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Generation of coherent x rays by a relativistic charged particle traveling through a crystal

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The radiation due to the coherent excitation of the electric dipole moments of the atoms in a crystal has been studied. These dipole moments are induced by the electric field of a relativistic charged particle traveling through the crystal. In this context, coherent excitation refers to the correlation of the phases of the dipole moments which are induced by a single relativistic charged particle. The phases of dipole moments which are induced by different charged particles are, of course, uncorrelated. The electric field of the incident relativistic charged particle is analyzed into its frequency spectrum and the effect of each frequency component on the crystal is determined. Expressions for the fields far away from the crystal and the radiated energy are derived for transitions between bound states, for transitions from a bound state into the continuum, and for the case where the frequency components are much larger than the ionization potentials of the atoms divided by Planck's constant. It is shown that the generated coherent radiation is emitted in the Bragg directions. Moreover, the polar and azimuthal angular spreads, as well as the frequency width, divided by the frequency of radiation, are of the order $1/\gamma$, where $\gamma = (1-\beta^2)^{-1/2}$, $\beta = v/c$, v being the velocity of the incident charged particle and c being the velocity of light. A comparison is made with x-ray diffraction and it is shown that, for a small crystal, the radiated energy per incident charged particle is less than the radiated energy per incident photon by a factor approximately equal to $Q^2/\hbar c$, where Q is the charge of the particle and $\hbar$ is Planck's constant divided by 2π.

I. INTRODUCTION

In contrast to previous investigations of coherent bremsstrahlung,[1,2] this paper is concerned with the radiation due to the coherent excitation of the electric dipole moments of the atoms in a crystal. These dipole moments are induced by the electric field of a relativistic charged particle traveling through the crystal. In this context, coherent excitation refers to the correlation of the phases of the dipole moments which are induced by a single relativistic charged particle. The phases of dipole moments which are induced by different charged particles are, of course, uncorrelated. In this paper, the characteristics of the emitted coherent radiation will be presented.

The following approach to the problem will be used. The electromagnetic field of the incident relativistic charged particle will be analyzed into its frequency spectrum and the effect of each Fourier component on the crystal will be determined. Certain similarities are expected then in this work with the diffraction of x-rays in crystals. For example, the maximum intensity of radiation occurs approximately at frequencies and directions for which the Bragg condition is satisfied. The symmetry properties of the crystal then specify these frequencies and directions. Thus, the radiation induced by the relativistic charged particle takes place approximately in the Bragg directions, the deviation from these directions being smaller, the larger γ is. Here, $\gamma = (1-\beta^2)^{-1/2}$, where $\beta = v/c$, v is the velocity of the relativistic charged particle, and c is the velocity of light. Moreover, since the wavelength of the emitted radiation satisfies approximately Bragg's law, it should be less than $2d$, where d is the distance between adjacent parallel lattice planes. On the other hand, the frequency width divided by the average frequency, as well as the polar and azimuthal angular spreads are of the order $1/\gamma$.

Transitions between bound states and from bound states into the continuum will be considered. The former case applies for frequency components smaller than the ionization potentials, divided by $\hbar$, of electrons in the inner shells of the atoms in the crystal, while the latter case applies for frequency components which are larger ($\hbar = h/2\pi$ and h is Planck's constant). In either of the above cases, it will be assumed that the wavelength of the emitted radiation is much larger than the dimensions of each atom, so that the retardation effects within the atoms will be neglected. It will be shown that the radiated energy in the former type of transition is, in general, less than that in the latter type, but both types lead to the same amount of radiation if γ becomes much larger than unity. Another case that will be considered is that in which the frequency components are much larger than the ionization potentials of the electrons, divided by $\hbar$. Under these conditions, the atomic polarizability is the same as that of free electrons. Thus, it is the actual density of the "electron cloud" surrounding each atom in its ground state that will interact with the electric field of the incident relativistic

charged particle and no transition from the ground state to an excited state is involved in the process.[3] Moreover, since the wavelength of the radiation is of the same order of magnitude as the dimensions of the atoms, the retardation that may take place within each atom will be included. The last case can be compared directly with x-ray diffraction. For a small crystal, the radiated energy per incident charged particle is less than the radiated energy per incident photon by a factor approximately equal to $Q^2/\hbar c$, where Q is the charge of the particle. In the presence of high-current electron beams the generation of coherent x-rays should be an observable effect.

II. MODEL

The crystal is in the form of a slab of width L. The z axis is chosen normal to the two surfaces of the slab and the origin of the coordinate system is chosen so that these plane surfaces lie at $z = \pm\frac{1}{2}L$. A charged particle moves with constant velocity v along the z axis, in the positive direction. The origin of time is chosen so that at time $t = 0$ the particle is at $z = 0$. Its electric field, in the frequency domain, is equal to[4]

$$\vec{E}_0(\vec{R}, \omega) = -\frac{2Q}{\beta c}\left(\vec{\nabla}_\rho + i\frac{\lambda_0}{\gamma}\vec{z}\right)K_0(\lambda_0\rho)e^{i(\omega/\beta c)z}, \quad (1)$$

where

$$\vec{\nabla}_\rho = \vec{x}\frac{\partial}{\partial x} + \vec{y}\frac{\partial}{\partial y}. \quad (2)$$

The symbols Q, β, γ, and c have already been defined. $K_0(x)$ is the modified Bessel function of order zero, $\lambda_0 = \omega/\gamma\beta c$, and $\vec{x}, \vec{y}, \vec{z}$ are unit vectors along the x, y, z axes, respectively. The position vector $\vec{R}$ in Eq. (1) has cylindrical coordinates (ρ, ϕ, z).

The function $K_0(z)$ has an exponentially decreasing asymptotic behavior.[5] Thus, the distance from the trajectory of the charged particle over which its electric field is large enough to induce radiation by the atoms in the crystal is approximately equal to $l_{\text{eff}} = \gamma\beta\lambda\!\!\!^{-}$, where $\lambda\!\!\!^{-} = c/\omega$. For example, if $\gamma = 100$, which corresponds to electrons with energy 50 MeV, and if $\lambda\!\!\!^{-} = 0.5$ Å, approximately 10^4 atoms per plane normal to the trajectory of the charged particle will contribute to the radiation. In this respect, the crystal does not have to extend more than two or three units of l_{eff} in directions normal to the z axis.

It will be assumed in the following that the amount of energy the charged particle loses is negligible compared to its total energy. In a real situation, however, the particle does lose energy as it travels through the crystal, mostly due to ionization and excitation of the atoms in the crystal and also due to bremsstrahlung. If coherent emission of x rays is to take place, the change in distance due to the change in velocity of the charged particle (since it slows down as it loses energy) should be less than half a wavelength of the emitted radiation. This condition sets an upper limit on the width of the crystal, given by the relation

$$L_{\max} = \left(\gamma^3\beta^2\frac{\frac{1}{2}\lambda}{(1/mc^2)\,\delta\epsilon/\delta x}\right)^{1/2}, \quad (3)$$

where $\lambda = 2\pi\lambda\!\!\!^{-}$, $\delta\epsilon/\delta x$ is the energy lost per unit length and m is the rest mass of the particle. As an example, for Al, $\delta\epsilon/\delta x = 9.57$ MeV/cm when $\gamma = 100$ and the particle is an electron.[6] For $\lambda = 3$ Å, one obtains from the above relation $L_{\max} = 2.8\times10^{-2}$ cm. For heavier elements $\delta\epsilon/\delta x$ is larger and, therefore, $L_{\max}$ becomes smaller than the above value.

