Density of the generalized oscillator strength of atomic hydrogen: A semiclassical approach

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An expression of the density of the generalized oscillator strength (GOS) for electron impact ionization of atomic hydrogen using a classical trajectory to describe the state of the ejected electron is presented with the help of its linear-response representation in the framework of the first Born approximation (FBA). Based on the reproduction of the GOS density of the FBA, the target polarization and the postcollision interaction (PCI) effect are included within the expression. The target polarization expressed by the decreasing of the initial expectation momentum of the atomic electron decreases the GOS density for small energy transfer E and moves the Bethe ridge toward higher momentum transfer K for larger E. The PCI effect should not be remarkable for the GOS density. [S1050-2947(98)03511-2]

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I. INTRODUCTION

The inelastic collision of an electron with matter is one of the elementary processes in various fields of physics such as plasma physics, atmosphere physics, astrophysics, and electron microscopy [1]. The study of the ionization of atomic hydrogen by electron impact which leads to three free particles in the final state is of fundamental importance for understanding the collision processes [2]. Many efforts have been made to deal with this many-body Coulomb problem, especially the description of the final state [3].

Pioneer works [1,4] studied the case in which the incident electron is fast. In this case most of the ionizing collisions proceed with asymmetric geometry, i.e., one of the outgoing electrons (scattered) is fast and the other (ejected) is slow. So the collision can be well studied by the first Born approximation (FBA) in which the states of the incident and scattered electrons are described by plane waves and the state of the ejected electron is described by the Coulomb wave. Within the same framework, corrections can be made by considering the correlation of the two outgoing electrons and the interaction between the scattered electron and the residual ion outside the reaction zone [5–7]. As in this region the electrons are in their continuum states, this postcollision interaction (PCI) effect can be represented with the help of the classical trajectories of the two electrons [5–8].

In the framework of FBA, i.e., with the states of the incident and the scattered electrons described by the plane waves, the generalized oscillator strength (GOS) is the key dynamic factor which characterizes the response of the target to the transient field of the charged particles. For H it is written as [1]

$$\frac{\partial f(E,K)}{\partial E}=\sum_n \frac{2E}{K^2}|\langle n|\exp(i\boldsymbol{K}\cdot\boldsymbol{r})|0\rangle|^2\delta(E_n-E), \qquad (1)$$

where $0,n$ are initial and final target eigenstates, respectively, the summation runs over all excited states (discrete and continuum), $\boldsymbol{K}=\boldsymbol{k}_0-\boldsymbol{k}_1$ is the momentum transfer with $\boldsymbol{k}_0,\boldsymbol{k}_1$ the momenta of the incident and the scattered electrons, respectively, and $E=E_0-E_1$ is the energy transfer with E_0,E_1 the energies of the incident and the scattered electrons, respectively.

The GOS density per unit range of excitation for impact ionization of H(1s) is exactly known in FBA, written as [1,4]

$$\frac{\partial f(E,K)}{\partial E}=\frac{2^9E(K^2+2E/3)}{[(K+\sqrt{2E-1})^2+1]^3[(K-\sqrt{2E-1})^2+1]^3}\times\left[1-\exp\left(\frac{-2\pi}{\sqrt{2E-1}}\right)\right]^{-1}\times\exp\left[-\frac{2}{\sqrt{2E-1}}\arctan\left(\frac{2\sqrt{2E-1}}{K^2-2E+2}\right)\right]. \qquad (2)$$

Beyond FBA, for the GOS density, there is only one calculation carried out by integrating the triple-differential cross section (TDCS) in the Coulomb-wave Born approximation (CWBA) over the solid angle of the ejected electron [9].

The linear-response representation of the GOS density given by Inokuti [1] is a more general expression with which the concept of GOS can be adapted to electron impact ionization in condensed matter by the relationship between the GOS density for electron impact ionization and the generalized complex dielectric constant describing the response of the medium to a small electromagnetic disturbance. It is deduced from Eq. (1) using

$$\sum_n |n\rangle\langle n|=1 \qquad (3)$$

and

$$\int_{-\infty}^{\infty}\exp(ixt)dt=2\pi\delta(x), \qquad (4)$$

given as [1]

