How the Klein–Nishina formula was derived: Based on the Sangokan Nishina Source Materials

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Abstract: In 1928, Klein and Nishina investigated Compton scattering based on the Dirac equation just proposed in the same year, and derived the Klein–Nishina formula for the scattering cross section of a photon. At that time the Dirac equation had the following unsettled conceptual questions: the negative energy states, its four-component wave functions, and the spin states of an electron. Hence, during their investigation struggles, they encountered various difficulties. In this article, we describe their struggles to derive the formula using the “Sangokan Nishina Source Materials” retained in the the Nishina Memorial Foundation.

Keywords: Klein–Nishina formula, Dirac equation, semi-classical treatment, field quantization, negative energy states

1. Introduction

In Compton scattering, the scattering of an X-ray by an electron, the wavelength of the scattered X-ray varies with the scattering angle. In 1923, using the light quantum theory for X-rays, A.H. Compton1) explained the wavelength shift upon scattering by using the conservation principle of energy and momentum of the light quantum and electron system. This analysis showed that the Compton effect was one of the important experimental facts confirming the quantum theory of light.

In his analysis concerning the angular distribution of the intensity of the scattered wave, Compton used relativistic theory and the Doppler effect. In 1926, Breit2) discussed this problem using the correspondence principle in the old quantum theory, and obtained the same result as what Dirac3) and subsequently Gordon4) obtained independently, using quantum mechanics.

They deduced the energy and momentum conservation law on the light-quantum and electron system quantum mechanically, which Compton hypothesized, and derived a formula giving the angular distribution of the intensity of the scattered wave. In 1927, Klein5) discussed how the interaction between an electron and an electromagnetic field including Compton scattering should be treated quantum mechanically. As for Compton scattering, he obtained energy-momentum conservation for the Compton scattering, but did not show the intensity distribution of the scattered wave. In 1927, Gordon4) and Klein5) independently developed the so-called Klein–Gordon equation to describe the behavior of an electron to include relativistic effects in Compton scattering. The energy and momentum relation of an electron used by Dirac3) was equivalent to that of the Klein–Gordon equation.

Soon after Dirac presented his relativistic electron theory,5),7) O. Klein and Y. Nishina succeeded to derive the famous Klein–Nishina formula,8),9) calculating the intensity distribution of the scattered wave in the Compton scattering based on the Dirac equation. The Klein–Nishina formula has been firmly accepted and widely used, even now.

When Klein and Nishina started to attack this problem, they intended in part to confirm the validity of the Dirac equation, as stated in Introduction of Ref. 8. Recalling that time, Bohr wrote to Nishina in 193410),11) that “the striking confirmation which this formula has obtained became soon the main support for the correctness of Dirac’s theory when it was apparently confronted with so many grave difficulties.” Ekspong discussed in Ref. 12, that the experiments conducted to confirm the Klein–Nishina formula were to suggest the existence of then unknown phenomena, namely the pair production and annihilation of positive and negative electrons.

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The following arguments in this article are based on the Sangokan Nishina Source, preserved by the Nishina Memorial Foundation. In Section 2 through Section 5, we survey Klein–Nishina’s theory and consider the process they undertook when deriving their formula. In Section 6 and Section 7, we look back their efforts to solve the most difficult problem for them, namely how to set the final states of the electron after scattering, and consider why they adopted the semi-classical method in treating electromagnetic waves. Finally, in Section 8, we discuss the equivalence between Klein–Nishina’s semi-classical method and the quantum field theoretical method.

2. Works preceding to Klein–Nishina’s theory

In this section we give the energy and momentum conservation law on the Compton scattering presented by Compton, himself, and the equation of the frequency shift accompanying the scattering. The energy and momentum conservation laws were regarded as being a basic hypothesis in Compton’s and Breit’s papers. In Section 2 through Section 5 we adopt the notations used by Klein and Nishina: \( h \) denotes Planck’s constant divided by \( 2\pi \) and \( \nu \) denotes frequency multiplied by \( 2\pi \), while \( m \) and \( -e \) are the mass and charge of an electron and \( c \) is the velocity of light in a vacuum.

The energy and momentum of a light quantum having frequency \( \nu \) and propagating direction \( \mathbf{n} \) are given by \( h\nu \) and \((h\nu/c)\mathbf{n}\). Suppose the frequency and propagating direction of a light quantum before and after the scattering are \( \nu, \mathbf{n} \) and \( \nu', \mathbf{n}' \), respectively, and the momenta of an electron before and after the scattering are \( 0 \) and \( \mathbf{p} \), respectively, then the energy and momentum conservation laws are given by

\[
\begin{align*}
\nu' &= \frac{\nu}{1 + \alpha(1 - \cos \theta)}, \\
\alpha &= \frac{h\nu}{mc^2}
\end{align*}
\]

2.1 Dirac’s theory. Dirac3) treated Compton scattering based on quantum mechanics for the first time, using his \( q \)-number algebraic method. As the first step, he developed a general theory of a quantum mechanical multi-periodic system.

For simplicity, we take here a system in which the degree of freedom is unity. The periodic system is defined by the following properties 1), 2) and 3) (we consider a system consisting only electrons without any electromagnetic field):

1) The system is to be described by a set of canonical variables, \( J \) and \( w(J) = ih \).
2) The Hamiltonian, \( H \), of this system is to be expressed by a function of \( J \) only, namely \( H(J) \).
3) The coordinate \( x \) and momentum \( p \) of this system are both to be expanded in the form \( x = \sum_n C_n(J)e^{i\omega n} \) and \( p = \sum_n D_n(J)e^{i\omega n} \), where \( C_n(J) \) and \( D_n(J) \) are amplitudes and \( \alpha \)'s are integers.

The term \( e^{i\omega n} \) is related to the transition of the system from the state \( J' \) to the state \( J' - h \). The frequency of radiation due to this transition is \( \nu = [H(J') - H(J' - h)]/h \). Then, the intensity of the emitted radiation observed in the direction perpendicular to the \( x \)-axis is obtained by substituting \( C_n(J') \) for the amplitude of the displacement of the charged particle in the formula for the intensity of dipole radiation, namely

\[
I = \frac{\nu^4}{8\pi^2c^2} \left| C_0(J') \right|^2,
\]

where \( r \) denotes the distance between the position of the charged particle and the observation point. This is the fundamental assumption of Dirac’s theory. This indicates that the interaction between a charged particle and an electromagnetic field should be handled by replacing quantities in the classical theory with their quantum mechanical alternatives, as was done in the semi-classical treatment of the electromagnetic field used by Gordon and Klein, as shown later.

We apply the above-mentioned general theory to an electron in an incident electromagnetic wave. Taking into account only the oscillating term, we can apply the definition of the periodic system to the electron considered here. Using his proper mathematical insight, Dirac succeeded to construct a set of canonical variables, \( J \) and \( w \), which describe scattering with the original variables \( x, p, t \), and \( E \). The transition from \( J \) to \( J' - h \) corresponds to a scattering process; in addition he showed that \( \nu' = [H(J') - H(J' - h)]/h \), \( \Delta J = -h \) and \( \Delta J_2 = \Delta J_3 = 0 \), where \( J_2 \) and \( J_3 \) were remaining variables commut-able with \( J \) corresponding to the energy and momentum conservation laws. Then the intensity of the scattered wave can be obtained using Eq. [2-3] as

\[
I = \frac{\nu^4}{r^2m^2c^4} I_0 \frac{\sin^2 \phi}{[1 + \alpha(1 - \cos \theta)])},
\]
where $I_0$ is the intensity of the initial wave, $\theta$ is the scattering angle, and $\phi$ is the angle between the propagating direction of the scattered wave and the direction of the electric field accompanying the incident wave.

