Fig. 1b.

Another type of solution which could and indeed has been used by Scherzer may be obtained from Eq. (17) by replacing z by $-z$ and taking the complex conjugate. Since $\eta=r-z$ and $\xi=r+z$, it is readily seen that replacing z by $-z$ is equivalent to changing η to ξ wherever it appears. Hence when these changes are made

$$e^{ikz}L_n(ik\eta)\rightarrow e^{ikz}L_n(-ik\xi).$$

By referring to Eq. (16), it is readily seen that this represents the asymptotic situation shown in Fig. 1c.

Having obtained a solution which represents the initial situation, the next problem is to ascertain whether there exists an orthonormal set of which it is a member. An indication of what we might expect these additional solutions to be should be obtained by seeking functions which would represent all of the possible final states of the electron. The functions which represent the final states must have the asymptotic form which gives a nearly plane wave leaving the nucleus in an arbitrary direction in space and having a certain velocity. Such functions can be obtained by referring Eq. (17) to a set of axes rotated with respect to the fixed set, to which the initial state is referred. Since the original differential equation is invariant with respect to rotations of the axes, the function found by rotation will still be a solution of the wave equation. If the infinite number of solutions thus found are to form an orthonormal set, then two such solutions with different spacial rotations must be orthogonal.

In order to test this heuristic argument it will be necessary to determine the solution (17) referred to a new system of axes x', y', z' in which the new z' axis makes an angle α with the fixed z axis and the $x'z'$ plane makes an angle β with the xz plane and then test the resulting solutions for orthogonality. Let the solution (17) with respect to the rotated system of axes be

$$\psi=e^{ikz'}L_n(ik\eta').$$

This solution referred to the fixed system x, y, z can be found by giving the expression for z' and η' in terms of the fixed system. Since the two systems are orthogonal $r=r'$ so that,

$$z'=x\sin\alpha\cos\beta+y\sin\alpha\sin\beta+z\cos\alpha$$

and

$$\eta'=r'-z'=r-z'=\tfrac{1}{2}(\xi+\eta)-\sin\alpha(x\cos\beta+y\sin\beta)-z\cos\alpha$$
$$=\xi\sin^2\tfrac{1}{2}\alpha+\eta\cos^2\tfrac{1}{2}\alpha-2(\xi\eta)^{\frac{1}{2}}\sin\tfrac{1}{2}\alpha\cos\tfrac{1}{2}\alpha\cos(\varphi-\beta).$$

It can now be shown that

$$\int_0^\infty\int_0^\infty\int_0^{2\pi}\tfrac{1}{4}(\xi+\eta)d\xi d\eta d\varphi e^{ik'z}L_{n'}(ik'\eta')\int_{\Delta\beta''}\int_{\Delta\alpha''}\int_{\Delta k''}e^{-ik''z}L_{-n''}(-ik''\eta'')k''^2dk''d\omega''$$
$$=\begin{cases}(2\pi)^3/|\Gamma(n'+1)|^2e^{in'\pi}\\ 0\end{cases} \tag{18}$$

The upper or the lower values are to be taken in Eq. (18) according as the volume elements, $k'^2dk'd\omega'$ and $k''^2dk''d\omega''$ in momentum space *do* or *do not* overlap in part. This is the customary normalization for the solutions when the parameters specifying the states are continuous. It means that any two solutions (17) representing states where the electron has different momenta both as regards absolute value or angular direction, are orthogonal. When the states are the same Eq. (18) gives the square of the normalizing factor. We have therefore generated an orthonormal set of solutions of Eq. (9)

by space rotation of the function given by Eq. (17), each member of which is suitable to describe the atomic states we are interested in. The normalized solutions are

$$u(\alpha, \beta, k|q)=[|\Gamma(n+1)|e^{\frac{1}{2}n\pi i}/(2\pi)^{\frac{3}{2}}]e^{ikz}L_n(ik\eta'). \tag{19}$$

That this orthonormal set is complete has been shown by Scherzer (reference 2, pp. 137).

§4. Calculation of the Matrix Elements Neglecting Retardation

Much of the mathematical analysis required to evaluate the requisite matrix elements will be omitted when it can be found in the literature already referred to. The mathematical details involved in extensions or original contributions will be found in the notes in the appendix.

The matrix elements to be evaluated first are those which refer to a transition from a state of the atom in which the electron is advancing toward the nucleus in the direction of the positive z axis with a momentum measured by $k_1=mv_1/\hbar$ to a state where the electron is leaving the nucleus in some small solid angular region specified by α and β with a momentum k. In terms of the momentum space the extremity of the momentum vector sweeps over the small volume element l in the initial state (see Fig. 2). In the final state the extremity of the momentum vector lies in some volume element 2. In accordance with the notation adopted in Eq. (8), the desired matrix elements for the three components of polarization are

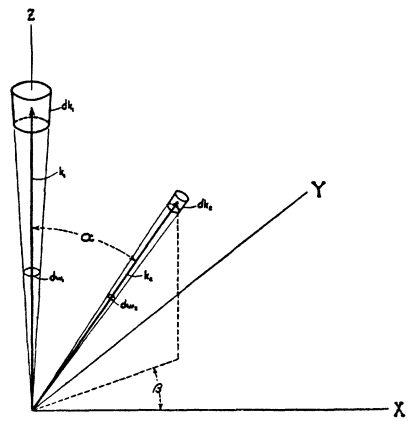

FIG. 2. The momentum space in terms of which the atomic states are specified.

$$\left(00k_1\left|\begin{matrix}x\\y\\z\end{matrix}\right|\alpha, \beta, k\right)=\int_0^\infty\int_0^\infty\int_0^{2\pi}u(00k_1|\xi\eta\varphi)\left\{\begin{matrix}x\\y\\z\end{matrix}\right\}u^*(\alpha\beta k/\xi\eta\varphi)(\eta+\xi)/4d\xi d\eta d\varphi, \tag{20}$$

where the normalized wave functions of Eq. (19) are used. The values of these integrals as calculated by Sommerfeld (reference 1, Eq. (17)), are

$$\left(00k_1\left|\begin{matrix}x\\y\end{matrix}\right|\alpha\beta k\right)=B\sin\alpha\left\{\begin{matrix}\cos\beta\\\sin\beta\end{matrix}\right\}n_1(1-n_2)F(1+n_1; 2-n; 2; w)$$

$$(00k_1|z|\alpha\beta k)=-B[(n-n_1\cos\alpha)F(1+n_1; 1-n; 1; w)+(1+\cos\alpha)n_1n_2F(1+n_1; 1-n; 2; w)], \tag{21}$$

where $F(\alpha, \beta, \gamma, x)$ is the hypergeometric function which is defined by the series

$$F(\alpha, \beta, \gamma, x)=1+\frac{\alpha\beta}{\gamma}x+\frac{\alpha(\alpha+1)\beta(\beta+1)}{\gamma(\gamma+1)}\frac{x^2}{2!}+\cdots|x|<1; \tag{22}$$

also

$$B=\frac{16\pi\Gamma(n_1+1)\Gamma(-n+1)k_1ke^{\frac{1}{2}(n-n_1)\pi i}}{(2\pi)^3(k_1^2-k^2)^2(k_1+k)^2}\left(\frac{k_1-k}{k_1+k}\right)^{n_1-n} \tag{23}$$

and $w=[4k_1k/(k_1+k)^2]\cos^2(\alpha/2)$.