$$\frac{\partial f(E,K)}{\partial E}=\frac{E}{\pi K^2}\int_{-\infty}^{\infty}dt\,\exp[-i(E-K^2/2)t]\times\left\langle \exp\left[i\int_0^t dt\boldsymbol{K}\cdot\boldsymbol{p}(t)\right]\right\rangle, \tag{5}$$

where the angular brackets denote the initial-state expectation value and $\boldsymbol{p}(t)$ is the Heisenberg momentum operator of the atomic electron, which is given by

$$\boldsymbol{p}(t)=\exp(iHt)\boldsymbol{p}\exp(-iHt)=\boldsymbol{p}+it[\boldsymbol{H},\boldsymbol{p}]+\tfrac{1}{2}(it)^2[\boldsymbol{H},[\boldsymbol{H},\boldsymbol{p}]]+\cdots. \tag{6}$$

In this linear-response representation, the information of the ejected electron state $|n\rangle$ in Eq. (1) is transformed into $\boldsymbol{p}(t)$. The GOS density expressed by Eq. (5) was studied by Inokuti [1] in the simplest case when the second and higher terms of $\boldsymbol{p}(t)$ in Eq. (6) were neglected, i.e., the ejected electron was approximated by the free one. A simple formula of the GOS density for ionization from H$(1s)$ was then obtained, which is in accord with the binary-encounter approximation (BEA) result [1,10]

$$\frac{\partial f(E,K)}{\partial E}=\frac{2^9EK^3}{3\pi[(2E-K^2)^2+4K^2]^3}. \tag{7}$$

The purpose of this paper is to obtain further information given by the linear-response representation from the state description of the ejected electron, i.e., the factor $\boldsymbol{p}(t)$ and the initial momentum distribution so as to make some corrections to the standard FBA result Eq. (2) within the same framework limited by Eq. (5).

An expression is presented in Sec. II which allows the use of the classical trajectory to describe the ejected electron. The FBA result for GOS is reproduced by the expression in Sec. III, which demonstrates the reliability of the expression and serves as a base to include some corrections in Sec. IV, such as the target polarization, by considering the change of the initial expectation momentum of the atomic electron and the PCI effect by evaluating the contributions from the scattered and ejected electrons with the help of the new expression. Conclusions are made in Sec. V. Atomic units are used.

II. AN EXPRESSION FOR GOS

The time limits in Eq. (5) indicate that the Heisenberg operator of momentum of the atomic electron $\boldsymbol{p}(t)$ may contain the information of the polarization process of the target by the incident electron from $t=-\infty$ to $t=0$, and the affection of the surrounding field to the ejected electron including the PCI effect from $t=0$ to $t=\infty$. Because $\boldsymbol{p}(t=-\infty\rightarrow 0)$ describes the state of the bounded atomic electron, and this time-dependent state cannot be described by classical mechanics and is also complicated for quantum-mechanics description, we just consider here $\boldsymbol{p}(t\geqslant 0)$, where the polarization effect can be expressed by the change of the initial momentum distribution at $t=0$.

So first, we rewrite Eq. (5) for $t\geqslant 0$, using

$$\int_0^{\infty}\exp(ixt)dt=\pi\delta(x)+ix^{-1}, \tag{8}$$

instead of Eq. (4), as

$$\frac{\partial f(E,K)}{\partial E}=\frac{2E}{\pi K^2}\mathrm{Re}\int_0^{\infty}dt\,\exp[-i(E-K^2/2)t]\times\left\langle \exp\left[i\int_0^t dt\boldsymbol{K}\cdot\boldsymbol{p}(t)\right]\right\rangle. \tag{9}$$

Then we break up $\boldsymbol{p}(t)$ into two parts according to the concept of the reaction zone and the postcollision region used for treatment of the PCI effect in Refs. [5–8], as

$$\boldsymbol{p}(t)=\boldsymbol{p}(0)+\int_{0^+}^t\dot{\boldsymbol{p}}(t)dt, \tag{10}$$

where $\boldsymbol{p}(0)$ is the momentum of the atomic electron in the reaction zone at the moment of collision and $\dot{\boldsymbol{p}}(t)$ reflects the effect on the ejected electron by the potential field of the ion and the scattered electron from the boundary of the reaction zone to infinity.