### 2.2 Gordon’s theory.

We now explain Gordon’s theory in some detail, since his work has a close relation to Klein–Nishina’s work. Gordon treated the scattering of an electromagnetic wave by an electron based on the correspondence principle, which means that at first writing down the classical equations of the interaction between an electron and an electromagnetic wave, and then replacing the quantities, such as the current density or the charge density, with the corresponding quantum mechanical expressions. Gordon’s theory can be characterized by compromising the use of classical and quantum mechanical theories, which came to be called a “semi-classical treatment” later.\(^1\)\(^1\)\(^2\) Gordon discussed the dynamics of an electron in an electromagnetic field using purely classical theory and quantum-mechanical theories, which came to be called a “semi-classical treatment” later.\(^1\)\(^1\)\(^2\) Gordon treated the scattering of an electromagnetic wave, and operated it on the wave function, replacing the Hamiltonian, we derived his non-relativistic wave equation, we analyze the Klein–Nishina formula was derived: Based on the Sangokan Nishina Source MaterialsNo. 6, Gordon discussed the semi-classical treatment, which came to be called a “semi-classical treatment” later.\(^1\)\(^1\)\(^2\). Gordon called this treatment as “the correspondence principle”, and took it as a basis for the validity of the semi-classical treatment, while Klein\(^5\) called the semi-classical treatment, itself, as the “correspondence principle method”.

(a) Klein–Gordon equation. In classical theory, the basic equations of an electron in an electromagnetic potential $A$ and $V$ are given by the relativistic Hamilton–Jacobi’s equation,

$$ -\frac{1}{c^2} \left( \frac{\partial W}{\partial t} - eV \right)^2 + \sum_{k=1}^{3} \left( \frac{\partial W}{\partial x_k} + \frac{e}{c} A_k \right)^2 + m^2 c^2 = 0 $$

Following the procedure that Schrödinger took when he derived his non-relativistic wave equation, we replace $\frac{\partial W}{\partial x_k}$ and $\frac{\partial W}{\partial t}$ in the Hamilton–Jacobi’s equation by

$$ \frac{\partial W}{\partial x_k} \rightarrow \frac{\hbar}{i} \frac{\partial}{\partial x_k}, \quad \frac{\partial W}{\partial t} \rightarrow i\hbar \frac{\partial}{\partial t} $$

and operate it on the wave function, $\psi$.

We then obtain the following Klein–Gordon equation:

$$ \left[ -\frac{1}{c^2} \left( i\hbar \frac{\partial}{\partial t} + eV \right)^2 + \sum_{k=1}^{3} \left( \frac{\hbar}{i} \frac{\partial}{\partial x_k} + \frac{e}{c} A_k \right)^2 + m^2 c^2 \right] \psi = 0 \quad \text{[2-5]} $$

(b) Charge density and current density. We define $\psi$ as a solution of Eq. [2-5] and $\varphi$ as its complex conjugate. We can then express the charge density, $\rho$, and the current density, $J$, as

$$ \rho = \frac{ie}{c^3} \left( \varphi \frac{\partial \varphi}{\partial t} - \varphi \frac{\partial \varphi}{\partial t} + \frac{2ie}{\hbar} V \varphi \psi \right), $$

$$ J = \frac{e}{i} \left( \varphi \text{grad} \psi - \psi \text{grad} \varphi - \frac{2i}{\hbar} \cdot \frac{e}{c} A \varphi \right) \quad \text{[2-6]} $$

Since these relations satisfy the equation of continuity, $\partial \rho / \partial t + div J = 0$, we can interpret $\rho$ and $J$ as being the charge density and the current density, respectively. Hereafter, the letter $J$ denotes the current density, though in sub-section 2.1, the letter $J$ denotes a canonical variable.

(c) Electromagnetic potential produced by an electron. We conjecture that the electromagnetic potential produced by an electron can be obtained by inserting $\rho$ and $J$ into the expression of the retarded potential in classical electromagnetic theory,

$$ A' = \frac{1}{c} \int \frac{|J|e^{-\frac{r}{R}}}{R} \, dr, \quad V' = \int \frac{|\rho|e^{-\frac{r}{R}}}{R} \, dr \quad \text{[2-7]} $$

where $R$ denotes the distance between the volume element $dr$ and the observation point. This is the fundamental hypothesis of the semi-classical treatment.

(d) Compton scattering. We assume here that the incident wave is a linearly polarized plane wave, and denote its electromagnetic potential as $\Phi_i = a_i \cos \nu(t - \mathbf{n} \cdot \mathbf{r} / c)$, where $i = 0, 1, 2, 3$; $\Phi_0 = V$; $\Phi_i = A_i$.

The solution of the Klein–Gordon Equation [2-5] can be obtained in the perturbed form of the solution of a free electron with momentum $p$.

$$ \psi(p) = C(p) e^{i(p \cdot r - E \nu)} \left( 1 + \text{[quantity of } O(a_i) \text{]} \times \sin \nu \left( t - \frac{\mathbf{n} \cdot \mathbf{r}}{c} \right) \right), $$

where $E$ denotes the energy of the free electron with momentum $p$, namely $E = \sqrt{c^2 p^2 + m^2 c^4}$. The coefficient $C(p)$ is the normalization factor, determined by the requirement of the correspondence principle in the $\hbar \rightarrow 0$ limit, resulting in normalization of the $\delta$-function type. Multiplying $\psi(p)$ by the weight factor, $z(p)$ (real quantity), and superposing them, we can write down the general solution as

$$ \Psi = \int z(p) C(p) \psi(p) dp. $$
When $\Psi$ is inserted into the expression of $\rho$ and $J$ of eq. [2-6], the electromagnetic potential of the scattered wave can be obtained using Equation [2-7] as

$$\Phi'_\nu = \frac{1}{r} \Re \int [\text{quantity of } O(\alpha_i)] \times z(p) z(p') e^{i \Phi(p - p') r - \nu(t - \frac{r}{c})} dp dp' dr',$$

where

$$\nu' = \frac{E + h\nu - E'}{h}, \quad P = p + \frac{h\nu}{c} n - \frac{E + h\nu}{c} n', \quad P' = p' - \frac{E'}{c} n'.$$

Here, the equation of $\nu'$ gives the energy conservation law of the photon and electron system, and integration over $r'$ gives $\delta(P - P')$, which reduces to the momentum conservation law. Taking the weight factor $z(p)$ and $z(p')$ into account, we obtain the electromagnetic potential related to the elementary process of the scattering $p \to p'$,

$$\Phi'_\nu(p \to p') = \frac{e c}{2r} \begin{pmatrix} [\text{quantity of } O(\alpha_i)] & \cos \nu' \left( t - \frac{r}{c} \right) \end{pmatrix},$$

[2-8]

where $\Delta \Delta'$ denotes the Jacobian of the transformation $p, p' \to P, P'$. Setting the initial state of the electron as $p = 0$, we can calculate the intensity of the scattered wave using the electromagnetic potential [2-8] and obtain the same conclusion as that of Dirac, given by Equation [2-4].

3. Klein–Nishina’s theory

Klein and Nishina calculated the intensity of the scattered wave in the Compton scattering based on the same framework as Gordon and Klein, except for adopting the Dirac equation as the equation for describing the behavior of an electron. In the following we briefly discuss how they did this. Note that we use the same equation numbers as those used by Klein and Nishina in their paper, for example [KN-1].

(a) Dirac equation. Under the electromagnetic field $(A, V)$ the Dirac equation is written as

$$\frac{1}{c} \left( i \hbar \frac{\partial}{\partial t} + eV \right) \psi + \rho_1 \left( \sigma, -i \hbar \frac{\partial}{\partial r} + \frac{e}{c} A \right) \psi + \rho_3 mc \psi = 0,$$

[KN-1]

where $\sigma$ is a 3-dimensional vector of 4×4 spin matrices; $\rho_1, \rho_2$ and $\rho_3$ are 4×4 matrices that are mutually anti-commutate, and each is commutate with $\sigma$; the notation $(\ldots, \ldots)$ in the second term denotes the scalar product (henceforth, we write down a scalar product of $A$ and $B$ as $(A B)$ following the original authors’ notation). The wave function $\psi$ has four components and is expressed as a 4×1 matrix. By denoting the Hermitian conjugate wave function of $\psi$ as $\varphi$, the charge density $\rho$ and the current density $J$ are given by

$$\rho = -e\varphi \psi, \quad J = c e \varphi \sigma_3 \psi,$$

[KN-3]

which satisfy the equation of continuity, $\partial \rho/\partial t + \text{div } J = 0$.