Each atom in the crystal has an induced dipole moment equal to

$$\vec{P}_i(\omega) = \alpha_i(\omega)\vec{E}(\vec{R}_i, \omega), \quad (4)$$

where $\vec{R}_i$ is the position of the ith atom, $\vec{E}(\vec{R}_i, \omega)$ is the electric field acting upon it and $\alpha_i(\omega)$ is the atomic polarizability. The expression for $\alpha_i(\omega)$ depends on the relation between the frequency under consideration and the ionization potentials, divided by $\hbar$, of the electrons bound to each atom. Thus, if the frequency component associated with the electric field of the incident charged particle is less than the ionization potentials, divided by $\hbar$, of electrons in the inner shells of the atoms, then only resonant transitions between bound states are possible and the atomic polarizability is equal to[7]

$$\alpha_d(\omega) = \frac{1}{2\pi}\sigma_d(\omega_r)c\frac{\Delta\omega_r}{\omega_r^2 - \omega^2 - i2\omega\Delta\omega_r}, \quad (5)$$

where

$$\sigma_d(\omega_r) = \pi\lambda\!\!\!^{-}_r^{\,2}(A_{21}/\Delta\omega_r). \quad (6)$$

Here, $\sigma_d(\omega_r)$ is the atomic absorption cross section at resonance, ω_r is the resonance frequency of the transition $\lambda\!\!\!^{-}_r = c/\omega_r$, $\Delta\omega_r$ is the broadening of the resonant line, and A_{21} is the spontaneous rate of radiation between the bound states. On the other hand, if frequency components are considered which are larger than the ionization potentials, divided by $\hbar$, of some electrons in the inner shells of the atoms, transitions will occur from a bound state into the continuum. It is shown in Appendix A that the atomic polarizability can be expressed, to a good approximation, in terms of the atomic absorption cross section as follows:

$$\alpha_{\text{cont}}(\omega) = (i/4\pi)(c/\omega)\sigma_{\text{cont}}(\omega), \tag{7}$$

where $\omega > \omega_c$. Here, ω_c is the cutoff frequency associated with the ionization potential I_c of the electrons in some inner shell, which make the transition into the continuum, i.e., $\omega_c = I_c/\hbar$. For simplicity, it has been assumed that the main contribution to the atomic polarizability comes from one particular shell and all the electrons in this shell have approximately the same ionization potential. In Eqs. (5)–(7) any retardation effects within the atoms have been neglected. This is justified if for each atom the inequality $\lambda\!\!\!^{-} \gg a_0/Z^{1/3}$ is satisfied, where a_0 is the Bohr radius and Z is the atomic number. The right-hand side of the above inequality provides a measure of the dimensions of an atom in the Thomas-Fermi model. Finally, if the frequency components under consideration are much larger than the ionization potentials, divided by $\hbar$, of the electrons bound to each atom, then these electrons behave like free charges and, as shown in Appendix B, the atomic polarizability is equal to

$$\alpha_f(\omega) = -(e^2/\mu)[f(\Delta\vec{K})/\omega^2], \tag{8}$$

where

$$f(\Delta\vec{K}) = \int_V n(\vec{r}) e^{-i\Delta\vec{K}\cdot\vec{r}}\, d^3r. \tag{9}$$

Here e, μ are the charge and mass of the electron, $f(\Delta\vec{K})$ is the atomic scattering factor, $n(\vec{r})$ is the electron concentration around the atom and $\Delta\vec{K} = \vec{K} - \vec{K}_0$, where $\vec{K}_0 = (\omega/\beta c)\hat{z}$ and $\vec{K} = (\omega/c)\hat{\vec{R}}$ are the wave vectors associated with the electric field of the incident charged particle and with the generated coherent radiation, respectively. The unit vector $\hat{\vec{R}}$ is directed towards the point of observation outside the crystal. The integration in Eq. (9) is over an infinite volume, while the exponential term in this equation provides any retardation that may occur in the atom, and $f(\Delta\vec{K})$ is so normalized that $f(\Delta\vec{K}=\vec{0}) = Z$, where Z is the atomic number. For a spherically symmetric electron concentration and for a relativistic incident particle with $\gamma \gg 1$, Eq. (9) reduces approximately to[8]

$$f(\Delta K) = 4\pi \int_0^\infty n(r) \frac{\sin \Delta K r}{\Delta K r} r^2\, dr, \tag{10}$$

where $\Delta K = (2/\lambda\!\!\!^{-})\sin\theta$ and (θ, ϕ) are the spherical coordinates of the unit vector $\vec{R}$.

III. RADIATION FIELDS

It will be assumed in the following that the wavelength of the x-ray radiation emitted by the atoms is of the same order of magnitude as the interatomic distances in the crystal. Moreover, it will be assumed that the inequality $|\alpha_i(\omega)|/\lambda\!\!\!^{-3} \ll 1$ is satisfied for all relevant frequencies. In this case, the effective field $\vec{E}(\vec{R}_i, \omega)$ in Eq. (4) may be replaced by the external field $\vec{E}_0(\vec{R}_i, \omega)$, since the electric field at the ith atom, which is due to its neighbors, is negligible in comparison to the external electric field.

Under this assumption, the electromagnetic field of the scattered x-ray radiation at the point of observation $\vec{R}$ outside the crystal is equal to

$$\mathbf{E}(\mathrm{R}, \omega) = \sum_{i=1}^{N} \sum_{j=1}^{M} \alpha_j(\omega) \vec{\nabla}_R \times \vec{\nabla}_R \times [G(\vec{R} - \vec{R}_i - \vec{r}_j; \omega/c) \vec{E}_0(\vec{R}_i + \vec{r}_j, \omega)], \tag{11a}$$

$$\vec{B}(\vec{R}, \omega) = \sum_{i=1}^{N} \sum_{j=1}^{M} \frac{-i\omega}{c} \alpha_j(\omega) \vec{\nabla}_R \times [G(\vec{R} - \vec{R}_i - \vec{r}_j; \omega/c) \vec{E}_0(\vec{R}_i + \vec{r}_j, \omega)], \tag{11b}$$

where

$$G(\vec{R}; K) = e^{iKR}/R, \tag{12}$$

is the retarded Green's function and $R = |\vec{R}|$. Here, N is the number of unit cells in the crystal, while the vector $\vec{R}_i$ determines the position of the ith cell. Also, M is the number of atoms in each cell. The location of the jth atom in a unit cell, e.g., the ith cell, is determined by the vector $\vec{r}_j$ whose origin lies at the position where the vector $\vec{R}_i$ ends. Now, use will be made of the identity

$$\sum_{i=1}^{N} \sum_{j=1}^{M} \alpha_j(\omega) f(\vec{R}_i + \vec{r}_j) = \frac{1}{V_c} \sum_{\vec{G}} \sum_{j=1}^{M} \alpha_j(\omega) \int_V f(\vec{R}' + \vec{r}_j) e^{i\vec{G}\cdot\vec{R}'}\, d^3R', \tag{13}$$

which reflects the periodicity of the crystal. The summation on the right-hand side of the above identity is over all vectors $\vec{G}$ of the reciprocal lattice, V is the volume of the crystal, V_c is the volume of the unit cell, and $f(\vec{R})$ is any function of $\vec{R}$. Moreover, since the radiation field far away from the crystal is of interest, use will be made of the far-field approximation of the retarded Green's function, which is given by the expression

$$G(\mathrm{R} - \mathrm{R}'; \omega/c) = [e^{i(\omega R/c)}/R]\, e^{-\omega \hat{\vec{R}}\cdot\vec{R}'/c}. \tag{14}$$