With the y axis representing the outgoing direction of the ejected electron and the x axis representing the other axis in the trajectory plane, we can write

$$\boldsymbol{K}\cdot\dot{\boldsymbol{p}}(t)=K_x\ddot{x}(t)+K_y\ddot{y}(t). \tag{11}$$

Because of the symmetry of the process and the integration of the outgoing directions of the ejected electron, the averaged values

$$K_x=0,\quad K_y=K\,\overline{\cos\theta}, \tag{12}$$

where θ is the angle between the outgoing direction of the ejected electron and the direction of $\boldsymbol{K}$. The averaged value $\overline{\cos\theta}$ is a function of K and E, related to the distribution of the outgoing directions of the ejected electron at the boundary of the reaction zone. From Eqs. (10)–(12) we have

$$\int_0^t dt\boldsymbol{K}\cdot\boldsymbol{p}(t)=\boldsymbol{K}\cdot\boldsymbol{p}(0)t+K\,\overline{\cos\theta}f(t), \tag{13}$$

with

$$f(t)=y(t)-\dot{y}(0^+)t. \tag{14}$$

If the ejected electron is free, $y(t)=\dot{y}(0^+)t$. Generally $y(t)\leqslant\dot{y}(0^+)t$, therefore $f(t)\leqslant 0$. With Eqs. (13) and (14), noting that the only term related to the initial state expectation value is $\boldsymbol{p}(0)$, we have

$$\left\langle \exp\left[i\int_0^t dt\boldsymbol{K}\cdot\boldsymbol{p}(t)\right]\right\rangle=\langle\exp[i\boldsymbol{K}\cdot\boldsymbol{p}(0)t]\rangle\exp[iK\,\overline{\cos\theta}f(t)]. \tag{15}$$

Now inserting Eq. (15) with Eq. (14) into Eq. (9), we obtain an expression for the GOS density of H as

$$\frac{\partial f(E,K)}{\partial E}=\frac{2E}{\pi K^2}\mathrm{Re}\int_0^\infty dt\,\exp\{i[(K^2/2-E)t+K\,\overline{\cos\theta}f(t)]\}\times\langle\exp[i\boldsymbol{K}\cdot\boldsymbol{p}(0)t]\rangle. \quad (16)$$

To obtain the GOS density from Eq. (16), three factors have to be determined: the momentum distribution of the atomic electron at $t=0$ to calculate the initial-state expectation value denoted by $\langle\rangle$; $f(t)$, which is related to the trajectory of the ejected electron from the boundary of the reaction zone to infinity; and $\overline{\cos\theta}$, which describes the averaged outgoing direction of the ejected electron at the boundary of the reaction zone.

The BEA result given by Eq. (7) is approached by Eq. (16) with an unpolarized initial momentum distribution when E becomes larger so that $f(t)\rightarrow 0$.

With the proper determination of these factors, the FBA result Eq. (2) should be reproduced and some corrections to FBA such as target polarization and PCI effects can be included conveniently.

III. REPRODUCTION OF GOS DENSITY OF FBA

For H$(1s)$, the momentum distribution of the atomic electron for the projection axis z gives

$$\langle f(p_z)\rangle=\int_{-\infty}^{\infty}f(p_z)\frac{8}{3\pi}\frac{p_0^5dp_z}{(p_z^2+p_0^2)^3}, \quad (17)$$

where p_0 is the expectation value of momentum of the atomic electron. The integration results in

$$\langle\exp[i\boldsymbol{K}\cdot\boldsymbol{p}(0)t]\rangle=\langle\cos[\boldsymbol{K}\cdot\boldsymbol{p}(0)t]\rangle=(p_0^2K^2t^2/3+p_0Kt+1)\exp(-p_0Kt). \quad (18)$$

Inserting Eq. (18) into Eq. (16) gives the expression for H$(1s)$,

$$\frac{\partial f(E,K)}{\partial E}=\frac{2E}{\pi K^2}\int_0^\infty dt\,\cos[(K^2/2-E)t+K\,\overline{\cos\theta}f(t)]\times(p_0^2K^2t^2/3+p_0Kt+1)\exp(-p_0Kt). \quad (19)$$

For unpolarized H, $p_0=1$.