(b) Free electron. The Dirac equation for a free electron is obtained by setting $A = V = 0$ in [KN-1], and the solution is written in the following form:

$$\psi_0(p) = \psi(p) e^{-i(E(t - p)/c)},$$

[KN-4]

where $\psi(p)$ is a 4×1 matrix independent on $r$ and $t$, and satisfies the equation

$$\begin{pmatrix} E/c + \rho_1 (\sigma p) + \rho_3 mc \end{pmatrix} \psi(p) = 0.$$  

[KN-5]

Here, $E$ and $p$ are the energy and momentum, respectively, satisfying the relativistic relation $E^2/c^2 = m^2c^2 + p^2$. Note that $E$ can take both positive and negative values for a given $p$, and $\psi(p)$ has four solutions, two of which belong to negative values of $E$. The two solutions of each sign of $E$ reflect degenerate spin states. Normalization of the wave function is given by

$$\int \psi_0(p)^* \psi_0(p') \psi(p) \psi(p') dp dp' = \delta(p - p').$$

Note that $E > 0$.

Solutions for $p \neq 0$, $v^\pm(p)$ can be obtained by operating the Lorentz transformation unitary operator $S^{-1}(p) = \alpha - i\beta p_4(\sigma p)$ to the solutions for $p = 0$, i.e., $v^\pm(0)$,

$$v^+(p) = S^{-1}(p) v^+(0).$$  

[KN-18]

Klein elaborated on this method of the Lorentz transformation, which played an important role in the “problem of final states”, discussed in Sec. 6.

(c) Solutions of the Dirac equation under radiation field. We write down the perturbed solution of the Dirac equation under an incident radiation field described by the vector potential,

$$A = a e^{i \nu t (\mathbf{r} - \mathbf{r}')} + \text{c.c.}$$

[KN-22]
The perturbed solution is written down in the form of the solution of a free electron with momentum $p$, modified by the incident radiation field as

$$\psi(p) = [1 + g(p)e^{i\psi(t-(nr)/c)} + \tilde{g}(p)e^{-i\psi(t-(nr)/c)}] \psi_0(p),$$

where $g(p)$ does not mean the complex conjugate of $g(p)$, but merely means the coefficient of $e^{-i\psi(t-(nr)/c)}$. Rewriting the Dirac equation in the second-order equation and inserting the form of [KN-23] into the wave function, $\psi$, in the rewritten Dirac equation, we find $g(p)$, $\tilde{g}(p)$ in the first-order approximation of the amplitude $a$ of the field. Then, $g(p)$ is given by

$$g(p) = [\text{sum of three terms including } (ap), \sigma, \text{ and } a, \rho_1, \sigma \text{ and } a]$$

and $\tilde{g}(p)$ is given by a similar form.

\(\text{(d) The field of the scattered wave.}\) Superposing the perturbed solutions described above, we obtain the general solution

$$\Psi = \int \psi(p) dp, \quad \Phi = \int \Phi(p) dp$$

This is the necessary process to extract the term describing the elementary process of the transition $p \rightarrow p'$, as we discussed concerning Gordon’s theory earlier. The current density, $J$, in this general solution is given by

$$J = \frac{cc}{\hbar} \int \phi(p) \rho_1 \sigma \psi(p') dp dp'$$

Inserting the expression $\psi(p)$ [KN-23] into [KN-29] and extracting linear terms in the amplitude of the incident wave $a$, we obtain the current density produced by the incident wave, which in turn produces the scattered wave. The vector potential of the scattered wave is obtained by inserting the above current density into the classical expression of the retarded potential [2-7]. This is an essential procedure of the corresponding principle method. Hence, as in the Gordon’s analysis, the energy and momentum conservation laws for the photon-electron system can be derived and the vector potential, $A(p, p')$, of the $p \rightarrow p'$ scattering process is given by

$$A(p, p') = \frac{e(2\pi \hbar)}{r\sqrt{\Delta \Delta'}} (e^{i\psi(t-\Delta')} u(p) | \rho_1 \sigma \tilde{g}(p) | + f(p) | \rho_1 \sigma | \tilde{v}(p') | + \text{c.c.})$$

Here, $f(p)$ denotes the Hermitian conjugate of $g(p)$ and $\Delta \Delta'$ denotes the Jacobian of transformation. The magnetic field, $H(p, p')$, of the scattered wave is given by $H(p, p') = \text{rot} \ A(p, p') = \dot{u}'/c A(p, p') \times n'$. Assuming that the initial momentum, $p$, of the electron is zero, we define $H(0, p) = H_0$. The terms $g(p)$ and $\tilde{g}(p)$ in [KN-36] contain the terms $\sigma$ and $\rho_0 \sigma$, as shown in [KN-25], and [KN-36] has such a structure that $g(p)$ and $f(p)$ multiplied by $\rho_0 \sigma$ are placed between $u(p)$ and left and $v(p')$ on right. Using the arithmetic rule on $\sigma$ and the equation that each of $u(p)$ and $v(p')$ satisfies, we can express each term in $[\text{KN-36}]$ in terms of $d = u(p) v(p')$, $s = u(p) \sigma v(p')$, and their complex conjugates. We then obtain

$$H_0 = [\text{sum of linear terms in } d, \text{ s}] e^{i\psi(t-\Delta')} + \text{c.c.}$$

\(\text{(e) Calculation of the intensity of the scattered wave.}\) The intensity of the scattered wave, $I$, is given by the time average of the Poynting’s vector,

$$I = \frac{c}{4\pi} \langle E_0 \times H_0 \rangle_{\text{time average}} = \frac{c}{4\pi} \langle H_0^2 \rangle_{\text{time average}}$$

Here, $E_0 = E(0, p')$, just like $H_0 = H(0, p')$. A calculation of $H_0^2$ requires calculating the bilinear products of $d, s, \bar{d}$, and $\bar{s}$. Because of the spin degeneration, we should take two mutually independent states into consideration as the final states of the electron with momentum $p'$. In the calculation of $H_0^2$, we take the sum of the contribution from these two spin states, unless we discuss a certain spin state as the final state. Klein–Nishina’s \(s^3\) treated this matter as follows. They assumed $v(p')$ to be expressed as the sum of $v^+(p')$ and $v^-(p')$ with arbitrary phases $\delta_1$ and $\delta_2$,

$$v(p') = v^+(p')e^{-i\delta_1} + v^-(p')e^{-i\delta_2}$$

In calculating the bilinear products of $d, s, \bar{d}$, and $\bar{s}$, we take the average on these phases. This procedure corresponds to taking the sum of the contributions from two final states, $v^+(p')$ and $v^-(p')$. Taking the average over phases of $\delta_1$ and $\delta_2$, we obtain the necessary calculation rules, given by

$$[\langle BS \rangle(CS) = \gamma[(BC) + il \cdot (B \times C)]]$$

Here, $B$ and $C$ are arbitrary constant vectors and $l$ is a unit vector along the spin direction in the initial state of the electron; long bars denote the average over the phases and short bars over $d$ and $s$ denote complex conjugates. Using the above calculation rules we can perform arithmetic calculations for $H_0^2$ and obtain the following result for a linearly polarized incident wave:
\[ \overline{H}_0^2 = \frac{e^4}{m^2c^2\rho^2} \left( \frac{\nu}{\nu'} \right)^3 \left[ \left( \frac{\nu}{\nu'} + \frac{\nu'}{\nu} \right) \varepsilon^2 - 2(n'\varepsilon)^2 \right]. \]

where \( \varepsilon \) denotes the amplitude of the electric field of the incident wave and \( n' \) denotes the scattering direction. Setting the scattering angle as \( \theta \) and the angle between the scattering direction and the direction of the polarization of the incident wave as \( \phi \), and taking into account \[2-2], \( \nu' = \nu/[1 + \alpha(1 - \cos \theta)] \), we obtain the intensity, \( I \), of the scattered wave:

\[ I = I_0 \frac{e^4}{m^2c^4\rho^2} \cdot \frac{\sin^2 \phi}{(1 + \alpha(1 - \cos \theta))^3} \cdot \left[ 1 + \alpha^2 \left( \frac{1 - \cos \theta}{2\sin^2 \phi(1 + \alpha(1 - \cos \theta))} \right)^2 \right] \]

Here, \( I_0 \) denotes the intensity of the incident wave, \((c/4\pi)2e^2\); the factor 2 comes from the electric field of the incident wave, being written as \( \varepsilon \left[ e^{i\nu(t-\nu/\rho)} + e^{-i\nu(t-\nu/\rho)} \right] \). Comparing [KN-59] with [2-4], we see that the difference between Klein–Nishina’s theory and Dirac’s or Gordon’s theories is in the second term added in the brackets of [KN-59]. By multiplying both sides of [KN-59] by \( (I/h\nu')/(I_0/h\nu) \), we obtain the differential cross section of photons as

\[ \frac{d\sigma}{d\Omega} = \frac{1}{2} \frac{e^4}{m^2c^4} \left( \frac{\nu}{\nu'} \right)^2 \left[ \left( \frac{\nu}{\nu'} + \frac{\nu'}{\nu} \right) - 2(n'\varepsilon_0)^2 \right] \]

This result is obtained after summing over the electron spin and over the polarization of the scattered photon.\[11,12\] This indicates that the correspondence principle method used to derive [KN-59] implicitly included the above-mentioned procedure.