The unit vector $\hat{\vec{R}}$ is in the direction of the point of observation $\vec{R}$. Finally, it will be assumed that there is no overlap in the radiation pattern from terms with different $\vec{G}$ on the right-hand side of Eq. (13), so that each term can be treated independently. With the help of Eqs. (11), (13),

and (14) the following expressions are obtained for the scattered x-ray radiation fields for a particular vector $\vec{G}$

$$\vec{E}_{\rm rad}(\vec{R},\omega)\sim\chi_{\vec{G}}(\omega)\left(\frac{\omega}{c}\right)^2\frac{e^{i(\omega/c)R}}{R}\hat{\vec{R}}\times\left[\hat{\vec{R}}\times\vec{\pi}\left(\frac{\omega\hat{\vec{R}}}{c},\omega\right)\right], \tag{15a}$$

$$\vec{B}_{\rm rad}(\vec{R},\omega)\sim\chi_{\vec{G}}(\omega)\left(\frac{\omega}{c}\right)^2\frac{e^{i(\omega R/c)}}{R}\hat{\vec{R}}\times\vec{\pi}\left(\frac{\omega\hat{\vec{R}}}{c},\omega\right), \tag{15b}$$

where

$$\vec{\pi}(\vec{K},\omega)=\int_V\vec{E}_0(\vec{R}',\omega)\,e^{-i(\vec{K}-\vec{G})\cdot\vec{R}'}\,d^3R', \tag{16}$$

and

$$\chi_{\vec{G}}(\omega)=\frac{1}{V_c}\sum_{j=1}^{M}\alpha_j(\omega)\,e^{-i\vec{G}\cdot\vec{r}_j}. \tag{17}$$

When Eq. (1) is substituted into Eq. (16), the integration can be performed analytically[9] and it leads to the relation

$$\vec{\pi}(\vec{K},\omega)=-i\frac{4\pi Q}{\beta^2c^2}\,\omega\frac{(\beta c/\omega)(\vec{K}_\rho-\vec{G}_\rho)+(1/\gamma^2)\vec{z}}{(\vec{K}_\rho-\vec{G}_\rho)\cdot(\vec{K}_\rho-\vec{G}_\rho)+(\omega/\gamma\beta c)^2}\times\frac{\sin(K_z-\omega/\beta c-G_z)\frac{1}{2}L}{\frac{1}{2}(K_z-\omega/\beta c-G_z)}, \tag{18}$$

where $\vec{K}_\rho=K_x\vec{x}+K_y\vec{y}$ and $\vec{G}_\rho=G_x\vec{x}+G_y\vec{y}$.

It is well known that every vector $\vec{G}$ of the reciprocal lattice is normal to a lattice plane of the crystal lattice.[10] Moreover, if the distance between two adjacent lattice planes normal to $\vec{G}$ is d, all the vectors $\vec{G}_n$ of the reciprocal lattice which are normal to $\vec{G}$ have a magnitude equal to

$$|\vec{G}_n|=n(2\pi/d), \tag{19}$$

where n is a positive integer. For each vector $\vec{G}_n$, the values of ω_n, θ_n, ϕ_n may be defined by means of the Bragg condition

$$\vec{K}_n-\vec{K}_{0n}=\vec{G}_n, \tag{20}$$

where

$$\vec{K}_n=(\omega_n/c)\hat{\vec{R}}_n, \tag{21a}$$

$$\vec{K}_{0n}=(\omega_n/c)\vec{z}, \tag{21b}$$

and the unit vector $\hat{\vec{R}}_n$ has spherical coordinates θ_n, ϕ_n. The solution of Eqs. (20) and (21) is as follows:

$$\lambda\!\!\!^{-}_n=2\cos\theta_G/|\vec{G}_n|, \tag{22a}$$

$$\theta_n=\pi-2\theta_G, \tag{22b}$$

$$\phi_n=\phi_G, \tag{22c}$$

where $(|\vec{G}_n|,\pi-\theta_G,\phi_G)$ are the spherical coordinates of the vector $\vec{G}_n$. Also, $\omega_n=c/\lambda\!\!\!^{-}_n$. From Eqs. (19) and (22), Bragg's law follows, i.e., $2d\sin(\theta_n/2)=n\lambda_n$, where $\lambda_n=2\pi\lambda\!\!\!^{-}_n$ and n is a positive integer.

IV. RADIATION PATTERN AND RADIATED ENERGY

The amount of energy radiated per unit frequency interval and per unit solid angle is equal

$$\frac{d^2W}{d\omega\,d\Omega_{\vec{R}}}=\frac{c}{(2\pi)^2}\left(\frac{\omega}{c}\right)^4|\chi_{\vec{G}_n}(\omega)|^2\times[\vec{\pi}(\vec{K},\omega)\cdot\vec{\pi}^*(\vec{K},\omega)-(\vec{\pi}(\vec{K},\omega)\cdot\hat{\vec{R}})(\vec{\pi}^*(\vec{K},\omega)\cdot\hat{\vec{R}})], \tag{23}$$

where $\vec{K}=(\omega/c)\hat{\vec{R}}$ and $\vec{\pi}(\vec{K},\omega)$ is given by Eq. (18). The vector $\vec{G}_n$ as given by Eq. (20), is substituted into Eq. (18). Then, it follows from the new expression for $\vec{\pi}(\vec{K},\omega)$ and from Eq. (23) that

$$\frac{d^2W}{d\omega\,d\Omega_{\vec{R}}}=\frac{4Q^2}{c}\left(\frac{\omega}{c}\right)^2|\chi_{\vec{G}_n}(\omega)|^2\Phi(\theta,\phi,\omega)\times\left[\frac{\sin X(\theta,\omega)L}{X(\theta,\omega)}\right]^2, \tag{24}$$

where (θ,ϕ) are the spherical coordinates of the unit vector $\hat{\vec{R}}$ in the direction of observation, and

$$X(\theta,\omega)=\left(\beta(\cos\theta-\cos\theta_n)-\frac{\omega-\omega_n}{\omega_n}(1-\beta\cos\theta)-\frac{1}{(1+\beta)\gamma^2}\right)\frac{\omega_n}{2\beta c}. \tag{25}$$

Also,

$$\Phi(\theta,\phi,\omega)=-\frac{1}{4\beta^2}+\frac{1-(1/2\beta^2)N(\theta,\omega)}{D(\theta,\phi,\omega)}-\frac{\beta^2/\gamma^2+(1/4\beta^2)N^2(\theta,\omega)}{D^2(\theta,\phi,\omega)}, \tag{26}$$

where

$$N(\theta,\omega)=\beta^2\sin^2\theta-\beta^2\left(\frac{\omega_n}{\omega}\right)^2\sin^2\theta_n+\frac{2\beta\cos\theta-1}{\gamma^2}, \tag{27a}$$

$$D(\theta,\phi,\omega)=\beta^2\left(\sin\theta-\frac{\omega_n}{\omega}\sin\theta_n\right)^2+2\beta^2\frac{\omega_n}{\omega}\sin\theta\sin\theta_n[1-\cos(\phi-\phi_n)]+\frac{1}{\gamma^2}. \tag{27b}$$

The last term within square brackets in Eq. (24) becomes maximum when $X(\theta,\omega)=0$, or else when θ is determined from the relation

$$\cos\theta=1/\beta-(\omega_n/\omega)(1-\cos\theta_n). \tag{28}$$

Since $-1\leq\cos\theta\leq1$, it follows that ω/ω_n must satisfy the inequalities

$$\beta\,\frac{1-\cos\theta_n}{1+\beta} \leq \frac{\omega}{\omega_n} \leq \beta\,\frac{1-\cos\theta_n}{1-\beta}\,. \tag{29}$$

The function $\Phi(\theta,\phi,\omega)$ becomes maximum when

$$D(\theta,\phi,\omega) = -N(\theta,\omega) = 2\beta^2/\gamma^2\,, \tag{30}$$

and its maximum value is $\gamma^2/4\beta^2$.