§5. Fundamental Transition Probabilities

The exact meaning of the transition probability $|A|^2$ given by Eq. (4) when any one of the matrix elements of Eq. (21) are used should be made clear so that it can be converted into a quantity useful in comparing with experiment. $|A|^2k^2dkd\omega$ is the probability that after a time t a light quantum of angular frequency ν_m, is emitted in the direction κ_m, with electric vector in the x, y, or z direction as the case may be, and simultaneously therewith the atomic system has changed from the state specified by the element of volume in momentum space $k_1^2dk_1d\omega_1$ to the state determined by the element of volume $k^2dkd\omega$, where $d\omega$ is the element of solid angle. For definiteness this probability will be denoted by

$$P_1\begin{pmatrix} 00k_1\|\alpha\beta k\,|\,\nu_m\kappa_m, \begin{matrix}x\\y\\z\end{matrix}\end{pmatrix}k^2dkd\omega=\frac{4\pi e^2}{Q\nu_m\hbar}[\omega(k_1)-\omega(k)]^2 \times\left|\begin{pmatrix}00k_1\left|\begin{matrix}x\\y\\z\end{matrix}\right|\alpha\beta k\end{pmatrix}\right|^2\frac{1-\cos[\omega(k)-\omega(k_1)+\nu_m]t}{[\omega(k)-\omega(k_1)+\nu_m]^2}\cdot k^2dkd\omega. \quad (24)$$

The quantity P_1 is then the probability per unit volume of momentum space.

The probability which is more useful is that which gives the probability of a photon being emitted in an element of solid angled Ω with a frequency between ν and $\nu+d\nu$. This may be found by multiplying Eq. (24) by the number of radiation components of the type ν_m, κ_m which fall in this angular frequency interval and solid angle range. This number is

$$[Q/(2\pi)^3]|\kappa|^2d|\kappa|d\Omega=[Q/(2\pi c)^3]\nu^2d\nu d\Omega.$$

In addition to this it is usually required to know the radiation energy emitted in the range. This is of course obtained by multiplying by $\hbar\nu$. This probability will be denoted by

$$P_2\begin{pmatrix}00k_1\|\alpha\beta k\,|\,\nu\begin{matrix}x\\y\\z\end{matrix}\end{pmatrix}k^2dkd\omega d\nu d\Omega=\frac{4\pi\nu^2e^2}{(2\pi c)^3}[\omega(k_1)-\omega(k)]^2|(00k_1|x|\alpha\beta k)|^2\frac{1-\cos[\omega(k)-\omega(k_1)-\nu]t}{[\omega(k)-\omega(k_1)+\nu]^2} \cdot k^2dkd\omega d\nu d\Omega. \quad (25)$$

P_2 is then the radiation energy emitted during time t per unit angular frequency, per unit solid angle, per unit volume in momentum space.

The expression for P_1 shows that unless $\omega(k)+\nu$ is nearly equal to $\omega(k_1)$ the transition probability is small and remains small for all time, which means that the energy is approximately conserved during the transition. Since the characteristic momenta of the final state form a continuous range, the only transitions of any consequence will be to those states for which the absolute value of the momentum lies in the region

$$k_2-\Delta k<k<k_2+\Delta k,$$

where k_2 satisfies the relation

$$\omega(k_2)-\omega(k_1)+\nu=0. \quad (26)$$

In terms of the momentum space, this means that the important final states of the atom will be those whose momenta lie in a spherical shell whose mean radius is k_2.

It is convenient to integrate Eq. (25) with respect to k thus obtaining the total probability of transitions to momentum states in the spherical shell subtended by the angular region $d\omega$. This integration can readily be carried out approximately on account of the circumstances mentioned above. We have to evaluate

$$\int_{k_2-\Delta k}^{k_2+\Delta k}[\omega(k_1)-\omega(k)]^2|(00k_1|\alpha\beta k)|^2\frac{1-\cos[\omega(k)-\omega(k_1)+\nu]t}{[\omega(k)-\omega(k_1)+\nu]^2}k^2dk.$$

This may be facilitated by the change of variable

$$s=[\omega(k)-\omega(k_1)+\nu]t; \qquad ds=t\omega'(k)dk=(t\hbar/m)kdk.$$

For rather large values of t the cosine factor and resonance denominator will be a rapidly varying function of s having a sharp maximum at $s=0$. The remaining terms will be slowly varying functions of s over the region where the rapidly varying part is appreciably different from zero. Hence we may expand them about the point $s=0$ or what amounts to the same thing about the point for which $k=k_2$ and retain only the first term in the expansion. Under these circumstances the above integral to a first approximation becomes

$$\frac{tmk_2}{\hbar}[\omega(k_1)-\omega(k_2)]^2|(00k_1|\alpha\beta k_2)|^2\int_{-\infty}^{+\infty}\frac{1-\cos s}{s^2}ds\cdot\frac{t\pi mk_2\nu^2}{\hbar}|(00k_1|\alpha\beta k_2)|^2. \tag{27}$$

Making use of this expression and Eq. (25) we may find a new probability, i.e.,

$$P_3\left(00k_1\|\alpha\beta k_2|\,\nu\begin{matrix}x\\y\\z\end{matrix}\right)=\frac{(2\pi)^2\nu^4mk_2e^2}{(2\pi c)^3\hbar}\left|\left(00k_1\left|\begin{matrix}x\\y\\z\end{matrix}\right|\alpha\beta k_2\right)\right|^2. \tag{28}$$

This gives the probable radiation energy of the prescribed polarization emitted per unit time, per unit angular frequency per unit solid angle due to an electron transition from a mean momentum k_1 to a mean momentum k_2 in the solid angular domain $d\omega$ where ν and k_2 are connected by the relation (26).

The probability P_3 is still not quite that desired for comparing with experimental results in certain cases, because it refers to a transition of one electron while what is actually desired is the probability in question when at a great distance from the nucleus precisely one electron per square centimeter per second approaches the nucleus. To obtain this it is only necessary to multiply P_3 by $(2\pi)^3m/\hbar k_1$. This can be seen by noting that $e|u(00k_1|q)|^2$ is the charge density so that the current is $v_1e|u(00k_1|q)|^2$. If this is to correspond with a current of one electron per square centimeter then $v_1|u|^2=1$. Using the asymptotic expressions Eq. (16) we note that $|u(00k_1|q)|^2=1/(2\pi)^3$ so that we must multiply Eq. (28) by $(2\pi)^3/v_1=(2\pi)^3m/\hbar k_1$. We have therefore obtained the desired fundamental probability function which we set out to calculate. We denote it by:

$$P\left(00k_1\|\alpha\beta k_2|\,\nu\begin{matrix}x\\y\\z\end{matrix}\right)d\nu d\Omega d\omega=C\left|\left(00k_1\left|\begin{matrix}x\\y\\z\end{matrix}\right|\alpha\beta k_2\right)\right|^2 d\nu d\Omega d\omega, \tag{29}$$

where $C=2\pi m^2e^2\nu^4k_2/c^3\hbar^2k_1$.