4. Nishina’s individual paper

Immediately after joint papers with Klein, Nishina by himself wrote subsequent papers\[13,14\] concerning polarizations of the scattered electromagnetic wave. In the classical theory for Thomson scattering, electron spins are not considered, and a linearly polarized incident wave remains to be linearly polarized even after it is scattered by an electron. The same condition holds, in Dirac\[3\] and Gordon’s theories. On the other hand, in the Klein–Nishina theory based on the Dirac equation, the incident wave is linearly polarized, but the scattered wave is generally elliptically polarized, consisting of two mutually incoherent elliptical polarizations, produced by the transition of the electron to two mutually independent final states. This point is clearly different from the result of Dirac’s and Gordon’s theories. Therefore, experiments on this can confirm the validity of Klein–Nishina theory and, moreover, of the Dirac equation. For this purpose, using the experimental conditions at that time, Nishina calculated the intensity distribution of the doubly scattered wave with the scattering direction being normal to each other on the result of the Klein–Nishina work.

Here, we follow Nishina’s calculation. First we rewrite the expression for the magnetic field of the scattered wave [KN-44] in Klein–Nishina’s paper; we separate the scattered wave into two mutually independent elliptically polarized components in the following way. In this section we use the same equation numbers as those used in Nishina’s paper:\[11\]:

\[ H_0 \propto (A - iB)e^{i\nu/(-\nu + \delta_1)} - (D + iC)e^{i\nu/(-\nu + \delta_2)} + c.c. \]

\[ N-2 \]

where \( \delta_1 \) and \( \delta_2 \) are arbitrary phases, as in section 3, expressing the final states of the electron, \( v^+(p')e^{i\nu_1} + v^-(p')e^{i\nu_2} \). Here, \( A, B, C \) and \( D \) denote vector functions, though in other places \( A \) denotes the vector potential. The electric field of the scattered wave, \( E_0 = H_0 \times n' \), can be written as

\[ E_0 \propto (A' - iB')e^{i\nu/(-\nu + \delta_1)} - (D' + iC')e^{i\nu/(-\nu + \delta_2)} + c.c. \]

\[ N-3 \]

Then, the magnetic field of the scattered wave for an elliptically polarized incident wave can be obtained on the basis of [KN-44] by setting the electric field \( E \) of the incident wave as

\[ E = (\varepsilon_a + i\varepsilon_b)e^{i\nu/(-\nu + \delta_2)} + c.c. \]

\[ N-5 \]

The intensity of the scattered wave depends on the spin direction, \( I \), of the electron in the initial state. This is different from that of a linearly polarized incident wave. If we average over the direction \( I \), we can obtain the intensity as a simple sum of the intensities in a linearly polarized incident wave given by [KN-59], with replacing \( \varepsilon \) in \( I_0 \) by \( \varepsilon_a \) and \( \varepsilon_b \). Thus, we obtain the intensity for elliptically polarized incident wave as

\[ I = \frac{e^4}{4\pi m^2c^2\rho^2} \cdot \frac{1}{(1 + \beta)^3} \left[ \frac{2 + 2\beta + \beta^2}{1 + \beta} (\varepsilon_a^2 + \varepsilon_b^2) - 2[(n'\varepsilon_a)^2 + (n'\varepsilon_b)^2]^2 \right] \]

\[ N-7 \]

where \( \beta = (hc/m\nu)(1 - nn') \), \( n \) denotes the incident direction, and \( n' \) denotes the scattered direction. We then obtain the intensity of the doubly scattered wave under the experimental conditions at that time;
the linearly polarized incident plane wave along the \(x\)-axis is scattered to the \(y\)-axis direction, and is then scattered again by the second electron on the \(y\)-axis. This secondly scattered wave is observed in the \(x-z\) plane. The electric fields of the two mutually incoherent elliptically polarized waves scattered by the first electron are determined by \([N-3]\). Inserting the obtained electric fields into \(\varepsilon_x\) and \(\varepsilon_y\) in \([N-7]\) and summing them, we obtain the intensity of the secondly scattered wave. Averaging over the direction of polarization of the linearly polarized incident wave, we obtain the averaged intensity, \(I_t\), given by

\[
I_t = \frac{e^8}{2m^4c^2r^2r^2} \frac{I_0}{(1 + 2\alpha)^3} \times \left[ \sin^2 \Theta + \frac{\alpha^2(2 + 4\alpha + 3\alpha^2)}{2(1 + \alpha)^2(1 + 2\alpha)} \right], \quad [N-14]
\]

where \(\Theta\) denotes the angle between the direction of observation and the \(z\)-axis, \(r\) denotes the distance between the first and the second electron and \(r^2\) is the distance between the second electron and the point of observation. The equation for \(I_t\), based on Dirac’s or Gordon’s theories, contains only the first term, \(\sin^2 \Theta\) in \([N-14]\). Note that Nishina’s result has an additional constant term that is independent of \(\Theta\).

5. The derivation process of the Klein–Nishina formula revealed through the “Sangokan Nishina Source Materials”

Concerning the background of the start of Klein and Nishina’s work, Klein wrote in his private note\(^{(5)}\) as follows:

Our nearer acquaintance, which then grew into friendship began in the spring 1928, I believe a little before Eastern\cite{sic}. He had just returned from a visit to Hamburg then, where he had met Pauli and Gordon, while I had been in Cambridge to see Dirac, whose first paper on the electron had just appeared. At about the same time also Gordon came on a little visit to the Bohr institute. He and I had earlier worked on the Compton effect independently of each other— he with Schrödinger in Berlin, I in Copenhagen— his paper with the complete solution appearing before mine was finished. And naturally we had both of us been thinking how this effect would come out according to Dirac’s new theory. I remember Gordon saying, when we all three were standing together: “Das mag ein gutes Problem für Herrn Nishina sein” (This might be a good problem for Mr. Nishina), and I, who had intended to attack that problem myself, agreed immediately.

As for Nishina, this problem was related to his previous work at Copenhagen on an experimental study of the absorption spectra of X-rays. Since then he had constantly paid attention to X-ray spectroscopy studies, although he became deeply interested in theory at the advent of quantum mechanics.\(^{(6)}\) Moreover, in the fall of 1927, he moved to Hamburg, and then in collaboration with I.I. Rabi he theoretically investigated the absorption coefficient of X-rays\(^{(11), (17)}\) while learning quantum theory under Pauli. He was thus deeply involved in X-ray research. Therefore, it was natural that the idea of treating Compton scattering based on the Dirac equation occurred to Nishina in Hamburg where they encountered the appearance of the Dirac equation with great enthusiasm.\(^{(11), (18)}\) Indeed he wrote to Dirac on 25th Feb. 1928,\(^{(19), (20)}\) “I hope to calculate Compton effect according to your new theory”, while he was studying in Hamburg before he came back to Copenhagen in March, 1928.

Here, in Sec. 5, we trace the approach Klein and Nishina took to obtain the Klein–Nishina formula using the “Sangokan Nishina Shiryo” (Building No. 3 Nishina source materials) retained in the Nishina Memorial Foundation, Tokyo. Their details have been reported in References 21 and 22: how they became noticed, how they were investigated, and a summary of their contents. The main part of the Sangokan source materials consists of Nishina’s documents concerning his study abroad, especially in Copenhagen from 1923 to 1928, such as memorandum concerning his investigations, colloquium notes, correspondences.