Equations (28) and (30) determine the values of $\omega=\omega_{\max}$, $\theta=\theta_{\max}$, and $\phi=\phi_{\max}$ for which the radiated energy per unit frequency interval and per unit solid angle is maximum. The exact expression for $\omega_n/\omega_{\max}$ is equal to

$$\frac{\omega_n}{\omega_{\max}} = \frac{\beta}{2}\left[1+\left(1+\frac{4}{\beta^2\gamma^2(1-\cos\theta_n)}\right)^{1/2}\right]. \tag{31}$$

The expressions for $\theta_{\max}$, $\phi_{\max}$ are too lengthy and will not be given. An approximate solution of Eqs. (28) and (30) is as follows, when $\gamma\gg1$

$$\omega_n/\omega_{\max} \simeq 1+1/\gamma^2(1-\cos\theta_n)\,, \tag{32a}$$

$$\theta_{\max}-\theta_n \simeq 1/2\gamma^2\sin\theta_n\,, \tag{32b}$$

$$\phi_{\max}-\phi_n \simeq \pm 1/\gamma\sin\theta_n\,. \tag{32c}$$

Hence, there are two maxima of radiation which lie very close to the Bragg direction. If $\omega=\omega_n$, $\theta=\theta_n$, and $\phi=\phi_n$, then $X(\theta,\omega)=-1/[2\beta(1+\beta)\gamma^2\chi_n]$, so that the last term within brackets in Eq. (24) does not take its maximum value. Also, $\Phi(\theta,\phi,\omega)=\sin^2\theta_n$, which is much less than $\gamma^2/4\beta^2$, the maximum value of $\Phi(\theta,\phi,\omega)$. Thus, the maxima do not occur exactly in the Bragg directions.

The ratio ω/ω_n must lie within the boundaries determined by Eq. (29). If

$$\omega_n/\omega = (1/\beta\gamma^2)[1/(1-\cos\theta_n)]\,, \tag{33a}$$

$$\theta = \arcsin(1/\gamma)\,, \tag{33b}$$

while ϕ is arbitrarily chosen, then $X(\theta,\omega)=0$ and $\Phi(\theta,\phi,\omega)\simeq\frac{1}{4}\gamma^2$, where it has been assumed that $\gamma\gg1$. It follows then that frequency components much larger than ω_n are emitted in the forward direction and are independent of the azimuthal angle. But as it can be seen from Eqs. (17), (5), (A9), (A10) and (8), the susceptibility of the crystal $\chi_{\vec{G}_n}(\omega)$ decreases with increasing frequency. Therefore, the main contribution to the radiation comes from frequencies and angles determined approximately by the Bragg condition when $\gamma\gg1$.

An order of magnitude of the angular spreads and the frequency width can be estimated as follows: Eq. (27b) can be written in the form

$$D(\theta,\phi,\omega) = (\vec{A}-\vec{B})\cdot(\vec{A}-\vec{B}) + 1/\gamma^2\,, \tag{34}$$

where the vectors $\vec{A}$ and $\vec{B}$ are equal to

$$\vec{A} = (\beta\sin\theta\cos\phi, \beta\sin\theta\sin\phi)\,, \tag{35a}$$

$$\vec{B} = \left(\beta\,\frac{\omega_n}{\omega}\sin\theta_n\cos\phi_n, \beta\,\frac{\omega_n}{\omega}\sin\theta_n\sin\phi_n\right). \tag{35b}$$

Thus, for any value of θ,ϕ,ω the inequality $D(\theta,\phi,\omega)\geq 1/\gamma^2$ holds. Now, the functions $U(\theta,\omega)$ and $V(\theta,\phi,\omega)$ will be defined by means of the relations

$$N(\theta,\omega) = (2\beta^2/\gamma^2)[-1+U(\theta,\omega)]\,, \tag{36a}$$

$$D(\theta,\phi,\omega) = (2\beta^2/\gamma^2)[1+V(\theta,\phi,\omega)]\,. \tag{36b}$$

Since $D(\theta,\phi,\omega)\geq 1/\gamma^2$, it follows that $V(\theta,\phi,\omega)\geq -1+1/(2\beta^2)$ for any values of θ,ϕ,ω. Substitution of Eqs. (36) into Eq. (26) leads to the relation

$$\Phi(\theta,\phi,\omega) = \frac{\gamma^2}{4\beta^2}\,\frac{1}{(1+V)^2}\left[1+2V-\frac{2}{\gamma^2}(U+V) - \frac{1}{\gamma^2}(U+V)^2\right]. \tag{37}$$

The maximum of $\Phi(\theta,\phi,\omega)$ occurs when $U=V=0$ [cf. Eqs. (30) and (36)]. For values of U, V around the maximum, the main contribution in the above equation comes from the first two terms within the square brackets, if $\gamma\gg1$, so that a good approximation

$$\Phi(\theta,\phi,\omega) \simeq (\gamma^2/4\beta^2) f[V(\theta,\phi,\omega)]\,, \tag{38}$$

where

$$f(x) = (1+2x)/(1+x)^2\,, \tag{39}$$

and $x\geq -1+1/2\beta^2$. For such values of x, $f(x)$ is positive and less than or equal to one, and it has only one maximum at $x=0$, where $f(0)=1$. Also, $f(2.5)=24/49\simeq 0.5$ and $f[-1+1/(2\beta^2)]=1/(2\gamma^2)$. Thus, the width ΔV around $V=0$ within which $f(V)$ takes appreciable values is approximately equal to $\Delta V\simeq 3$. Moreover, it follows from Eq. (36b) and the result just obtained that the width ΔD around $D=2\beta^2/\gamma^2$ within which the function $\Phi(\theta,\phi,\omega)$ takes appreciable values is equal to $\Delta D\simeq 6\beta^2/\gamma^2$. Now, the functions $X(\theta,\omega)$ and $D(\theta,\phi,\omega)$ around the point $(\omega_n,\theta_n,\phi_n)$ are given approximately by their Taylor expansions, namely,

$$X(\theta,\omega) \simeq -\left(\beta\sin\theta_n\Delta\theta + (1-\beta\cos\theta_n)\times\frac{\Delta\omega}{\omega_n}+\frac{1}{(1+\beta)\gamma^2}\right)\frac{\omega_n}{2\beta c}\,, \tag{40}$$

$$D(\theta,\phi,\omega) \simeq \beta^2[\cos\theta_n\Delta\theta+\sin\theta_n(\Delta\omega/\omega_n)]^2 + \beta^2\sin^2\theta_n(\Delta\phi)^2 + 1/\gamma^2\,, \tag{41}$$