To avoid confusion it will be repeated that this gives the radiant energy emitted per unit time in the element of solid angle $d\Omega$ with angular frequency between ν and $\nu+d\nu$ polarized in the direction x, y or z when electrons with initial mean momentum k_1 approach the nucleus at the rate of one per second, are deflected into the element of solid angle $d\omega$ with a final mean momentum k_2 where k_2 is given by Eq. (26). If the intensity at a distance R away from the nucleus is desired, the above result must be multiplied by $[R^2d\Omega]^{-1}$.

If the energy of the photons emitted in the direction specified by Θ and Φ is desired, then it is convenient to select components of polarization which are transverse to the direction of propagation of the photon. Let one of these transverse components lie in the plane determined by the z axis (initial direction of electron) and the direction of the photon and directed toward increasing Θ. Let the other component be perpendicular to this plane and directed toward increasing Φ. Then the expressions giving the probability corresponding to expression (29) for the two components of

polarization are

$$P_\Theta(00k_1\|\alpha\beta k_2|\nu\Theta\Phi)=C|(00k_1|x|\alpha\beta k_2)\cos\Theta\cos\Phi + (00k_1|y|\alpha\beta k_2)\cos\Theta\sin\Phi-(00k_1|z|\alpha\beta k_2)\sin\Theta|^2, \quad (30a)$$

$$P_\Phi(00k_1\|\alpha\beta k_2|\nu\Theta\Phi)=C|-(00k_1|x|\alpha\beta k_2)\sin\Phi+(00k_1|y|\alpha\beta k_2)\cos\Phi|^2. \quad (30b)$$

The transition probabilities given in this section serve as the basis for all the intensity, polarization, and electron scattering formulae which will be developed in the next section. To check the expressions (30) in detail, experiments would have to be performed in which the deflection of an electron is measured and at the same time the direction, frequency, etc., of the emitted photon.

§6. Total Intensity

In the actual measurement of radiation intensity, the total radiation due to all possible electron deflections is measured. This total intensity measured at a distance R away from the nucleus in a direction determined by Θ and Φ with electric vector directed toward increasing Θ or Φ is found by integrating the expressions (30) over all of the electron directions. Hence.

$$I_\Theta(\nu\Theta\Phi)d\nu=(d\nu/R^2)\int_0^\pi\int_0^{2\pi}P_\Theta(00k_1\|\alpha\beta k_2|\nu\Theta\Phi)\sin\alpha d\alpha d\beta, \quad (31a)$$

$$I_\Phi(\nu\Theta\Phi)=(d\nu/R^2)\int_0^\pi\int_0^{2\pi}P_\Phi(00k_1\|\alpha\beta k_2|\nu\Theta\Phi)\sin\alpha d\alpha d\beta. \quad (31b)$$

The total intensity regardless of polarization will be the sum of the above expressions.

It is customary to measure the intensity distribution in a plane at right angles to the direction of the initial electron beam or in a plane containing it. The corresponding intensity can be found from Eq. (31) by setting $\Theta=\pi/2$ or $\Phi=0$. Eqs. (31) becomes somewhat simpler for these particular conditions and for the first case may be written

$$I_z(\nu,\pi/2,\Phi)d\nu=(C/R^2)d\nu\int_0^\pi\int_0^{2\pi}|(00k_1|z|\alpha\beta k_2)|^2\sin\alpha d\alpha d\beta, \quad (32a)$$

$$I_\Phi(\nu,\pi/2,\Phi)=(d\nu/R^2)\int_0^\pi\int_0^{2\pi}|(00k_1|x|\alpha\beta k_2)|^2\sin\alpha d\alpha d\beta. \quad (32b)$$

Use has been made of the fact that

$$\int_0^{2\pi}(00k_1|x|\alpha\beta k_2)(00k_1|y|\alpha\beta k_2)d\beta=0.$$

The first expression gives the intensity of the radiation in a plane perpendicular to the z axis (initial electron beam) with electric vector along the z axis, the second refers to the intensity with the electric vector in the direction of increasing Φ.

Corresponding expressions for the intensity in a plane containing the z axis (initial electron beam) are

$$I_\Theta(\nu,\Theta,0)d\nu=(Cd\nu/R^2)\int_0^\pi\int_0^{2\pi}\{|(00k_1|x|\alpha\beta k_2)|^2\cos^2\Theta+|(00k_1|z|\alpha\beta k_2)|^2\sin^2\Theta\}\sin\alpha d\alpha d\beta, \quad (33a)$$

$$I_y(\nu,\Theta,0)d\nu=(Cd\nu/R^2)\int_0^\pi\int_0^{2\pi}|(00k_1|y|\alpha\beta k_2)|^2\sin\alpha d\alpha d\beta. \quad (33b)$$

Use has been made of the circumstance that

$$\int_0^{2\pi} (00k_1|x|\alpha\beta k_2)(00k_1|z|\alpha\beta k_2)d\beta = 0.$$

The indicated integrations over α and β must now be performed. In Sommerfeld's treatment these integrations were carried out for two limiting cases only, namely for $|n_1|^2 \ll 1$ and $|n_1|^2 \gg 1$. Unfortunately much of the experimental data are for regions which lie between these two limiting cases. It should also be pointed out that the limiting case $|n_1|^2 \ll 1$ is to a certain extent incompatible with the non-relativistic theory which requires $\beta_1^2 = (v_1/c)^2 \ll 1$. n_1 is defined as Z/iak_1 hence $|n_1| = Z/ak_1 = Z/137\beta_1$. Since $|n_1|$ and β_1 are connected by this reciprocal relation, the requirement that $\beta_1 \ll 1$ and $|n_1|^2 \ll 1$ cannot always be fulfilled, especially if Z is large. In order to make the non-relativistic theory as useful as possible it seemed necessary to evaluate the integrals with respect to α and β for quite general n_1 and n_2. This has been done by the writer in Appendix B.