In the Nishina Memorial Foundation, a voluntary investigation group, called “Tamaki Group”, was set up by Hideniko Tamaki together with Fukutaro Shimamura, Hajime Takeuchi and Yuji Yazaki. Besides a historical investigation on Nishina’s study abroad, they took up the task to list and assign consecutive numbers to each of the Sangokan Nishina Shiryo, for which H. Takeuchi was responsible. In 1991, they prepared a pamphlet called “Sangokan Nishina Shiryo no Naiyou Ichiran” (the contents of the Sangokan Nishina source materials). This pamphlet was edited by H. Takeuchi, T. Iwaki, H. Tamaki, F. Shimamura and Y. Yazaki. In 1994 this pamphlet was printed by the Nishina Memorial Foundation.
The Sangokan source materials contain documents on the Klein–Nishina formula, with assigned numbers of [166] through [218]. These documents contain Klein’s memorandums, Nishina’s memorandums, and correspondences between Klein and Nishina, Waller and Nishina, Skobeltzyn and Nishina, Skobeltzyn and Jacobsen.

5.1 Source materials concerning to Klein–Nishina’s joint paper. No draft or manuscript of the Klein–Nishina paper was found in the sources. This is probably because Klein undertook the writing of the final manuscript, although it is clear from Klein’s letters to Nishina (Ref. 23 and 24) that they discussed closely until they reached the final stage of the manuscript, just before Nishina’s departure from Copenhagen. Nevertheless, we find a note in Nishina’s handwriting (source No. [174]) corresponding to a semidraft with expository writing in German, in which the main points before the calculation of the intensity of the scattered wave were elaborately stated. This indicates important suggestions concerning the development of their ideas to treat the final states of the electron, discussed later in Sec. 6.

Now we divide the evolution of Klein–Nishina’s theory into four stages, with sources at each stage:

1. Finding solutions of the Dirac equation perturbed by an external electromagnetic field ([KN-23]–[KN-27]).
2. Formulating an expression of the vector potential of the scattered wave ([KN-36]).
3. Formulating the vector potential and magnetic field of the scattered wave in the form of a linear combination of $d = u(0)v(p')$, $s = u(0)\sigma v(p')$ and $d, s$ ([KN-44]).
4. Finding expressions of the magnetic field of the scattered wave$^2$ and the intensity of the scattered wave ([KN-58]–[KN-60]).

Many calculation memorandums can be categorized to not only one particular stage, but to several stages. Since they have overlapping contents, we conjecture that the same kinds of calculations were repeated. In addition we find several errors in the calculations or ways of theorizing and assemblies of fragmental memorandums without meaningful procedures.

(a) The first stage (Perturbed solution of the Dirac equation).

Source [197]: Calculation memorandums (from the 1st stage to the middle of the 3rd stage)

The method taken to find the perturbed solution is essentially equivalent to that in the Klein–Nishina’s paper$^5$, though the procedure to reform the Dirac equation into the 2nd-order equation is somewhat different, and the obtained form of the perturbed solution is also apparently different from that in their joint paper.

Source [198]: Calculation memorandums (from the 1st stage to the middle of the 3rd stage)

The method taken to find the perturbed solution is the same as that taken in their joint paper, though here are contained in part errors in sign.

Source [204]: Calculation memorandums (the 1st stage)

The method taken to find the perturbed solution is the same as that in their joint paper with the correct answer.

Source [212]: Calculation memorandums by Klein (the 1st stage)

(i) the method in terms of the Fourier transformation

(ii) the same method as their joint paper are given.

(b) The second stage (Expression of the vector potential of the scattered wave).

Source [197]: Calculation memorandums (from the 1st stage to the middle of the 3rd stage)

The development process is discussed in detail, and the result is derived correctly, except for the point discussed below.

Source [198]: Calculation memorandums (from the 1st stage to the middle of the 3rd stage)

The calculation is advanced under an incorrect expression for $J = ce\phi(p_2\sigma)\psi$. In the aforementioned note [174], only the result obtained in [197] is written down, and in both sources the Jacobian of the transformation factor, $1/\sqrt{\Delta \Delta'}$, is missing. This factor, which appeared in the Gordon’s paper$^6$, is necessary to obtain the correct intensity. In the Klein–Nishinas’ paper$^6$ they stated that the integration was performed using the variable transformation “nach dem Vorgang von Gordon” (according to the precedent by Gordon) (Ref. 8, p. 861). However, since in the source [196] they at last took the Jacobian transformation factor into account, they must have realized the necessity of the factor sometime later.

Source [200]: Calculation memorandums (from the 2nd stage to the middle of the 3rd stage)

They adopted the expression of $J$, not $ce\phi(p_2\sigma)\psi$, but the same form written in terms of wave function and its derivatives as that used by Klein$^7$ and Gordon$^4$, and they calculated the vector potential. Klein’s calculation memorandums for deriving such an expression of $J$ are found in the source [203], and Nishina’s calculation memorandums for the same purpose are found in fragmented assembly sources [201] and [214]. Though this
The expression of $\mathbf{J}$ is not convenient for the calculation, they might have been interested in it because of former theories by Klein and Gordon, and tried to examine such a procedure. We note that minor errors exist in the expression of $\mathbf{J}$ in the above-mentioned sources: [200], [203], [201] and [214].

(c) The third stage (Concrete expression of the vector potential and the magnetic field of the scattered wave).

While in the second stage the expression of the vector potential contains 2nd-order terms in wave (from the 1st stage to the middle of the 3rd stage), in this third stage a technique to transform the vector potential into the linear combination of $d = u(0)v(\mathbf{p}^{'})$, $s = u(0)\mathbf{\sigma}v(\mathbf{p}^{'})$ and $\tilde{d}$, $\tilde{s}$ was employed based on the properties of the spin operator, $\mathbf{\sigma}$, and the solution of the Dirac equation for free electrons. Source [192]: Calculation memorandums (from the 3rd stage to the middle of the 4th stage)

Correct expressions are derived, except for the Jacobian factor. The result obtained here is taken into the note [174], which is mentioned in the beginning of this subsection 5.1.

Sources [197], [198], [200]: Calculation memorandums (from the 1st stage to the middle of the 3rd stage)

The vector potential is transformed into linear forms in $\mathbf{\sigma}$, though there remains $\rho_i$. Therefore, these sources should be regarded as representing the middle stage of the formulation.

Source [201-(i)]

The source [201] is an assembly of the fragmented calculation memorandums. We classified and reorganized it into several parts, each of which has some meaningful contents.

[201-(i)] is the calculation memorandums for the stages from the 2nd stage to the middle of the 4th stage. In the 2nd stage the vector potentials are not expressed in terms of $d$ and $s$, as above, but are expressed by substituting the direct matrix expressions into $\rho_i$ and $\mathbf{\sigma}$ in the expression of the vector potential [KN-36]: the vector potential is expressed in terms of the components of the wave functions of the initial and final states: $u_0$, $u_4'$, $u_2'$, $u_3'$ and $u_4'$. Here, a primitive calculation method is adopted instead of using the properties of spin operators. The result gives the correct expression of the vector potential, except for the Jacobian factor mentioned above. This method, however, does not give a clear view, and has to be judged as being inferior to that of their joint paper from the view point of the beauty of the theory. Therefore, this calculation method should be judged as no more than a primitive attempt.

(d) The fourth stage (Magnetic field of the scattered wave, the intensity of the scattered wave).

Since the expression for the magnetic field of the scattered wave obtained in the 3rd stage consists of 8 terms, each of which contains $d$ and $s$ in different ways and takes complicated forms containing scalar products and vector products, the algebraic calculation of the square of the magnetic field became very tedious. Regarding this point, Klein wrote an episode in Ref. 15:

But we still had to make some lengthy algebraic calculations in order to get the practical result. This involved the addition of a great many terms, and to be certain not to make any mistakes in the summation we decided to work separately each in his place, and finally our independent results agreed.

Source [189]: Calculation memorandums (the 4th stage, interrupted in the middle)

This source contains the same sort of calculation as those in their joint paper, mistakes in the calculations interrupted their calculation.

Source [196]: Calculation memorandums (the 4th stage, completed)

This is the only one source showing the procedure to the final result of the intensity of the scattered wave. The Jacobian is taken into account. These memorandums indicate that to proceed calculations properly they needed to manage to reshape the terms that appeared in the development, and to accumulate them into compact forms, using the relations between $\nu$, $\nu'$ (the frequencies of the incident and scattered wave) and $\mathbf{n}$, $\mathbf{n}'$ (the propagating directions of the incident and scattered wave), instead of blindly calculating.