where $\Delta\omega=\omega-\omega_n$, $\Delta\theta=\theta-\theta_n$, and $\Delta\phi=\phi-\phi_n$. The function within square brackets in Eq. (24) and $\Phi(\theta,\phi,\omega)$ take significant values when the functions $X(\theta,\omega)$ and $D(\theta,\phi,\omega)$ satisfy the inequalities $|X(\theta,\omega)|\leq\pi/L$ and $|D(\theta,\phi,\omega)-2\beta^2/\gamma^2|\leq 6\beta^2/\gamma^2$, respectively. If Eqs. (40) and (41) are substituted into these inequalities, one concludes that signifi-

cant radiation is obtained when $\Delta\theta$, $\Delta\phi$, and $\Delta\omega$ satisfy the inequalities

$$|\Delta\phi| \leq \sqrt{7}/\gamma \sin\theta_n \tag{42a}$$

$$|\cos\theta_n \Delta\theta + \sin\theta_n(\Delta\omega/\omega_n)| \leq \sqrt{7}/\gamma\,, \tag{42b}$$

$$\left|\sin\theta_n \Delta\theta + (1-\cos\theta_n)\frac{\Delta\omega}{\omega_n}\right| \leq \frac{\lambda_n}{L} + \frac{1}{2\gamma^2}\,, \tag{42c}$$

where it was assumed that $\gamma \gg 1$. As may be noted from Eq. (32c), the difference $\phi_{\max} - \phi_n$ is of the same order of magnitude as the right-hand side of the inequality in Eq. (42a). Since the azimuthal spread $\langle\Delta\phi\rangle$ is measured with respect to $\phi_{\max}$ rather than ϕ_n, it follows that

$$\langle\Delta\phi\rangle = (\sqrt{7}+1)/\gamma \sin\theta_n\,. \tag{43}$$

Similarly, the polar spread $\langle\Delta\theta\rangle$ and frequency width $\langle\Delta\omega/\omega_n\rangle$ are obtained from Eqs. (42b) and (42c), namely,

$$\langle\Delta\theta\rangle = \frac{\sqrt{7}}{\gamma} + \frac{\sin\theta_n}{1-\cos\theta_n}\left(\frac{\lambda_n}{L} + \frac{1}{2\gamma^2}\right), \tag{44}$$

$$\left\langle\frac{\Delta\omega}{\omega_n}\right\rangle = \frac{\sin\theta_n}{1-\cos\theta_n}\frac{\sqrt{7}}{\gamma} + \frac{|\cos\theta_n|}{1-\cos\theta_n}\left(\frac{\lambda_n}{L} + \frac{1}{2\gamma^2}\right). \tag{45}$$

In most cases $\lambda_n/L \ll 1/\gamma$, so that the second term on the right-hand side of the above equations can be neglected.

Integration of Eq. (24) over the angles leads to the following relation[11]:

$$\frac{1}{L}\frac{dW}{d\omega} = \frac{(2\pi)^2 Q^2}{c}\,|\chi_{\tilde{G}_n}(\omega)|^2\,\frac{\omega}{c}\,F\left(\frac{\omega_n}{\omega}\right), \tag{46}$$

where

$$F(x) = -\frac{1}{4\beta^2} + \frac{1-(1/2\beta^2)N_1(x)}{B(x)} - A(x)\,\frac{\beta^2/\gamma^2 + (1/4\beta^2)N_1^2(x)}{B^3(x)}\,, \tag{47}$$

and

$$N_1(x) = -2(1-\cos\theta_n)\beta x\,(\beta x - 1 + 1/\gamma^2)\,, \tag{48a}$$

$$A(x) = 2(1-\cos\theta_n)\beta x(\beta x\cos\theta_n + 1)\,, \tag{48b}$$

$$B(x) = 2(1-\cos\theta_n)\beta x\,[(\beta x - 1)^2 + \delta^2]^{1/2}\,. \tag{48c}$$

Also

$$\delta = \sin\theta_n/\gamma(1-\cos\theta_n)\,. \tag{49}$$

If $\gamma \gg 1$, one may set $x = 1 + \xi\delta$ and $F(x)$ becomes approximately equal to

$$F(x) = \frac{\gamma}{4\sin\theta_n}\,\frac{1+(2-\sin^2\theta_n)\xi^2}{(1+\xi^2)^{3/2}} + \frac{1}{4}\,\frac{\xi}{(1+\xi^2)^{1/2}}\left(1 - \frac{1-2\cos\theta_n + 1/\sin^2\theta_n}{1+\xi^2}\right) - \frac{1}{4}\,. \tag{50}$$

Terms of order $1/\gamma$ and higher have been neglected. If only the first term is retained in the above equation, since it is the dominant term, it follows that the maximum of $F(\omega_n/\omega)$ lies approximately at $\omega = \omega_n$, when $\sin\theta_n \geq 1/\sqrt{2}$, and $F(1) \simeq \gamma/4\sin\theta_n$. On the other hand, when $\sin\theta_n < 1/\sqrt{2}$, there are two maxima lying at $\omega = \omega_n/(1 \pm \xi_0\delta)$, where

$$\xi_0 = \left(\frac{1-2\sin^2\theta_n}{2-\sin^2\theta_n}\right)^{1/2} \tag{51}$$

and

$$F(1 \pm \xi_0\delta) \simeq \frac{\gamma}{6\sqrt{3}}\,\frac{(2-\sin^2\theta_n)^{3/2}}{\sin\theta_n|\cos\theta_n|}\,. \tag{52}$$

If $\theta_n \simeq \pi/2$, it may be seen from Eq. (50) that the width $\Delta\omega/\omega_n$ of $F(\omega_n/\omega)$ is of the order $1/\gamma$.

In order to integrate over the frequency domain, it will be assumed for simplicity that the crystal consists of identical atoms and that there is only one atom in each unit cell. Then the summation extends only over one term in Eq. (17) and the volume V_c of the unit cell is the inverse of the number of atoms per unit volume $\hat{N}$. From Eqs. (17) and (5) the following expression is obtained for $\chi_{\tilde{G}_n}(\omega)$ for resonant transitions between bound states

$$\chi_{\tilde{G}_n}(\omega) = \frac{1}{4\pi}\,\tau_a(\omega_r)\frac{c}{\omega_r}\,\frac{\Delta\omega_r}{\omega_r - \omega - i\Delta\omega_r}\,, \tag{53}$$

where

$$\tau_a(\omega_r) = \hat{N}\sigma_a(\omega_r)\,, \tag{54}$$

is the absorption coefficient at resonance. Since in most cases $\Delta\omega/\omega_r \ll 1/\gamma$ integration over the frequency domain in Eq. (46) gives the relation

$$\frac{W_a}{\hbar\omega_r} = \frac{Q^2}{\hbar c}\,\tau_a^2(\omega_r)\lambda_r L\pi F\left(\frac{\omega_n}{\omega_r}\right)\frac{\Delta\omega_r}{\omega_r}\,. \tag{55}$$

For transitions from a bound state to the continuum, it follows from Eqs. (17) and (7) that

$$\chi_{\tilde{G}_n}(\omega) = (i/4\pi)(c/\omega)\tau_{\text{cont}}(\omega), \tag{56}$$

where

$$\tau_{\text{cont}}(\omega) = \hat{N}\sigma_{\text{cont}}(\omega)\,, \tag{57}$$

is the absorption coefficient of the transition under consideration. Also, ω_n/ω must lie within the limits

$$\frac{1-\beta}{\beta(1-\cos\theta_n)} \leq \frac{\omega_n}{\omega} \leq Min\left(\frac{\omega_n}{\omega_c}\,,\ \frac{1+\beta}{\beta(1-\cos\theta_n)}\right), \tag{58}$$