Referring to Eqs. (21), (B1), (B11), (B13) and (B17), the intensity expressions (32) and (33) can be written

$$I_z(\nu, \pi/2, \Phi)d\nu = (C|B|^2/R^2)d\nu K_2(n_1; n_2), \tag{34a}$$

$$I_\Phi(\nu, \pi/2, \Phi)d\nu = (C|B|^2 d\nu/R^2)K_1(n_1; n_2), \tag{34b}$$

$$I_\Theta(\nu, \Theta, 0)d\nu = (C|B|^2 d\nu/R^2)[K_1(n_1 n_2)\cos^2\Theta + K_2(n_1 n_2)\sin^2\Theta], \tag{35a}$$

$$I_y(\nu, \Theta, 0)d\nu = (C|B|^2 d\nu/R^2)K_1(n_1; n_2), \tag{35b}$$

where from Appendix B Eqs. (B9), (B11) and (B17):

$$K_1(n_1 n_2) = (2\pi/s^2)\sum_{l=1}^{\infty} l(l+1)(2l+1)|G_l(n_1; 1-n_2; s)|^2,$$

$$K_2(n_1 n_2) = (\pi|n_1|^2/s^2)\sum_{l=0}^{\infty} (2l+1)|(s+n_2 s/n_1 - 2)G_l(1+n_1; 1-n_2; s) + 2G_l(n_1; 1-n_2; s)|^2,$$

$$G_l(\alpha, \beta, s) = \frac{2s^l}{\Gamma(\alpha)\Gamma(\beta)} \frac{\Gamma(\alpha+l)\Gamma(\beta+l)}{\Gamma(2l+2)} F(\alpha+l; \beta+l; 2l+2; s), \qquad s = 4k_1 k_2/(k_1+k_2)^2. \tag{36}$$

The above series are all absolutely convergent for $s^2 < 1$ (see Appendix B). The maximum value s can assume is $s = 1$ which corresponds to the long wave-length limit. At first sight the above series may seem quite complicated, but they converge so rapidly in most cases that three terms are all that are required to compute the intensity with considerable accuracy.

The total intensity without regard to the direction of the electric vector in the plane perpendicular to the initial electron beam or parallel thereto is the sum of expressions (34) or (35).

Short wave-length limit

An important limiting case of the above formulae is that for which $k_2 \to 0$, i.e., the short wave-length limit. In order to determine the limiting expressions for the intensity, the following limits are required, namely

$$\lim_{k_2 \to 0} C|B|^2 K_1(n_1; n_2) \qquad \text{and} \qquad \lim_{k_2 \to 0} C|B|^2 K_2(n_1; n_2).$$

It can be shown without difficulty (see Appendix D) that on passing to the limit $k_2 = 0$ the above expressions become

$$\lim_{k_2 \to 0} C|B|^2 K_1(n_1; n_2) = DK_1^0(n_1) \qquad \text{and} \qquad \lim_{k \to 0} C|B|^2 K_2(n_1; n_2) = DK_2^0(n_1),$$

where

$$D=e^2|n_1|^2\hbar^2/2\pi(2m)^2c^3(e^{2|n_1|\pi}-1) \tag{37}$$

$$K_1^0(n_1)=\frac{8\pi}{|\Gamma(n_1)|^2}\sum_{l=1}^{\infty}\frac{l(l+1)}{\Gamma(2l+1)\Gamma(2l+2)}|\Gamma(n_1+l)(-4n_1)^l F(n_1+l;\,2l+2;\,-4n_1)|^2, \tag{38}$$

$$K_2^0(n_1)=16\pi|n_1|^2\sum_{l=0}^{\infty}\frac{|4n_1|^{2l}}{\Gamma(2l+1)\Gamma(2l+2)}\left|\frac{\Gamma(1+n_1+l)}{\Gamma(1+n_1)}F(1+n_1+l;\,2l+2;\,-4n_1)+\frac{\Gamma(n_1+l)}{\Gamma(n_1)}F(n_1+l;\,2l+2;\,-4n_1)\right|^2. \tag{39}$$

The function $F(\alpha,\,\beta,\,x)$ is the ordinary confluent hypergeometric function defined by the series

$$F(\alpha,\,\gamma,\,x)=1+\frac{\alpha}{\gamma}x+\frac{\alpha(\alpha+1)}{\gamma(\gamma+1)}\frac{x^2}{2!}+\cdots.$$

The intensities perpendicular to the initial electron beam at the short wave-length limit will be denoted by $I_z^0(\nu,\,\pi/2,\,\Phi)$ and $I_\Phi^0(\nu,\,\pi/2,\,\Phi)$. Using the above limits, we have from Eqs. (34)

$$I_z^0(\nu,\,\pi/2,\,\Phi)d\nu=(D/R^2)K_2^0(n_1)d\nu, \tag{40a}$$

$$I_\Phi^0(\nu,\,\pi/2,\,\Phi)d\nu=(D|R^2)K_1^0(n_1)d\nu. \tag{40b}$$

The intensities in the plane containing the initial electron beam are obtained in a similar manner from Eqs. (35), namely

$$I_\Theta^0(\nu,\,\Theta,\,0)=(D/R^2)d\nu[K_1^0(n_1)\cos^2\Theta+K_2^0(n_1)\sin^2\Theta], \tag{41a}$$

$$I_y^0(\nu,\,\Theta,\,0)=(D/R^2)d\nu K_1^0(n_1). \tag{41b}$$

The sum of the expressions (40) or (41) give the total intensities in the respective planes. From the intensity formulae just given it is easy to determine the degree of polarization.

§7. Degree of Polarization

The polarization characteristics of the radiation in the continuous spectrum has been the subject of considerable investigation. A number of theories have been given which sought in particular to account for the high degree of polarization at the short wave-length limit. The first wave mechanical calculation of degree of polarization at the short wave-length limit was made by Oppenheimer.[9]

The degree of polarization can easily be obtained in terms of the intensity formulae of the preceding section with the help of the so-called depolarization ratio d. This is the ratio of the intensity of the radiation whose electric vector lies in the plane at right angles to the direction of the initial electron beam to the intensity whose electric vector is parallel to the initial electron beam. Thus

$$d=I_\Phi(\nu,\,\pi/2,\,\Phi)/I_z(\nu,\,\pi/2,\,\Phi).$$

In terms of d, the degree of polarization P in percent is

$$P=100(1-d)/(1+d). \tag{42}$$

[9] J. R. Oppenheimer, Zeits. f. Physik **55**, 725 (1929).

From Eqs. (34), the above value of d becomes

$$d=K_1(n_1, n_2)/K_2(n_1, n_2), \tag{43}$$

so that

$$P=100[K_2(n_1, n_2)-K_1(n_1, n_2)/K_2(n_1, n_2)+K_1(n_1, n_2)]. \tag{44}$$

If the degree of polarization for the short wave-length limit be denoted by P^0 then:

$$P^0=100[K_2^0(n_1)-K_1^0(n_1)/K_2^0(n_1)+K_1^0(n_1)]. \tag{45}$$

It appears superfluous to develop expressions for the degree of polarization of the radiation in directions other than in the plane perpendicular to the initial electron beam since they can readily be obtained from the preceding intensity formulae for any special case.