Corresponding to the description of the state of the ejected electron by the Coulomb wave in FBA, $f(t)$ in the expression is determined by the classical trajectory in the Coulomb field, written as [11]

$$y=\frac{Z}{2E_a}\sqrt{e^2-1}\,\sinh\xi,\quad t=\frac{Z}{(2E_a)^{3/2}}(e\sinh\xi-\xi), \quad (20)$$

where Z is the charge of the ion and E_a is the energy of the atomic electron, for H$(1s)$,

$$E_a=E-\tfrac{1}{2},\quad Z=1, \quad (21)$$

The eccentricity e can be determined by the initial velocity of the ejected electron at the boundary of the reaction zone:

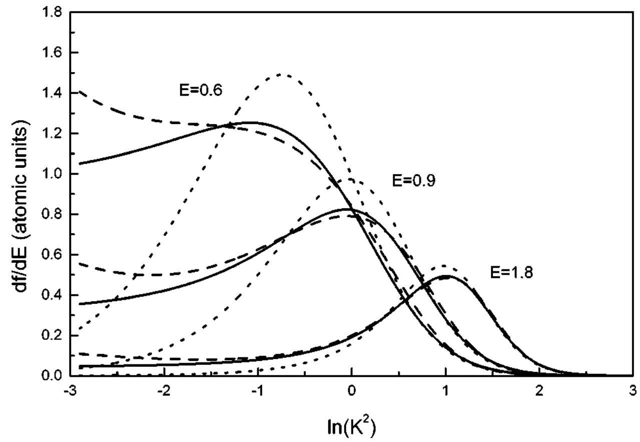

FIG. 1. GOS densities per unit range of excitation for impact ionization of H$(1s)$ for different energy transfers calculated by Eq. (19) with $\overline{\cos\theta}=1$ and $p_0=1$ (dashed lines) along with the FBA ones by Eq. (2) (full lines). BEA results (dot lines) are plotted to show improvement by introducing the factor $f(t)$.

$$\dot{y}(0^+)=\sqrt{2E}. \quad (22)$$

The trajectory Eq. (20) gives

$$\dot{y}(0^+)=\sqrt{2E-1}\sqrt{(e+1)/(e-1)}. \quad (23)$$

Comparing Eq. (22) with Eq. (23), we have

$$e=4E-1. \quad (24)$$

Inserting Eqs. (21) and (24) into Eq. (20), the trajectory of the ejected electron from H$(1s)$ as a function of the energy transfer is obtained as

$$y=2\sqrt{\frac{2E}{2E-1}}\sinh\xi,$$

$$t=\frac{1}{(2E-1)^{3/2}}[(4E-1)\sinh\xi-\xi]. \quad (25)$$

$f(t)$ is now determined by Eq. (14) with the trajectory Eq. (25).

To examine the role played by $f(t)$, i.e., the classical trajectory given by Eq. (25), we first consider the factor $\overline{\cos\theta}$ in the case of large K, when the outgoing direction of the ejected electron can be approximated by the direction of $\boldsymbol{K}$, i.e.,

$$\lim_{K\rightarrow\infty}\overline{\cos\theta}=1. \quad (26)$$

Figure 1 shows the GOS densities as a function of the momentum transfer K for different energy transfers E calculated by Eq. (19) with $p_0=1$ for large K along with the GOS densities by FBA [Eq. (2)]. The BEA results [Eq. (7)] are also plotted to show the improvement by the expression. Conforming with the large-K approximation, the whole peak for large E and the large-K side of the peak for small E of the GOS density are well reproduced. The GOS density is better reproduced with $\overline{\cos\theta}=1$ for larger E, because the binding

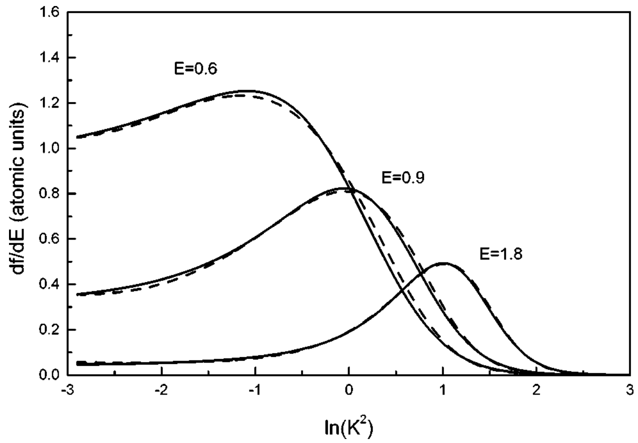

FIG. 2. The reproduction of the FBA GOS densities (full lines) by Eq. (19) with $\overline{\cos\theta}$ expressed by Eq. (29) and $\alpha=0.12$ (dashed lines).