[cf. Eqs. (7) and (29)]. For $\tau_{\rm cont}(\omega)$ the following empirical expression will be adopted:

$$\tau_{\rm cont}(\omega)=\tau_{\rm cont}(\omega_n)(\omega_n/\omega)^{\sigma}, \tag{59a}$$

where

$$\tau_{\rm cont}(\omega_n)=\rho_0 C\lambda\!\!\!^{-}_{n}^{\sigma}. \tag{59b}$$

Here, ρ_0 is the density of the crystal and C, σ are empirically determined parameters.[12] Integration of Eq. (46) leads to the expression

$$\frac{W_{\rm cont}}{\hbar\omega_n}=\frac{Q^2}{\hbar c}\tau^2_{\rm cont}(\omega_n)\lambda\!\!\!^{-}_{n} L H_{\rm cont}\left(\frac{\omega_n}{\omega_c}\right), \tag{60a}$$

if $1<\omega_n/\omega_c\leq(1+1/\beta)/(1-\cos\theta_n)$, and

$$\frac{W_{\rm cont}}{\hbar\omega_n}=\frac{Q^2}{\hbar c}\tau^2_{\rm cont}(\omega_n)\lambda\!\!\!^{-}_{n} L H_{\rm cont}\left(\frac{1+\beta}{\beta(1-\cos\theta_n)}\right), \tag{60b}$$

if $\omega_n/\omega_c>(1+1/\beta)/(1-\cos\theta_n)$. The function $H_{\rm cont}(x)$ is equal to

$$H_{\rm cont}(x)=\int_{x_0}^{x} x^{2\sigma-1}F(x)dx, \tag{61}$$

where $x_0=1/[\beta(1+\beta)\gamma^2(1-\cos\theta_n)]$ and $F(x)$ is given by Eq. (47). In general, a numerical integration of Eq. (61) should be performed for the various values[13] of the parameter σ. But when $\gamma\gg1$, the function $F(x)$ is given approximately by the term proportional to γ in Eq. (50). Since this term has a sharp peak at $x=1$, one may set $x^{2\sigma-1}\simeq1$ in Eq. (61). Also the lower limit x_0 may be set equal to zero, in which case $H_{\rm cont}(x)$ becomes approximately equal to

$$H_{\rm cont}(x)\simeq\frac{1+\cos^2\theta_n}{4(1-\cos\theta_n)}\left(\ln\frac{2}{\delta}+\ln\frac{x-1+R}{\delta}\right)-\frac{\cos^2\theta_n}{4(1-\cos\theta_n)}\left(\frac{x-1}{R}+1\right), \tag{62}$$

where

$$R=[(x-1)^2+\delta^2]^{1/2}, \tag{63}$$

and δ is given by Eq. (49). The main contribution comes from the logarithmic terms in the above expression and $H_{\rm cont}(x)$ is of order one even if γ takes very large values. Finally, for the case in which the frequency ω_n is much larger than the ionization potentials, divided by $\hbar$, of the inner shells of the atoms, it follows from Eqs. (17) and (8) that $\chi_{\vec{G}_n}(\omega)$ in Eq. (46) should be replaced by

$$\chi_f(\omega)=\chi_f(\omega_n)(\omega_n/\omega)^2, \tag{64}$$

where

$$\chi_f(\omega_n)=-\hat{N}(e^2/\mu)(f_n/\omega_n^2), \tag{65}$$

and f_n is given by Eq. (10) with $\Delta K=(2/\lambda\!\!\!^{-}_{n})\sin\theta_n$.

The total number of radiated photons is equal to

$$\frac{W_f}{\hbar\omega_n}=\frac{Q^2}{\hbar c}(4\pi)^2\chi_f^2(\omega_n)\frac{L}{\lambda\!\!\!^{-}_{n}}H_f\left(\frac{1+\beta}{\beta(1-\cos\theta_n)}\right), \tag{66}$$

where

$$H_f(x)=\int_{x_0}^{x} xF(x)dx. \tag{67}$$

The integration can be performed analytically, but the resulting expression is too lengthy and will not be given. If $\gamma\gg1$, the function $H_f(x)$ becomes equal to $H_{\rm cont}(x)$ as given by Eq. (62). Thus, $H_f(x)$ is also of order 1 even for very large values of γ. Equation (66) can be compared directly with the corresponding expression in x-ray scattering. The number of scattered photons per incident photon by a crystal of small dimensions is equal to[14]

$$\frac{W_{\rm ph}}{\hbar\omega_n}=(4\pi)^2\chi_f^2(\omega_n)\frac{L}{\lambda\!\!\!^{-}_{n}}\frac{\pi}{4}\frac{1+\cos^2\theta_n}{\sin\theta_n}. \tag{68}$$

Comparison of Eqs. (66) and (68) indicates that the ratio of the radiated energy per incident charged particle to the scattered energy per incident photon is approximately equal to $Q^2/\hbar c$.

Two numerical examples will be given here. First, for transitions between bound states, the following numbers are chosen: $\tau_d(\omega_r)\sim10^3$ cm^{-1}, $\lambda\!\!\!^{-}_{r}\sim10^{-8}$ cm, $L\sim10^{-2}$ cm, $\Delta\omega_r/\omega_r\sim10^{-3}$. Then it follows from Eq. (55) that for a 50-MeV and 1-mA incident beam of electrons, which corresponds to $\gamma\sim100$ and 10^{16} incident electrons/sec, there will be radiated approximately 10^{10} photons/sec. On the other hand, if $\hbar\omega_n$ is much larger than the ionization potentials, the following numbers are chosen: $\hat{N}f_n\sim10^{23}$ cm^{-3}, $\lambda\!\!\!^{-}_{n}\sim10^{-8}$ cm, $L\sim10^{-2}$ cm. Then it follows from Eqs. (65) and (66) that for the same incident beam of electrons there will be radiated again approximately 10^{10} photons/sec.

V. DISCUSSION

Transitions between bound states are possible only if there is a vacancy in the upper state. The light elements with atomic number $Z<10$ have a vacant L shell, but their resonant wavelengths for K to L transitions do not satisfy Bragg's law $\lambda\leq2d$. Hence, a transition between the K and L shells of these elements will give a very small amount of radiated energy. On the other hand, elements with an atomic number between 13 and 28 have a vacant M shell and their resonant wavelengths for transitions between the K and M shells do satisfy Bragg's law. For example,[15] Al with $Z=13$, has only three electrons in its M shell, it forms a cubic crystal and λ_{KM}

$= 7.96$ Å, $d = 4.05$ Å, while Ni with $Z = 28$, has 16 electrons in its M shell, it forms also a cubic crystal and $\lambda_{KM} = 1.5$ Å, $d = 3.52$ Å. Thus, for elements with $13 \leq Z \leq 28$, a transition between the K and M shells should provide a rather large amount of radiation. In Eq. (55), the ratio $\Delta\omega_r/\omega_r$ is quite a small number, but it is compensated by the function $F(\omega_n/\omega_r)$ which is very large at its maximum [cf. Eq. (50)]. Hence, for very large values of γ, the radiated energy, either for transitions between bound states or for transitions between a bound state and the continuum, could become of the same order of magnitude.