§8. Electron Scattering

In measurements on electron scattering by a nucleus, one is interested in the radiation emitted in connection with the scattering process only insofar as the radiative forces effect the angular distribution of the electrons. The probable number of electrons scattered into the solid angular region between ω and $\omega+d\omega$ with energies between $\frac{1}{2}mv_2^2$ and $\frac{1}{2}mv_2^2+dE$ with the radiative forces taken into account is found by adding the expressions (30a) and (30b) and integrating over all the directions of emission of the photons, i.e.,

$$N(00k_1|\alpha\beta k_2)dEd\omega=d\nu d\omega\int\{P_\Theta(00k_1\|\alpha\beta k_2|\nu\Theta\Phi)+P_\Phi(00k_1\|\alpha\beta k_2|\nu\Theta\Phi)\}d\Omega.$$

Substituting the actual expressions for the P, the integration over all solid angles can be performed without difficulty giving

$$N(00k_1|\alpha\beta k_2)dEd\omega=(8\pi C/3\hbar)\{|(00k_1|x|\alpha\beta k_2)|^2+|(00k_1|y|\alpha\beta k_2)|^2+|(00k_1|z|\alpha\beta k_2)|^2\}d\omega dE.$$

Since we are not primarily concerned with electron scattering we shall not discuss the above scattering formula any further. For further details the reader is referred to reference 2, page 152, where the form of the function N is given for certain interesting limiting cases.

§9. General Remarks

In the preceding sections the general formulae for the spacial intensity distribution, polarization, etc., of the continuous x-ray radiation have been developed which are entirely valid when $\beta_1=v_1/c\ll 1$. No comparison with existing experimental results will be made nor graphical representations of the formulae derived, as this will be done in Part II where similar relativistic formulae will be available and the comparisons can be made over the complete range of β_1. In this part an effort has been made to present as complete general formulae as is possible from the non-relativistic theory in a convenient form for numerical calculation.

In applying the formulae which concern the short wave-length limit, a certain amount of caution should be exercised since a direct comparison of these formulae with experimental results may not be justified. The reason for this is that the intensity changes quite rapidly in a region near $k_2=0$, so that if the wave-length interval of the radiation examined is not very small the intensity cannot be compared with the formulae obtained for the limit $k_2=0$. When the wave-length interval is not sufficiently small, the general intensity formulae should be expanded about a point k_2 which gives a wave-length in the interval observed and the result integrated over this range.

§10. Mathematical Appendix

Appendix A

The validity of Eq. (8) namely

$$(\hbar/mi)\int u(n\xi|q)\ \text{grad}\ u^*(n'\xi'|q)dq=[\omega(n\xi)-\omega(n'\xi')]\int u(n\xi|q)\mathfrak{r}u^*(n'\xi'|q)dq$$

can be briefly established with the help of the current vector

$$\mathbf{S}(n\xi|n'\xi')=(e\hbar/2mi)[\psi(n\xi|q)\ \text{grad}\ \psi^*(n'\xi')-\psi^*(n'\xi')\ \text{grad}\ \psi(n\xi)] \tag{A1}$$

associated with the transition $n\xi\rightarrow n'\xi'\cdot\psi(n\xi|q)$ is the solution of Eq. (1) with the time factor included so that

$$\psi(n\xi|q)=e^{i\omega(n\xi)}u(n\xi|q).$$

Adding the expression $(e\hbar/2mi)[\psi(n\xi|q)\ \text{grad}\ \psi^*(n'\xi'|q)+\psi^*(n'\xi')\ \text{grad}\ \psi(n\xi|q)]$ whose integral over the coordinates vanishes, to (A1) and integrating over the q's we have

$$e^{i[\omega(n\xi)-\omega(n'\xi')]}\int u(n\xi|q)\ \text{grad}\ u^*(n'\xi'|q)dq=(mi/e\hbar)\int\mathbf{S}(n\xi|n'\xi')dq,$$

but

$$\int\mathbf{S}(n\xi|n'\xi')dq=-\int\mathfrak{r}\ \text{div}\ \mathbf{S}(n\xi|n'\xi')dq$$

and from the equation of continuity

$$e\partial\psi\psi^*/\partial t=-\text{div}\ \mathbf{S}$$

we have

$$e[\omega(n\xi)-\omega(n'\xi')]e^{i[\omega(n\xi)-\omega(n'\xi')]}\int u(n\xi|q)u^*(n'\xi'|q)dq=-\int\text{div}\ \mathbf{S}(n\xi|n'\xi')dq$$

and finally

$$(\hbar/mi)\int u(n\xi|q)\ \text{grad}\ u^*(n'\xi'|q)dq=[\omega(n\xi)-\omega(n'\xi')]\int u(n\xi|q)\mathfrak{r}u^*(n'\xi'|q)dq.$$

Appendix B

In order to obtain the value of

$$\int_0^{2\pi}d\beta\int_0^{\pi}\left|\left(00k_1\left|\begin{matrix}x\\y\end{matrix}\right|\alpha\beta k_2\right)\right|^2\sin\alpha d\alpha$$

it will be necessary to evaluate an integral of the following type, namely

$$\frac{K_1}{|n_1(1-n_2)|^2}=\int_0^{2\pi}d\beta\left\{\begin{matrix}\cos^2\beta\\\sin^2\beta\end{matrix}\right\}\int_0^{\pi}F(1+n_1;2-n_2;2;w(\alpha))F(1-n_1;2-n_2;2;w(\alpha))\sin^3\alpha d\alpha. \tag{B1}$$

Introducing the new variable $\xi=\cos\alpha$, so that

$$w(\alpha)=[4k_1k_2/(k_1+k_2)^2]\cos^2\alpha/2=\tfrac{1}{2}s(1+\xi) \tag{B2}$$

and performing the integration over β, (B1) becomes

$$\pi\int_{-1}^{+1}F(1+n_1;2-n_2;2;\tfrac{1}{2}s(1+\xi))F(1-n_1;2+n_2;2;\tfrac{1}{2}s(1+\xi))(1-\xi^2)d\xi. \tag{B3}$$

In order to proceed further it is convenient to expand $(1-\xi^2)^{\frac{1}{2}}F$ in a series of associated Legendre

polynomials thus

$$(1-\xi^2)^{\frac{1}{4}}F(1+n_1;\,2-n_2;\,2;\,\tfrac{1}{2}s(1+\xi))=\sum_{l=1}^{\infty}a_lP_l^1(\xi). \tag{B4}$$

On account of the orthogonality of these polynomials the coefficients a_l are determined by the expression

$$a_l=\frac{2l+1}{2}\frac{(l-1)!}{(l+1)!}\int_{-1}^{+1}F(1+n_1;\,2-n_2;\,2;\,\tfrac{1}{2}s(1+\xi))(1-\xi^2)^{\frac{1}{4}}P_l^1(\xi)d\xi. \tag{B5}$$

Making use of the relation $P_l^1(\xi)=(1-\xi^2)^{\frac{1}{4}}(d/d\xi)P_l(\xi)$ and integrating once by parts remembering at the same time that

$$\int F(\alpha,\,\beta,\,\gamma,\,x)dx=[(\gamma-1)/(\alpha-1)(\beta-1)]F(\alpha-1;\,\beta-1;\,\gamma-1;\,x)$$

the integral (B5) becomes

$$a_l=-\frac{2l+1}{2}\frac{1}{l(l+1)}\cdot\frac{2}{s}\frac{1}{n_1(1-n_2)}\int_{-1}^{+1}F(n_1;\,1-n_2;\,1;\,\tfrac{1}{2}s(1+\xi))\left[\frac{d}{d\xi}(1-\xi^2)\frac{d}{d\xi}P_l(\xi)\right]d\xi.$$

From the differential equation satisfied by $P_l(\xi)$ we have

$$\frac{d}{d\xi}(1-\xi^2)\frac{d}{d\xi}P_l(\xi)=-l(l+1)P_l(\xi).$$

Using this expression the expression for a_l becomes

$$a_l=\frac{2l+1}{s}\frac{1}{n_1(1-n_2)}\int_{-1}^{+1}F(n_1;\,1-n_2;\,1;\,\tfrac{1}{2}S(1+\xi))P_l(\xi)d\xi. \tag{B6}$$

Instead of evaluating this integral directly we shall evaluate the more general integral

$$G_l(\alpha,\,\beta,\,s)=\int_{-1}^{+1}F(\alpha,\,\beta,\,1,\,\tfrac{1}{2}s(1+\xi))P_l(\xi)d\xi. \tag{B7}$$

The arbitrary quantities α and β have nothing to do with the angles α and β used before. Only a brief use will be made of them here so that no confusion will arise.