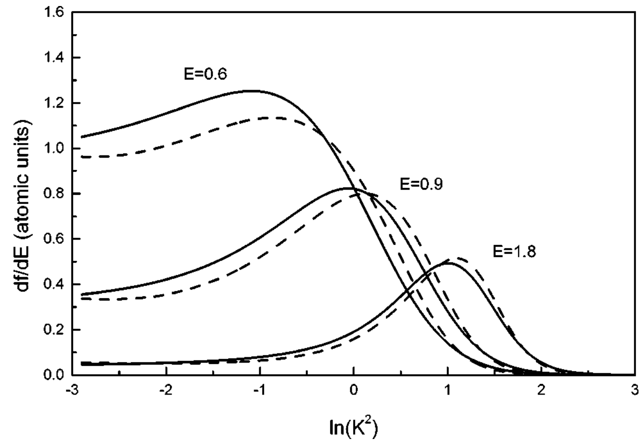

FIG. 3. Polarization effect to GOS densities given by Eq. (19) with $p_0=0.9$ (dashed lines) gives the correction to the FBA results (full lines).

energy of the atom becomes negligible in the involved collision and the ejected electron, behaving as if it were free, has an outgoing direction which is only determined by $\boldsymbol{K}$. This fact is reflected in the TDCS as a larger ratio of the binary-to-recoil intensity.

Further, we develop a simple formula for $\overline{\cos\theta}$ to give a better reproduction of GOS density of FBA which can serve as a base to make corrections to FBA. From Eq. (19) we have

$$\lim_{K\to 0}\frac{\partial f(E,K)}{\partial E}=\lim_{K\to 0}\frac{2E}{\pi K^2}\int_0^\infty dt[\cos(K^2/2-E)t+\sin(Et)K\overline{\cos\theta}f(t)]$$
$$=\lim_{K\to 0}\frac{2E\overline{\cos\theta}}{\pi K}\int_0^\infty dt\sin(Et)f(t). \quad (27)$$

When $K\to 0$, the GOS density of the electron impact ionization tends to the density of the optical oscillator strength, i.e., the photoabsorption cross section (apart from a universal constant), which has a limited value. So, according to Eq. (27), $\overline{\cos\theta}$ should have the tendency

$$\lim_{K\to 0}\overline{\cos\theta}=g(E)K, \quad (28)$$

where $g(E)$ is a function only depending on E. This behavior is easy to understand. If $K\to 0$, the ejected electron carrying the momentum $\sqrt{2E}$ will go out with uniform distribution of the direction as in the case of photoionization. With the increasing of K, the averaged direction of the ejected electron will be closer to the direction of K and depends on the ratio of K to $\sqrt{2E}$. With this consideration and Eqs. (26) and (28) we write

$$\overline{\cos\theta}=\frac{K}{K+\alpha\sqrt{2E}}, \quad (29)$$

where α is an adjustable parameter chosen to be 0.12.

Figure 2 shows the reproduction of the FBA for GOS density by Eq. (19) with Eq. (29).

IV. CORRECTIONS TO FBA

A. Target polarization

The polarization of the target by the incident electron has been included implicitly through the use of the Hartree-Fock wave function of the atomic electron [12,13] and explicitly by introducing an *ad hoc* polarization potential [14]. This effect was also studied by introducing into the Hamiltonian of the atomic electron a potential from the incident electron at a fixed distance [15].

In the expression Eq. (16) the polarization effect can be reflected in the initial-state momentum distribution of the atomic electron. In the first-order approximation, considering the total energy of the system, the attractive polarization potential used in the treatments in Refs. [9,14] should be in accord with the decreasing of the initial expectation momentum p_0 of the atomic electron in Eq. (19).

Figure 3 shows the polarization effect to GOS density with $p_0=1$ (FBA) being changed to $p_0=0.9$ calculated by Eq. (19). The left side of the Bethe ridge is decreased while the right side of the Bethe ridge is increased. For small E, the left side is changed more than the right side. For large E, the change is to move the Bethe ridge toward large K.