The treatment given above represents a rather idealized situation. For example, the absorption that takes place in the crystal, if resonant radiation is emitted, was neglected. This is a good approximation, if the dimensions of the crystal in the direction of the emitted radiation are much smaller than the inverse of the absorption coefficient at resonance. The crystal should also be small in the direction that the incident charged particle moves, if the loss of energy by the particle is to be negligible [cf. Eq. (3)]. Finally, the multiple scattering that the incident particle undergoes, due to its interaction with the nuclei, was not taken into consideration. As a result of it, there should be an additional broadening of the angular spreads of the emitted radiation. The root mean square of the angular deflection of the incident charged particle is inversely proportional to γ and it becomes very small for large γ. Thus,[16] for an aluminum crystal with thickness $L \sim 10^{-2}$ cm and electrons as incident particles with $\gamma = 100$, the angular deflection is of the order of 10^{-3} rad. This value is smaller than the polar and azimuthal spreads, as given by Eqs. (43) and (44). Therefore, there should not be a considerable broadening.

As it may be seen from Eqs. (55), (60), and (66), the total radiated energy is proportional to the density of atoms squared which indicates that the radiation is coherently emitted.

One may conclude then that the crystal acts as a filter on the generated coherent radiation by favoring the radiation at frequencies and angles for which the Bragg condition is approximately satisfied.

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APPENDIX A

From first-order perturbation theory it follows that the induced polarizability due to one of the electrons in the nth shell of an atom in the presence of an electric field is equal to

$$\alpha_e(\omega) = \int_{k_F}^{\infty} \frac{F(k)}{E_k + I_n - \hbar\omega - i\hbar\gamma_n} k^2\, dk\,, \tag{A1}$$

where

$$F(k) = \frac{1}{3}\,\frac{1}{2l+1} \sum_{l'm'm} |\langle kl'm'|\vec{D}|nlm\rangle|^2\,. \tag{A2}$$

Here, $\vec{D} = -|e|\vec{r}$, $E_k = (\hbar^2/2\mu)k^2$ is the kinetic energy of the ejected electron, I_n is the ionization energy of the nth shell, and γ_n is the lifetime width of the hole that is left by the removal of an electron in the shell. The eigenvalues of the orbital angular momentum l, m take the values $l = 0, 1, \ldots, n-1$, $m = -l, -l+1, \ldots, l-1, l$, while l', m' take the values $l' = 0, 1, \ldots$, $m = -l', -l'+1, \ldots, l'-1, l'$. For simplicity, the spin of the electron was neglected. If the transition is made into the conduction band of the crystal, k_F is the wave number associated with the Fermi energy E_F, i.e., $k_F = (2\mu E_F/\hbar^2)^{1/2}$. The wave functions of the discrete spectrum are normalized to unity, while for the continuous spectrum the normalization is chosen as follows:

$$\langle k'l'm'|k''l''m''\rangle = (1/k'^2)\delta(k' - k'')\delta_{l'l''}\delta_{m'm''}\,. \tag{A3}$$

A change of variables leads to the following expression of $\alpha_e(\omega)$, as given by Eq. (A1):

$$\alpha_e(\omega) = \frac{1}{4\mu\omega_1^2 a^5}\left(\frac{I_n}{I_1}\right)^{1/2} \int_{x_F}^{\infty} \left\{F\left[\frac{1}{a}\left(\frac{I_n}{I_1}x\right)^{1/2}\right]\Big/(x - \Delta\Omega - i\Gamma_n)\right\} x^{1/2}\, dx\,, \tag{A4}$$

where $x_F = E_F/I_n$, $\Gamma_n = \hbar\gamma_n/I_n$, $\Delta\Omega = (\hbar\omega - I_n)/I_n$, $I_1 = \hbar^2/(2\mu a^2)$, $a = a_0/Z$, and $\omega_1 = I_1/\hbar$. Here, a_0 is the Bohr radius and Z is the atomic number. For hydrogenic wave functions, the function $F(k)$ can be evaluated analytically. For example, for a transition from the K shell ($n = 1, l = 0$) into the continuum, $F(k)$ is given by the expression[17]

$$F(k) = \frac{2^8}{3}\,\frac{e^2\eta^{11}}{(1+\eta^2)^5}\, a^5 f\left(\frac{1}{\eta^2}\right), \tag{A5}$$

where

$$f(x)=\frac{\exp[-(4\arctan\sqrt{x})/\sqrt{x}]}{1-\exp(-2\pi/\sqrt{x})}, \tag{A6}$$

and $\eta=1/ka$. Also, for hydrogenic wave functions, the ionization potential I_n is equal to $I_n=I_1/n^2$. It may be noted from Eqs. (A5) and (A6) that the integral in Eq. (A4) is convergent. Also, if $\Delta\Omega \gg \Gamma_n$ the numerator of the integrand in Eq. (A4) varies much slower than the denominator within the range of integration. It will be assumed that this is always the case for transitions from the bound states into the continuum. The main contribution of the denominator comes from values of x around $x=\Delta\Omega$. Since the range of integration is positive, $\Delta\Omega$ must also be positive so that the polarizability may have significant values. If, in addition, $\Delta\Omega \gg x_F$, the real part of the denominator is an odd function of x around the point $x=\Delta\Omega$ where the most significant contribution comes from. Hence, the real part of the integral in Eq. (A4) is negligible in comparison to the imaginary part, if $\Delta\Omega \gg \Gamma_n$ and $\Delta\Omega \gg x_F$. On the other hand, the imaginary part of the denominator in Eq. (A4) is a Lorentzian with its peak at $x=\Delta\Omega$. Since $\Delta\Omega \gg \Gamma_n$ and $\Delta\Omega \gg x_F$, the value of x in the numerator in Eq. (A4) can be set equal to $x=\Delta\Omega$ and integration over the Lorentzian leads approximately to the relation

$$a_e(\omega)=(i/4\pi)(c/\omega)\sigma_e(\omega), \tag{A7}$$

where

$$\sigma_e(\omega)=\frac{\pi^2}{\mu\omega_1^2 a^5}\frac{\omega}{c}\left(\frac{I_n}{I_1}\Delta\Omega\right)^{1/2} \times F\left[\frac{1}{a}\left(\frac{I_n}{I_1}\Delta\Omega\right)^{1/2}\right]. \tag{A8}$$

Here, $\Delta\Omega$ must be positive, i.e., $\omega>\omega_n$. If there are N_n electrons in the nth inner shell, the atomic polarizability for transitions from that shell into the continuum is N_n times the value given by Eq. (A7), so that

$$\alpha_{\text{cont}}(\omega)=(i/4\pi)(c/\omega)\sigma_{\text{cont}}(\omega), \tag{A9}$$

where $\omega>\omega_n$ and $\sigma_{\text{cont}}(\omega)$ is N_n times the value given by Eq. (A8). In particular, for a K-shell transition, it follows from Eqs. (A5), (A6), and (A8) that

$$\sigma_{\text{cont}}(\omega)=\frac{2^9\pi^2}{3}\frac{e^2}{\mu c}\frac{\omega_1^3}{\omega^4}f\left(\frac{\omega-\omega_1}{\omega_1}\right), \tag{A10}$$

where $\omega>\omega_1$ and consideration was taken of the fact that there are two electrons in the K shell. But Eq. (A10) is equal to the atomic-absorption cross section for that transition.[18] In general, the imaginary part of the polarizability does provide the absorption, so that the particular case of Eq. (A10) may be generalized in the sense that $\sigma_{\text{cont}}(\omega)$ in Eq. (A9) is the atomic-absorption coefficient for any transition from a bound state into the continuum.