It is convenient to make use of Rodriques' formula for $P_l(\xi)$ namely

$$P_l(\xi)=(1/2^l l!)(d^l/d^l\xi)(\xi^2-1)^l$$

and the general formula for the lth derivative of the hypergeometric function, namely

$$\frac{d^l}{d\xi^l}F(\alpha,\,\beta,\,1,\,\tfrac{1}{2}s(1+\xi))=\frac{\Gamma(\alpha+l)}{\Gamma(\alpha)}\frac{\Gamma(\beta+l)}{\Gamma(\beta)}\frac{1}{\Gamma(l+1)}\left(\frac{s}{2}\right)^l F(\alpha+l;\,\beta+l;\,l+1;\,\tfrac{1}{2}s(1+\xi)).$$

If these expressions are used in (B7) and l partial integrations are performed, the integral becomes

$$(-1)^l\frac{\Gamma(\alpha+l)\Gamma(\beta+l)}{\Gamma(\alpha)\Gamma(\beta)\Gamma(l+1)}\left(\frac{s}{2}\right)^l\frac{1}{2^l l!}\int_{-1}^{+1}F(\alpha+l;\,\beta+l;\,1+l;\,\tfrac{1}{2}s(1+\xi))(\xi^2-1)^l d\xi.$$

It is convenient to substitute the series expression for the hypergeometric function, namely

$$F(\alpha+l;\,\beta+l;\,1+l;\,\tfrac{1}{2}s(1+\xi))=\frac{\Gamma(1+l)}{\Gamma(\alpha+l)\Gamma(\beta+l)}\sum_{\rho=0}^{\infty}\frac{\Gamma(\alpha+l+\rho)\Gamma(\beta+l+\rho)}{\Gamma(1+l+\rho)\rho!}\cdot\left(\frac{s}{2}\right)^\rho(1+\xi)^\rho$$

in the above integral and invert the order of integration in which case we have

$$(-1)^l\frac{1}{\Gamma(\alpha)\Gamma(\beta)}\cdot\left(\frac{s}{2}\right)^l\frac{1}{2^l l!}\sum_{\rho=0}^{\infty}\frac{\Gamma(\alpha+l+\rho)\Gamma(\beta+l+\rho)}{\Gamma(1+l+\rho)\rho!}\left(\frac{s}{2}\right)^\rho\int_{-1}^{+1}(1+\xi)^\rho(\xi^2-1)^l d\xi. \tag{B8}$$

The above integral can be written in the form

$$(-1)^l\int_{-1}^{+1}(1+\xi)^{l+\rho}(1-\xi)^l d\xi$$

which is an integral representation of the beta-function except for a factor, hence we have

$$(-1)^l\int_{-1}^{+1}(1+\xi)^{l+\rho}(1-\xi)^l d\xi=(-1)^l 2^{2l+\rho+1}B(l+\rho+1;\,l+1)=(-)^l 2^{2l+\rho+1}\frac{\Gamma(l+\rho+1)\Gamma(l+1)}{\Gamma(2l+\rho+2)}.$$

The expression (B8) then becomes

$$\frac{2}{\Gamma(\alpha)\Gamma(\beta)}s^l\sum_{\rho=0}^{\infty}\frac{\Gamma(\alpha+l+\rho)\Gamma(\beta+l+\rho)}{\Gamma(2l+\rho+2)P!}s^\rho$$

or

$$G_l(\alpha,\,\beta,\,s)=\frac{2s^l}{\Gamma(\alpha)\Gamma(\beta)}\frac{\Gamma(\alpha+l)\Gamma(\beta+l)}{\Gamma(2l+2)}F(\alpha+l;\,\beta+l;\,2l+2;\,s). \tag{B9}$$

The integral (B7) is therefore expressible in terms of another hypergeometric function and we have succeeded in evaluating the coefficients a_l which are given by the expression

$$a_l=\frac{2l+1}{s}\cdot\frac{2s^l\Gamma(n_1+l)\Gamma(1-n_2+l)}{\Gamma(1+n_1)\Gamma(2-n_2)\Gamma(2l+2)}F(n_1+l;\,1+l-n_2;\,2l+2;\,s). \tag{B10}$$

The integral (B3) can now be evaluated in terms of a series, by making use of the series (B4). Doing this we have

$$\frac{K_1}{|n_1(1-n_2)!|^2}=\pi\int_{-1}^{+1}|F(1+n_1;\,2-n_2;\,2;\,\tfrac{1}{2}s(1+\xi))|^2(1-\xi^2)d\xi=\pi\int_{-1}^{+1}\sum_{l=1}^{\infty}a_l P_l^1(\xi)\cdot\sum_{l'=1}^{\infty}a_{l'}{}^* P_{l'}{}^1(\xi)d\xi.$$

Inverting the order of integration and summation and again using the orthogonality of the P's, K_1 becomes

$$\frac{K_1}{|n_1(1-n_2)|^2}=\pi\sum_{l=1}^{\infty}\frac{2}{2l+1}\frac{(l+1)!}{(l-1)!}a_l a_l{}^*.$$

Putting in the expression (B10) found for a_l this becomes

$$K_1(n_1n_2)=(2\pi/s^2)\sum_{l=1}^{\infty}l(l+1)(2l+1)\,|G_l(n_1,\,1-n_2,\,s)|^2$$

$$=\frac{8\pi}{s^2|\Gamma(n_1)|^2|\Gamma(1-n_2)|^2}\sum_{l=1}^{\infty}l(l+1)\frac{|\Gamma(n_1+l)|^2|\Gamma(1-n_2+l)|^2}{\Gamma(2l+1)\Gamma(2l+2)}s^{2l}$$

$$\times|F(n_1+l,\,1+l-n_2,\,2l+2;\,s)|^2. \tag{B11}$$

This series appears somewhat complicated but as we shall now show it converges rather rapidly for $s<1$. The maximum value that s can assume in any physical case is $s=1$. By referring to Eq. (B2) this happens when $k_1=k_2$, or $v_1=v_2$, which means at the long wave-length limit of the spectrum, which is not of particular interest.