There are two sources that show different approaches from their joint paper.

Source [192]: Calculation memorandums (from the 3rd stage to the middle of the 4th stage)

Including the rotation operator in spin space, and averaging over the spin direction of the electron in the initial state led them to derive the calculation rules for the intensity, similar to [KN-56]. On the other hand, in their joint paper they fixed the spin direction, $\mathbf{l}$, in the initial state and for a linearly polarized incident wave, they showed that the final intensity of the scattered wave was independent of the spin direction, $\mathbf{l}$. The method in [192] could have led to the correct result, but the calculation of the intensity is interrupted in the middle.
Following the primitive method of calculation already mentioned, \([\text{the vector potential}]^2\) was calculated. They probably intended to take the average over the spin directions in the final state, and hence the cross terms \(u^*_i \frac{\hbar^2}{2m} (i \neq k)\) of the 4 components of the wave function of the electron in the final state were dropped out, which is not valid. In Ref. 23, Klein wrote to Nishina that he made an important improvement on their theory concerning two points after Nishina left Copenhagen: One was related to the handling of the final states of the electron, which will be discussed later; the other was a technical improvement of the calculation of [magnetic field] using the matrix \(\mu\) given in their joint paper (p. 865), which is the projection operator to the state of \(\sigma_z = 1/2\) (or \(\sigma_z = -1/2\)) with \(E > 0\) in the static system of the electron*. Indeed, this method of using the matrix \(\mu\) was not adopted in the source [196].

According to the matters discussed above, we managed to understand how the formulation methods and the calculation techniques in each stage were developed through various gropings, especially the calculation techniques using the properties of the spin operators and handling the spin states.

The solution of the Dirac equation under a static magnetic field. Although not mentioned in their joint paper, there are sources showing that Klein and Nishina attempted to find a solution of the Dirac equation under a static magnetic field. We will discuss later this point.

Comparison with experiment. There are sources that show numerical calculations based on the Klein–Nishina formula compared with experimental data. At that time (1928–29), \(\gamma\)-rays emitted from RaC were used in experiments concerning Compton scattering. They contained several wavelength components, but there were no reliable data on the ratio of each component. Accordingly, in a Klein–Nishina's note to Nature,\(^9\) they stated that a comparison with the experiment was difficult. Nishina performed numerical calculations using the value of the wavelength and the intensity rate of each component obtained at that time.

Source [183]: The angular distribution of the intensity of the scattered wave for each component of wavelength.

Source [185]: The angular distribution of the total intensity of the scattered wave (Values due to Klein–Nishina and Dirac or Gordon are given.)

Source [187]: Scattering coefficient and transmission attenuation factor (Values due to Klein–Nishina and Dirac or Gordon are given.)

The experimental data are given in sources [186] and [188].

Source [186]: Data of the intensity ratio of \(\gamma\)-rays emitted from RaC.

Source [188]: Data of the angular distribution of scattering and the transmission attenuation factor.

In addition sequential letters including experimental data and preprints were sent from Skobelzyn,\(^25\) who measured the angular distribution of the scattered electrons using the Wilson chamber.

5.2 Source materials on the Nishina's single-name papers.\(^{13,14}\) In the source materials we find handwritten manuscripts of Nishina's single-name papers and their preparation notes. These calculation memorandums are well regulated because the methods that Nishina used were already established through joint work with Klein. Therefore, these notes have different features from those of the joint papers.

Here we pick out some noteworthy sources:

Source [167]: Handwritten manuscript for Zs. f. Phys.\(^{(15)}\)

This manuscript is different from the published paper in the following two points: First, Nishina took the two final states for the electron, and stated clearly about those that one had the same spin direction as that of the initial state, and the other had the opposite direction; however, in the published paper such definite expression was deleted. This is probably because, as written in the letter from Klein to Nishina,\(^{11,24}\) Klein corrected this point in Nishina's manuscript. Second, there is an error in the calculation of double scattering of the electromagnetic wave by electrons, where the frequency of the incident wave for the second scattering is different from that for the first scattering. In [167] this modification of the frequency is not included, while in the published paper this error is corrected. On this point, Klein\(^{11,23}\) wrote to Nishina that Bohr suggested to C. Møller that he should check Nishina's calculation memorandums, and he discovered the error. Klein submitted the corrected version of Nishina's paper to Zs. f. Phys. In the above-mentioned letter, Klein added the words for relief “a thing one would easily forget”.

Source [170]: Typewritten manuscript of Nishina's Nature note.\(^{14}\)
Though there is little difference between the two sources, the published note is slightly different from both. In the manuscript, there is a passage that the spin direction of the electron is noted, but in the published note, this passage is deleted. Regarding the error that C. Møller discovered, Nishina’s Nature note was published without the correction, since it was submitted before Møller’s check. Nishina submitted the correction notice\textsuperscript{26} to Nature, however, on this point later, and Klein and Bohr provided intermediation for early publication of it. This is indicated in the letter\textsuperscript{11,27} from Klein to Nishina.

Source [177]: The note including explanations in English.

This note seems to be made for preparation of completing the paper for Zs. f. Phys. (Ref. 13), in which the process of the calculations are recorded in more detail and explanations in English are attached concerning the important points. The contents are almost the same as the source [167].

We find two sets of calculation memorandums ([172] and [181]), in which the calculation of the whole process are recorded. These two are different in the treatment of the initial conditions.

Source [172]: Calculation memorandums (for the whole process).

Similar to the published paper, the calculations proceed under the condition that the spin direction in the initial state of the electron for the first scattering is fixed at a certain direction, \( \mathbf{l} \), and then the averaging process is taken over the spin direction in the initial state of the electron for the second scattering.

Source [181]: Calculation memorandums (for the whole process).

Two calculation procedures are considered:

1. When the spin direction in the initial state of the electron for both the first and the second scattering are set along the \(+z\) direction, the same result is obtained, as in [172], after being averaged over the polarization of the linearly polarized incident wave.

2. When the spin direction for the first scattering is fixed along the general direction \( \mathbf{l} \) and the spin direction for the second scattering is fixed along the \(+z\) direction, the same result as in [172] is also obtained after averaging over the direction \( \mathbf{l} \). In the published paper (Ref. 13, p. 876) we find the statement:

“Wie eine genauere Betrachtung zeigt, gibt der Ausdruck (14) die Tertiärrstrahlintensität für den Fall, dass eins — gleichgültig welches — der beiden streuenden Elektronen unmagnetisiert ist, während das andere Elektron nach einer beliebigen Richtung magnetisiert oder auch unmagnetisiert sein kann.” (As a more detailed consideration shows, Equation (14) ([N-14]) gives the expression of the intensity of the third radiation in the following case, that one of the two scattering electrons (whether for the 1st or the 2nd scattering) is not magnetized, while the other electron is magnetized for an arbitrary direction or this also can be unmagnetized.)

The calculations in [181] give confirmation of this statement.

Source [182]: Calculation memorandums

The calculation of the intensity of the scattered wave for an elliptically polarized incident wave (not for the double scattering but for the single scattering) is described with the spin direction in the initial state of the electron fixed along \(+z\), for a linearly polarized incident wave. For a linearly polarized incident wave, it is shown in the Klein–Nishina paper,\textsuperscript{8} that the intensity of the scattered wave is independent on the spin direction in the initial state of the electron. On the other hand, for an elliptically polarized incident wave treated in source [182], the intensity of the scattered wave depends on the spin direction.\textsuperscript{12} The calculation here shows the actual matter. Regarding this point, the following footnote was added in the Klein–Nishina paper (Ref. 8, p. 864): Nishina would discuss this point in detail in a subsequent paper by Nishina. However, in the published paper\textsuperscript{13} by Nishina only the result of averaging over the spin directions was presented in [N-7]. Although in [182] the dependence of the result on \( \mathbf{l} \) is not explicitly described, where \( \mathbf{l} \) denotes the spin direction in the initial state of the electron, [182] is a noteworthy document because it proves that in the case of \( \mathbf{l} \parallel z \), at least, the calculations regarding this matter were certainly performed. Moreover, it is shown in [182] that the Equation [N-7] is obtained after averaging for \( \mathbf{l} \parallel +z \) and \( \mathbf{l} \parallel -z \).