APPENDIX B

In a classical theory of x-ray scattering, Eq. (8) can be deduced from Eq. (97.6), p. 399 in Landau and Lifshitz (Ref. 3). In the context of quantum electrodynamics, Eq. (97.9) in Landau and Lifshitz corresponds to Eqs. (3), (5), (7), and (8), pp. 190–191 in Heitler,[19] where $n=n_0$ in these equations, i.e., the initial and final atomic states are the same. The treatment in Heitler is for a single atom and a single electron (but compare pp. 192–194). Equation (7) should be amended by inserting the lifetimes of the bound states in the denominators of the first term inside the brackets. Moreover, the assumption that the wavelengths of $\vec{K}_0$ and $\vec{K}$ are large compared with the dimensions of the atom may not be true for x rays, so that the exponential term in Eq. (7) should be incorporated in the matrix elements as given by Eqs. (3) and (5) with $n=n_0$. Now, if the energies of the incident and scattered photons [actually, they are equal by Eq. (1) in Heitler] are much larger than the ionization potentials of the electrons in the atoms, then the main contribution in the first term of Eq. (7) comes from intermediate states for which the ejected electron has a kinetic energy approximately equal to the photon energy. This leads to a wavelength for the ejected electron approximately equal to $\lambda\!\!\!^{-}_e=(\lambda\!\!\!^{-}_c\lambda\!\!\!^{-}/2)^{1/2}$, where $\lambda\!\!\!^{-}_c=\hbar/\mu c$ is the electron Compton wavelength and $\lambda\!\!\!^{-}$ is the photon wavelength. Since for the light elements, $\lambda\!\!\!^{-}_e \ll a_0/Z^{1/3}$, the oscillatory intermediate states render the matrix elements in Eqs. (5) negligible in comparison to that in Eq. (3), so that the last term is the dominant term in Eq. (7). Substitution of Eqs. (3) and (7) into Eq. (8) leads to a relation identical to Eq. (97.9) in Landau and Lifshitz. In the context of ordinary quantum mechanics, a similar argument leads to the conclusion that the last term in Eq. (104), p. 85 in Kramers,[20] leads to a result identical to that of the classical theory. It should be pointed out again that in the present work the external electric field is that of the incident relativistic charged particle.

[1]H. Überall, Phys. Rev. 103, 1055 (1956).
[2]G. Diambrini Palazzi, Rev. Mod. Phys. 40, 611 (1968).
[3]For a classical approach to x-ray diffraction in crystals, see, for example, L. D. Landau and E. M. Lifshitz, *Electrodynamics of Continuous Media* (Pergamon, London, 1960, p. 398 *et seq*. In the present work, of course, the external electric field is due to the relativistic charged particle.
[4]See, for example, J. D. Jackson, *Classical Electrodynamics* (Wiley, New York, 1962), p. 437, Eqs. (13.29) and (13.30). Equation (1) differs by a factor $(2\pi)^{1/2}$ from the above equations. The absence of the exponential term in Jackson is due to the fact that the point $\vec{R}$ is taken on the x-y plane, where $z=0$ [cf. Eqs. (11.118) and Fig. 11.13, p. 381]. Also, here use has been made of the identity $K_0'(z)=-K_1(z)$ [cf. *Handbook of Mathematical Functions* (U.S. GPO, Washington, D.C., 1964), p. 376, Eq. (9.6.27)].
[5]Cf. Eq. (9.7.2), p. 378 in the latter part of Ref. 4.
[6]See, for example, p. 237 in Publ. 1133, *Studies in Penetration of Charged Particles in Matter*, 2nd printing, edited by U. Fano (National Acad. Sci.–Natl. Res. Council, Washington, D.C., 1967).
[7]E. U. Condon and G. H. Shortley, *The Theory of Atomic Spectra* (Cambridge U.P., London, 1964), Eq. (14), p. 108. It has been assumed that ω is so closely located to a particular resonant frequency that only one term of the sum in Eq. (14) contributes. Moreover, the broadening of the line was added as a phenomenological parameter and use was made of the relation $A_{21}=2(e^2/\mu c^3)\omega_r^2 f_{21}$, where e, μ are the charge and mass of the electron and f_{21} is the oscillator strength of the transition.
[8]See, for example, C. Kittel, *Introduction to Solid State Physics*, 3rd ed. (Wiley, New York, 1968), Eq. (69), p. 67. Numerical values of the atomic-scattering factor for various elements are given in Appendix IV, p. 780 *et seq*., in A. H. Compton and S. K. Allison, *X-Rays in Theory and Experiment* (Van Nostrand, New York, 1935). See also Fig. 31 on p. 66 and Fig. 34 on p. 73 in Kittel.
[9]For this purpose, use was made of Eq. (9.1.18), p. 360, in *Handbook of Mathematical Functions* (U.S. GPO, Washington, D.C., 1964), and also of Eq. (6.521.2), p. 672; in I. S. Gradshteyn and I. M. Ryzhik, *Table of Integrals, Series and Products* (Academic, New York, 1965).
[10]See, for example, p. 55 in Ref. 8.
[11]The integration over the azimuthal angle ϕ can be easily performed with the help of Eq. (3.661.4), p. 383 in Ref. 9. The integration over θ is based on the assumption that the function within brackets in Eq. (27) has a width which is much smaller than that of $\Phi(\theta,\phi,\omega)$. This is true if $\lambda_n/L \ll 1/\gamma$. Then, the value of θ for which $X(\theta,\omega)=0$ [cf. Eq. (28)] is substituted into $\Phi(\theta,\phi,\omega)$ and the limits of integration can be extended from $-\infty$ to $+\infty$ without introducing any significant error.
[12]See, for example, *Encyclopedia of X-Rays and Gamma Rays*, edited by G. L. Clark (Reinhold, New York, 1963), p. 10, Eq. (2).
[13]Reference 12, Table 1, p. 11.
[14]See, for example, A. H. Compton and S. K. Allison, *X-Rays in Theory and Experiment* (Van Nostrand, New York, 1935), Eq. (6.78), p. 414, and footnote p. 415.
[15]The given values were obtained from the *American Institute of Physics Handbook*, 3rd ed. (McGraw-Hill, New York, 1972), pp. 7-98 and p. 9-5.
[16]Cf. for example, *Experimental Nuclear Physics*, edited by E. Segrè (Wiley, New York, 1953), Vol. I, Eqs. (77), (78), and p. 285.
[17]Cf. for example, H. A. Bethe and E. E. Salpeter, *Quantum Mechanics of One- and Two-Electron Systems, Encyclopedia of Physics, Atoms I* (Springer-Verlag, Berlin, 1957), Vol. 35, Eq. (71.4), p. 390. It should be noted that the normalization of the wave functions in the continuum in Bethe and Salpeter is different from that in Eq. (A3).
[18]Cf. for example, Ref. 17, Eq. (71.7), p. 71. The difference of a factor 2π is due to the relation $\omega = 2\pi\nu$.
[19]W. Heitler, *The Quantum Theory of Radiation* (Oxford U.P., London, 1957).
[20]H. A. Kramers, *Quantum Mechanics* (North-Holland, Amsterdam, 1957).