In order to establish the convergence of (B11) and to get some idea of the order of magnitude of the individual terms, it is desirable to find a dominant series. This can readily be done by making use of the following definite integral representations for the hypergeometric functions:

$$F(-n_1+l,\ 1+l+n_2,\ 2l+2;\ s)=\frac{\Gamma(2l+2)}{\Gamma(1+l+n_2)\Gamma(1+l-n_2)}\int_0^1 t^{n_2+l}(1-t)^{l-n_2}(1-st)^{n_1-l}dt,$$

$$F(n_1+l,\ 1+l-n_2,\ 2l+2;\ s)=\frac{\Gamma(2l+2)}{\Gamma(n_1+l)\Gamma(2+l-n_1)}\int_0^1 t^{n_1+l-1}(1-t)^{1+l-n_1}(1-st)^{n_2-l-1}dt.$$

From these expressions we can conclude that

$$|F|\leq\frac{\Gamma(2l+2)}{|\Gamma(1+l-n_2)|^2}\int_0^1|t^{n_2+l}(1-t)^{l-n_2}(1-st)^{n_1-l}|dt=\frac{\Gamma(2l+2)}{|\Gamma(1+l+n_2)|^2}\int_0^1 t^l\left(\frac{1-t}{1-st}\right)^l dt$$

and

$$|F^*|\leq\frac{\Gamma(2l+2)}{|\Gamma(n_1+l)\Gamma(2+l-n_1)|}\int_0^1 t^{l-1}\left(\frac{1-t}{1-st}\right)^{l+1}dt.$$

In the range $0\leq t\leq 1$ the factor $(1-t/1-st)$ remains positive and has its greatest value at $t=0$ which is 1. Consequently

$$\int_0^1 t^l\left(\frac{1-t}{1-st}\right)^l dt\leq\int_0^1 t^l dt=\frac{1}{l+1}\qquad\text{and}\qquad\int_0^1 t^{l-1}\left(\frac{1-t}{1-st}\right)^{l+1}dt\leq\int_0^1 t^{l-1}dt=\frac{1}{l}$$

so that

$$|F(-n_1+l;\ 1+l+n_2;\ 2l+2;\ s)|\leqq\frac{\Gamma(2l+2)}{|\Gamma(1+l-n_2)|^2}\cdot\frac{1}{l+1},$$

$$|F(n_1+l;\ 1+l-n_2;\ 2l+2;\ s)|\leq\frac{\Gamma(2l+2)}{|\Gamma(n_1+l)\Gamma(2+l-n_1)|}\cdot\frac{1}{l}.$$

Placing these expressions in the series (B11), we have the dominant series:

$$\sum_{l=1}^{\infty}\frac{(2l+1)}{|(1+l-n_1)(l-n_1)|}s^{2l}=\sum_{l=1}^{\infty}\frac{(2l+1)s^{2l}}{[(1+l)^2+|n_1|^2]^{\frac{1}{2}}[l^2+|n_1|^2]^{\frac{1}{2}}}.\tag{B12}$$

It can be readily established that this series converges absolutely for $s^2<1$. In fact even if $|n_1|=0$ the individual terms are less than $(2s^{2l}/l)$.

We still have to evaluate the integrals involved in the integral

$$\int_0^{2\pi}d\beta\int_0^{\pi}|(00k_1|z|\alpha\beta k_2)|^2\sin\alpha d\alpha,$$

which, by referring to Eq. (21), may be written

$$K_2=\int_0^{2\pi}d\beta\int_{-1}^{+1}|(n_2-n_1\xi)F(1+n_1;\ 1-n_2;\ 1;\ \tfrac{1}{2}s(1+\xi))$$
$$+(1+\xi)n_1n_2F(1+n_1;\ 1-n_2;\ 2;\ \tfrac{1}{2}s(1+\xi))|^2d\xi,\tag{B13}$$

where the substitution given in (B2) has been made. It will be advantageous to express the integrand in terms of hypergeometric functions whose third parameter is unity in such a way that the variable ξ occurs only as the variable in the hypergeometric function. This can be accomplished by making use of recurrence relations between the hypergeometric functions. In particular, from the relation

$$(\alpha/\gamma)xF(\alpha+1;\ \beta+1;\ \gamma+1;\ x)=F(\alpha;\ \beta+1;\ \gamma;\ x)-F(\alpha;\ \beta;\ \gamma;\ x)$$

we have

$$n_1 n_2(1+\xi)F(1+n_1;\,1-n_2;\,2;\,\tfrac{1}{2}s(1+\xi))=(2n_2/s)[F(n_1;\,1-n_2;\,1;\,\tfrac{1}{2}s(1+\xi))-F(n_1;\,-n_2;\,1;\,\tfrac{1}{2}s(1+\xi))]. \quad \text{(B14)}$$

Also with the help of the relation

$$\alpha(1-x)F(\alpha+1;\,\beta;\,\gamma;\,x)=(\gamma-\beta)F(\alpha;\,\beta-1;\,\gamma;\,x)-(\gamma-\alpha-\beta)F(\alpha;\,\beta;\,\gamma;\,x)$$

and after making certain simplifications we have

$$(n_2-n_1\xi)F(1+n_1;\,1-n_2;\,1;\,\tfrac{1}{2}s(1+\xi))=[n_1+n_2-(2n_1/s)]F(1+n_1;\,1-n_2;\,1;\,\tfrac{1}{2}s(1+\xi))+(2n_1/s)F(n_1;\,1-n_2;\,1;\,\tfrac{1}{2}s(1+\xi))-(2n_2/s)[F(n_1;\,1-n_2;\,1;\,\tfrac{1}{2}s(1+\xi))-F(n_1;\,-n_2;\,1;\,\tfrac{1}{2}s(1+\xi))]. \quad \text{(B15)}$$

The integrand of (B13) is obtained by adding the relations (B14) and (B15). When this sum is substituted in (B13) and the integration with respect to β performed we have

$$K_2=2\pi\int_{-1}^{+1}|[n_1+n_2-(2n_1/s)]F(1+n_1;\,1-n_2;\,1;\,\tfrac{1}{2}s(1+\xi))+(2n_1/s)F(n_1;\,1-n_2;\,1;\,\tfrac{1}{2}s(1+\xi))|^2 d\xi. \quad \text{(B16)}$$

With the help of (B7) and (B9) we can expand the two hypergeometric functions in the integrand thus

$$F(1+n_1,\,1-n_2,\,1,\,\tfrac{1}{2}s(1+\xi))=\sum_{l=0}^{\infty}\tfrac{1}{2}(2l+1)G_l(1+n_1,\,1-n_2,\,s)P_l(\xi)$$

and

$$F(n_1,\,1-n_2,\,1,\,\tfrac{1}{2}s(1+\xi))=\sum_{l=0}^{\infty}\tfrac{1}{2}(2l+1)G_l(n_1,\,1-n_2,\,s)P_l(\xi).$$