As discussed above, we see that in the course of writing the Nishina’s single-name paper, several attempts were made concerning the electron spin, though not included in the published paper. Section 6 discusses the problem of the final states of the electron, which was the most elaborating problem for Klein and Nishina.
6. The problem of final states

Notes on notations: In Section 6 through Section 8 we adopt usual notations: \((\text{Planck constant})/2\pi = \hbar, \text{frequency} = \nu, \text{and } 2\nu = \omega.\)

As noted in Sec. 3, due to spin degeneration, there are two independent states in the solution of the Dirac equation for a free electron, even though the values of the energy and momentum are assigned. When we consider scattering problems, we must assign a set of two mutually orthogonal states for final states of an electron as two independent states, and sum up the contribution to the intensity from each final state. Today we usually assign these two states as two eigen states of helicity \(\sigma_z\) belonging to eigenvalues \(\pm 1\), but we can assign two arbitrary, mutually orthogonal states instead. Therefore, there is a simple and clear judgment condition for the validity of taking two states: the orthogonality of these two states. However, in 1928 when Klein and Nishina finished their calculation, the concept of helicity had not yet been introduced, and furthermore the concept of orthogonality was not well-defined for the 4-component wave-function solutions of the Dirac equation. It was only six months after the appearance of the Dirac equation, and Dirac’s electron theory, itself, was considered skeptically because of the existence of negative energy states. The physical meaning of these 4-component wave functions, and treating methods of these were not well established. Therefore, instead of taking the orthogonality condition, Klein and Nishina used the following argument to treat two final states of an electron after scattering: they gave each of the two set states its own physical meaning properly, and judged that setting as being valid if transitions of the electron from the initial state to the two final states were mutually exclusive in probability theory. For instance, the following two transitions to the states were mutually exclusive, one with the same spin direction as that of the initial state, and the other with the opposite spin direction to that of the initial state. And if they had dealt with the case of the non-relativistic Schrödinger equation, they could take the eigen states of \(\sigma_z\) with the eigenvalues \(\pm 1\) as its solution for arbitrary momentum, \(i.e.,\) setting the eigenstate \(\sigma_z = 1\) as the initial state and the eigenstates \(\sigma_z = \pm 1\) as the two final states could be considered to be valid. However, the situation was different for the Dirac equation. For the initial state with \(\mathbf{p} = 0\), they could take eigenstates of \(\sigma_z = \pm 1\), namely, \((\psi_1 = 1, \psi_2 = \psi_3 = \psi_4 = 0)\) and \((\psi_1 = 0, \psi_2 = 1, \psi_3 = \psi_4 = 0)\), as a solution of the Dirac equation. For the final state with \(\mathbf{p} \neq 0\), however, eigenstates of \(\sigma_z\) were not solutions of the Dirac equation unless \(p_x = p_y = 0\). Hence, it was impossible to assume a simple meaning of the final states; that one was in the same spin direction as the initial state, and the other was in the opposite direction. As a result, Klein and Nishina seemed to have felt some apprehension about the validity of their setting of the two final states until the final stage. At last Klein solved the problem at the very final stage. We argue about what happened based on two letters of Klein to Nishina in 1928, and testify it on the basis of other source materials. The first letter, dated 27th Oct. 1928, was found among calculation memorandums with no envelop and no creases, starting with the following text: “Just a few lines accompanying the manuscripts, which I hope reach you in time.” This sentence indicates that this letter was sent along with a copy of the manuscripts of Nishina’s single-name paper, \(^{13}\) which was corrected in part by Klein before submitting to Zs. f. Phys. Nishina left Copenhagen in early October of 1928 and set sail for America on 31st Oct. from London via Paris. Klein and Nishina’s paper \(^{9}\) and Nishina’s single-name paper \(^{13}\) were both received by Zs. f. Phys. on 30th Oct. 1928. We pick out the points related to the problem of the final states from this letter. The word “paper” in the passages below probably means Nishina’s single-name paper. The numbers \(1, 2, \ldots\) assigned to each passage are attached by the present author.

1. “though the form in which the degeneration of the free electron is now treated in the paper would seem to be unambiguous”

2. “The difficulty was the eigenfunction in the presence of a magnetic field, a point which I think is not completely cleared up yet”

3. “Therefore the eigenfunctions you have used in your paper are not so simply as we thought connected with the ‘spin’”

4. “but this has no influence on your results, only the sentences where spin comes in could not have quite the definite form you gave them”

The second letter, dated 2nd Dec. 1928, was sent to Nishina enclosed together with proofs of their joint paper and Nishina’s single-name paper for Zs. f. Phys. We pick out the necessary passages from this second letter assigning the numbers subsequent to those for the first letter:

5. “As to the spin difficulty it was this. In the paragraph about the eigenfunctions in the presence of a magnetic field, which I gave you...”
to read a few days before you left Copenhagen, I had tried to prove; that these functions for arbitrary velocities were those where \( \psi_1 = 0 \) and \( \psi_2 = 0 \) respectively.

6. “That this is wrong would follow from our considerations in the country already, but in the meantime I had forgotten some of our conclusions”

7. “I have limited myself to try to give a proper treatment of the degeneration in question. The result is the new §2 of the paper. I found this way of treating the degeneration rather convenient, since it gives a simple way of finding two independent eigenfunctions for each set of energy and momentum”.

8. “There are, however, an infinite amount of other eigenfunctions, for instance our solutions \( \psi_1 = 0, \psi_2 = 0 \). But you must not forget that our argument for regarding them as proper eigenfunctions was that we believed that they, apart from the transition to Bessel functions, would be the eigenfunctions in the presence of a magnetic field.”

9. “In fact, I did not feel certain that our intensity calculation was correct until I had derived all our \( dd, ds \) etc. relations by means of the new functions, which I have called \( u^*, v^* \). At present I am inclined to think that one could have been certain of it, but I do believe that the argument is easier when we make use of \( u^*, v^* \).”

From these statements altogether, we can presume their course of attacks on the problem of the final states as follows:

1. They choose solutions of the Dirac equation of which the types were \((0, \psi_2, \psi_3, \psi_4)\) and \((\psi_1, 0, \psi_3, \psi_4)\) as the two final states. They thought their choice was valid because these were connected to the eigenstates of energy with magnetic moments parallel to \( \pm z \) (in the limit of the magnetic field \( \to 0 \), as will be discussed later). (see 8)

2. Later they realized that it was wrong to conjecture that the eigenfunctions in the presence of a static magnetic field were the \( \psi_1 = 0 \) type and the \( \psi_2 = 0 \) type. (This happened when they were still in the summer resort). (see 2, 3, and 6)

3. They thought that choosing the \( \psi_1 = 0 \) type and the \( \psi_2 = 0 \) type solutions as the final states was not wrong, though those solutions could not be given the meaning of eigenfunctions in the presence of a static magnetic field. (see 1, 4)

4. However, they felt a little uneasy because the \( \psi_1 = 0 \) type and the \( \psi_2 = 0 \) type solutions could not lead to some definite meaning, and the problem remained as a pending issue. (see 2, 5, 9)

5. At last Klein devised a method to derive the solutions for \( p \neq 0 \) by performing the Lorentz transformation on the solutions for \( p = 0 \), and solved the problem. (This is stated in their joint paper, 8) (see 7, 9)

The solutions for \( p \neq 0 \) obtained through the Lorentz transformation on the solutions for \( p = 0 \), \( \sigma_z = \pm 1 \) can be given such a definite meaning as “the states with spin directions parallel to \( \pm z \) on the static system for the electron” and the transitions from the initial state \( p = 0, \sigma_z = 1 \) or \( \sigma_z = -1 \) to these final states can indeed be regarded as being mutually exclusive. Actually, the concrete forms of the solutions thus obtained are proved to be just the \( \psi_1 = 0 \) type and the \( \psi_2 = 0 \) type. Thus, the Lorentz transformation here does not introduce new types of solutions, but plays the role of giving a definite meaning to the pending solutions. However, it should be noted that this method of the Lorentz transformation can be applied to the solutions for \( p = 0 \) with an arbitrary spin direction, and therefore it is a method that has broader generality. This point might have been in his mind when Klein wrote “until I had derived all our \( dd, d\sigma \) etc. relations by means of the new functions”, in the citation 9. It was after Nishina left Copenhagen in early October of 1928, when this last improvement was carried out.