Because the integration of GOS density over K is related to the single-differential cross section (SDCS) as [1]

$$\frac{d\sigma}{dE}=\frac{2\pi}{E_0E}\int\frac{\partial f(E,K)}{\partial E}\frac{dK}{K}=\frac{\pi}{E_0E}\int\frac{\partial f(E,K)}{\partial E}d(\ln K^2) \quad (30)$$

and the higher total cross section (TCS) for H calculated by FBA at small and intermediate incident energy E_0 is due to the higher SDCS at small E, the decreasing of the GOS density for small E in Fig. 3 by the inclusion of the target polarization will improve the FBA calculations.

B. PCI effect

The postcollision interaction (PCI) effect, which is neglected in FBA, for the scattered electron, is the affection from the ion and the ejected electron system; for the ejected electron, it is affection from the scattered one. These affections can give the two outgoing electrons additional acceleration or deceleration, depending on the relative positions of the two electrons with respect to the residual ion or the outgoing direction of the ejected electron [6,7]. Because for GOS density the outgoing direction of the ejected electron has been integrated, the PCI effect contributed either by the scattered electron or by the ejected one should be less than for the TDCS.

For small E, when the collision process has an asymmetrical geometry, the scattered electron is far away from the ejected electron, and the ejected electron has an almost uniform distribution of the outgoing direction. So, for the scattered electron the ion field is almost fully screened and for the ejected electron the repulsion potential from the scattered electron is weak and averaged out.

For large E, the ion potential has less importance in the collision process, which corresponds to the fact that the factor $f(t)$ reflecting the contribution from the ejected electron tends to zero. And from Eq. (19) most of the collisions will take place at $E = K^2/2$; any changes of E and K which correspond to the contribution of the scattered electron will not affect much the GOS density. In fact, when the collision in this case is like the one between two free electrons, the PCI effect loses its meaning.

For intermediate E, the ejected electron no longer screens out the ion potential and feels the repulsion potential from the scattered one. We consider the relative contributions from the two electrons by Eq. (19). The contribution from the ejected electron can be included in the factor $f(t)$ with the correction to the classical trajectory in the Coulomb field. The contribution from the scattered electron can be included in the changes of E and K as in Refs. [6,7]. The relative positions of the two electrons can be classified into two kinds: The averaged position of the ejected electron and the position of the scattered one are on the same side or a different side with respect to the ion. In the former case, the ejected electron will be decelerated by the scattered electron in the outgoing direction and the scattered electron will be accelerated by the ion and the ejected electron system in its outgoing direction. This can be described by the decreasing of $y(t)$, and therefore the increasing of $|f(t)|$ and the increasing of E and K. In the latter case, the ejected electron will be accelerated and the scattered one decelerated, which makes $|f(t)|$, E, and K decrease.

With these changes of $|f(t)|$, E, and K in Eq. (19), the two electrons will give opposite PCI contributions to the GOS density. This can also be understood from Fig. 1. The lower $|f(t)|$ makes the GOS density more like the one for a free-electron collision, i.e., the BEA one, which is lower on the left side of the Bethe ridge and higher on the right, while the corresponding lower E and K will move the Bethe ridge forward left. In the other case, the contribution of the higher $|f(t)|$ is also opposite the one of higher E and K. So although for intermediate E the two electrons will give more contributions to the PCI effect separately, their total contribution is still small.

V. CONCLUSIONS

The linear-response representation of the GOS density can reproduce the FBA result by describing the initial state of the atomic electron with its momentum distribution and the final states of the ejected electron by its classical trajectory. Further, it makes it convenient to include some corrections to the FBA. The target polarization expressed by the decreasing of the initial expectation momentum of the atomic electron decreases the GOS density for small E and moves the Bethe ridge toward higher K for larger E. This effect can improve the FBA calculation for SDCS and TCS. The PCI effect should not be remarkable for GOS because the contributions from the scattered and ejected electron are not only small due to the integration of the outgoing direction of the ejected electron but also are opposite, as given by the expression.

With the other advantages of the linear-response representation of the GOS density such as the avoiding of the calculation of the nondiagonal matrix element between the initial and continuum state in Eq. (1) and the direct relation to the generalized complex dielectric constant of the medium, this expression can be extended to calculate the more complicated targets.

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