Substituting these expressions in (B16), inverting the order of summation and integration and observing the orthogonality of the P's we have

$$K_2=2\pi\left\{\begin{aligned}&|[n_1+n_2-(2n_1/s)]|^2\sum_{l=0}^{\infty}\tfrac{1}{2}(2l+1)\,|G_l(1+n_1,\,1-n_2,\,s)|^2\\&+[n_1+n_2-(2n_1/s)](2n_1/s)^*\sum_{l=0}^{\infty}\tfrac{1}{2}(2l+1)G_l(1+n_1,\,1-n_2,\,s)G_l^*(n_1,\,1-n_2,\,s)\\&+[n_1+n_2-(2n_1/s)]^*(2n_1/s)\sum_{l=0}^{\infty}\tfrac{1}{2}(2l+1)G_l^*(1+n_1,\,1-n_2,\,s)G_l(n_1,\,1-n_2,\,s)\\&+|(2n_1/s)|^2\sum_{l=0}^{\infty}\tfrac{1}{2}(2l+1)\,|G_l(n_1,\,1-n_2,\,s)|^2.\end{aligned}\right\}$$

Corresponding terms in each series may be combined to form one series since for $s^2<1$ all the series converge absolutely, thus

$$K_2=\frac{2\pi|n_1|^2}{s^2}\sum_{l=0}^{\infty}\frac{2l+1}{2}|[s+(n_2s/n_1)-2]G_l(1+n_1,\,1-n_2,\,s)+2G_l(n_1,\,1-n_2,\,s)|^2. \quad \text{(B17)}$$

Appendix C

Finding expressions for the energy radiated at the short wave-length limit involves taking the limit as $k_2 \to 0$. To do this it is necessary to determine the limit as $\beta \to \infty$ and $s \to 0$ in such a way that $\lim \beta s \to t$ of $G_l(\alpha, \beta, s)$. From Eq. (B9) we have

$$\lim_{\substack{\beta\to\infty \\ s\to 0 \\ \beta s\to t}} G_l(\alpha, \beta, s) = \frac{2\Gamma(\alpha+l)}{\Gamma(\alpha)\Gamma(2l+2)} \lim s^l \frac{\Gamma(\beta+l)}{\Gamma(\beta)} \lim F(\alpha+l, \beta+l, 2l+2, s).$$

It is well known that

$$\lim_{\substack{\beta\to\infty \\ s\to 0 \\ \beta s\to t}} F(\alpha+l, \beta+l, 2l+2, s) = F(\alpha+l, 2l+2, t),$$

where $F(\alpha+l, 2l+2, t)$ is the confluent hypergeometric function defined by

$$F(\alpha, \gamma, x) = 1 + \frac{\alpha}{\gamma}x + \frac{\alpha(\alpha+1)}{\gamma(\gamma+1)}\frac{x^2}{2!} + \cdots.$$

Also

$$\lim_{\substack{\beta\to\infty \\ s\to 0}} \frac{s^l\Gamma(\beta+l)}{\Gamma(\beta)} = s(\beta+l-1)s(\beta+l-2)s(\beta+l-3)\cdots s\beta\frac{\Gamma(\beta)}{\Gamma(\beta)} = t^l.$$

Hence the limit sought is

$$\lim_{\substack{\beta\to\infty \\ s\to 0 \\ \beta s\to t}} G_l(\alpha, \beta, s) = \frac{2\Gamma(\alpha+l)}{\Gamma(\alpha)\Gamma(2l+2)} t^l F(\alpha+l, 2l+2, t). \tag{C1}$$

The specific G's required are $G_l(-n_1, 1+n_2, s)$ an $G_l(1-n_1, 1+n_2, s)$. Since $s = 4k_1k_2/(k_1+k_2)^2$ and $\beta = 1+n_2 = 1+(Z/iak_2)$, then

$$\lim \beta s = t = \lim_{k_2\to 0} \frac{4k_1k_2}{(k_1+k_2)^2}\left(1+\frac{Z}{iak_2}\right) = \frac{4Z}{iak_1} = 4n_1.$$

Consequently

$$\lim_{k_2\to 0} G_l(-n_1, 1+n_2, s) = \frac{2\Gamma(-n_1+l)}{\Gamma(-n_1)\Gamma(2l+2)}(4n_1)^l F(-n_1+l, 2l+2, 4n_1), \tag{C2}$$

$$\lim_{k_2\to 0} G_l(1-n_1, 1+n_2, s) = \frac{2\Gamma(1-n_1+l)}{\Gamma(1-n_1)\Gamma(2l+2)}(4n_1)^l F(1-n_1+l, 2l+2, 4n_1). \tag{C3}$$

Appendix D

To obtain the limits

$$\lim_{k_2\to 0} C|B|^2 K_1(n_1, n_2) \qquad \text{and} \qquad \lim_{k\to 0} C|B|^2 K_2(n_1 n_2)$$

it is convenient to proceed as indicated by the following expressions.

$$\lim_{k_2\to 0} C|B|^2 K_{1,\,2}(n_1, n_2) = \lim_{k_2\to 0} (C|B|^2/s^2) \lim_{k_2\to 0} s^2 K_{1,\,2}(n_1 n_2).$$

The limit as $k_2 \to 0$ of $C|B|^2/s^2$ presents no difficulty since

$$\lim_{k_2 \to 0} \frac{C|B|^2}{s^2} = D = \frac{e^2 |n_1|^2 \hbar^2}{2\pi (2m)^2 c^3 (e^{2|n_1|\pi} - 1)}. \tag{D1}$$

Since $s^2 K_1(n_1, n_2)$ is represented by the uniformly convergent series

$$s^2 K_1(n_1 n_2) = 2\pi \sum_{l=1}^{\infty} l(l+1)(2l+1) |G_l(n_1, 1-n_2, s)|^2,$$

then

$$\lim_{k_2 \to 0} s^2 K_1(n_1 n_2) = 2\pi \sum_{l=1}^{\infty} l(l+1)(2l+1) \lim_{k_2 \to 0} |G_l(n_1, 1-n_2, s)|^2.$$

The limit of the G_l has been determined in note *C*. Using Eq. (C2) we have

$$\lim_{k_2 \to 0} s^2 K_1(n_1 n_2) = \frac{8\pi}{|\Gamma(n_1)|^2} \sum_{l=1}^{\infty} \frac{l(l+1)}{\Gamma(2l+1)\Gamma(2l+2)} |\Gamma(n_1+l)(-4n_1)^l F(n_1+l, 2l+2, -4n_1)|^2.$$

Similarly

$$\lim_{k_2 \to 0} s^2 K_2(n_1 n_2) = 16\pi |n_1|^2 \sum_{l=0}^{\infty} \frac{|4n_1|^{2l}}{\Gamma(2l+1)\Gamma(2l+2)} \left| \frac{\Gamma(1+n_1+l)}{\Gamma(1+n_1)} F(1+n_1+l, 2l+2, -4n_1) + \frac{\Gamma(n_1+l)}{\Gamma(n_1)} F(n_1+l, 2l+2, -4n_1) \right|^2.$$

From these expressions the desired limits can be found.