We now mention other sources that describe the circumstances presented above. First, the method of choosing two final states of the electron as the \( \psi_1 = 0 \) type and the \( \psi_2 = 0 \) type remained unchanged in Nishina’s single-name paper 13): Nishina stated clearly in p. 870 “Für den Endzustand wollen wir als unabhängige Eigenfunktionen diejenigen wählen, wo entweder \( u_1, v_1 \) oder \( u_2, v_2 \) gleich Null sind” (For the final states, we would like to choose as independent eigenfunctions those in which whether \( u_1, v_1 \) or \( u_2, v_2 \) are equal to zero). Moreover, in Source 174, it is stated that when taking these final states the intensity of the scattered wave comes to be independent of the spin direction of the electron in the initial state. This fact might be one support of the validity of their choice of the final states as the \( \psi_1 = 0 \) type and the \( \psi_2 = 0 \) type, although those states could not be interpreted as the eigenfunctions under a static magnetic field. (In fact, in Source 174, the
ψ_3 = 0 type and the ψ_4 = 0 type were taken instead of the ψ_1 = 0 type and the ψ_2 = 0 type, because of the different choice of ρ_v.

As pointed out in Sec. 5.2, comparing Nishina’s handwritten manuscripts of his single-name paper (Source [167]) with his published paper,13) we noticed different manners of regulating the final states in several passages: the direction of the magnetic moment of the electron is more clearly specified in the manuscript. This also is consistent with citations ③, ④ in the letter of 27th Oct. 1928.24)

Eigenstates in the presence of a static magnetic field. Though not mentioned in their joint paper, Klein and Nishina made considerable efforts in trying to solve the Dirac equation under a static magnetic field. As discussed above, it is obvious that their efforts were related to the problem of the final states. Klein seemed to put a lot of time on trials because his memorandum contained itemization of the whole trial procedure (Source [212-(iii)]), and his calculation memorandums had indicated many trials (Source [194], [205]–[209]). Because these calculation memorandums consist of fragmental assemblies, we can hardly read the line of his thoughts from these. But in Nishina’s note (Source [195]) the whole procedure of the trials is systematically explained in English, like a draft of a paper, from which we can conjecture the course of their trials to solve this problem. We give an outline below:

1. At first, they wrote down the Dirac equation in the presence of the vector potential, which gives the static magnetic field parallel to z.
2. They then showed that the z component of the angular momentum, J_z = ℓ_z + (ℏ/2)σ_z, was commutable with the Hamiltonian, and adopted its eigenstate as the solution.
3. Applying transformations that eliminated the z-component of the momentum and the angular variable θ of cylindrical coordinates (r, θ, z), the Dirac equation was reduced to an ordinary differential equation for each of the 4 components containing only r as an independent variable.
4. Solving the above equation within a first-order approximation on the magnetic field, they obtained an approximate solution in terms of Bessel functions.
5. They then set the boundary conditions to restrain the electron to within a cylinder (probably for obtaining discrete energy eigenvalues), in order to make the charge density, \( \varphi \psi \), on \( r = R \) (\( R \) = the radius of the cylinder) to be zero, where \( \varphi \) indicated the function conjugate to the wave function, \( \psi \). If \( \varphi \) is to be a Hermitian conjugate of \( \psi \), the above boundary condition cannot be satisfied. But Klein and Nishina seemed to have thought as follows: \( \varphi \) was to be determined as the solution of the conjugate equation to that of \( \psi \), and the coefficients of the 4 components of \( \varphi \) were to be determined independently of the coefficients of the 4 components of \( \psi \); therefore, they chose those coefficients so as to satisfy the boundary condition, and obtained discrete energy eigenvalues. We now know that this is wrong, but here we can see the situation at that time when the treating method of the 4 components of the wave function of the Dirac equation was not yet established.

6. Superposing Bessel function-type eigenstates thus obtained, they constructed a plain-wave solution of a free electron in the limit of a magnetic field \( H \to 0 \) and \( R \to \infty \). As a result, they showed that the \( \psi_3 = 0 \) type and the \( \psi_4 = 0 \) type solutions were obtained only in the case of \( p_x = 0 \) and \( p_y = 0 \).

Nishina’s note closed with the above statements. Note that regarding the problem of the final states, unless \( p_x = p_y = 0 \), the \( \psi_3 = 0 \) type and the \( \psi_4 = 0 \) type solutions cannot be obtained in the limit \( H \to 0 \), \( R \to \infty \). This seems to be consistent with the citation ⑥ in the Klein’s letter dated 2nd Dec. 1928: “That this (the \( \psi_3 = 0 \) type and the \( \psi_4 = 0 \) type solutions are eigenfunctions in the presence of a magnetic field) is wrong would follow from our considerations in the country already, but in the meantime I had forgotten some of our considerations’. Accordingly, it is impossible to clarify what sort of role the considerations in the Nishina’s note played on their efforts in trying to solve the problem of the final states. However, based on citation ⑧ in the same letter, there seemed to be times when they thought that the \( \psi_1 = 0 \) type and the \( \psi_2 = 0 \) type solutions were eigenfunctions in the presence of a magnetic field, and with the words “apart from the transition to Bessel functions” appearing there, they possibly reached this conclusion on the basis of the approximate solutions recorded in the note. Indeed, if we remove the artificial boundary condition to restrain the electron in the region \( r < R \), for a given value of \( J_x \), we can construct the \( \psi_1 = 0 \) type and the \( \psi_4 = 0 \) type solutions with the above-mentioned Bessel function-type approximate solutions, and these two solutions give the expectation values of the spin \( (\hbar/2)\sigma \) with...
the directions being directly opposite to each other. (As in Source [174], in this note Source [195] also, the form of $\psi_3 = 0, \psi_4 = 0$ were taken instead of $\psi_1 = 0, \psi_2 = 0$ because of the different choice of the expressions for $p_\tau$.)

Although Klein and Nishina’s attempt ended unsuccessfully, after all, due to the first-order approximation in the magnetic field, the ordinary differential equation that they obtained for one component of the wave function at the above-mentioned step 3 was completely correct, and should be regarded as reaching an important step for solving the Dirac equation in the presence of a magnetic field. Thus, this work is worth being evaluated as an exertion at that time. Today we know the exact solution of the differential equation in the presence of a magnetic field, to which Klein and Nishina reached. Applying an appropriate variable transformation, it can be reduced to a confluent hypergeometric differential equation. Solving it, we obtain a discrete set of energy eigenvalues (relativistic Landau level). Moreover, we can construct the $\psi_3 = 0$ type and the $\psi_4 = 0$ type solutions from the obtained exact solutions. These two solutions give a pair of values directed to the $\pm z$ direction as expectation values of the spin. However, unless $p_\tau = 0$, these states do not give the maximum value of $|\langle \sigma_z \rangle|$; hence, these cannot be considered to have any specific character in the presence of a magnetic field. In that sense, Klein and Nishina’s considerations may be judged as being valid, so that the $\psi_1 = 0$ type and the $\psi_2 = 0$ type solutions are not eigenstates under a static magnetic field.

The greatest problem for Klein and Nishina. As a conclusion of the investigation of Nishina’s source materials discussed in Sec. 5 and Sec. 6, we can state that the hardest problem to which Klein and Nishina made the greatest effort was a conceptual problem concerning the 4-component wave function solution of the Dirac equation, i.e., the problem of the physical meaning of the spin states. Although a semi-classical treatment of the interaction of electron and electromagnetic field had already been established by Gordon and Klein, spin was an entirely new matter, which did not appear in the Klein–Gordon equation. Hence, in the sources we find various groping and progressing processes for the spin operators and a treating method of the spin states, on both the intensity calculations and the verbal expressions. Though the tediousness of the intensity calculations has so far been emphasized as the hardest problem for Klein and Nishina, the greatest problem concerned the physical interpretation and the treating method of the spin states.

7. Reasons for Klein and Nishina’s adoption of the semi-classical treatment

As already noted in Sec. 3 Klein and Nishina adopted a semi-classical way to treat the interaction between electron and electromagnetic field, when they attacked the Compton-scattering problem. It is usually understood that they adopted the semi-classical way because no other way existed at that time. However, looking back at the situation concerning theories in the period of spring to summer of 1928 when their work was performed, we can see that another way had already appeared at that time.\(^{(12,47)}\)

To treat the problem of the Compton scattering in the framework of quantum mechanics more consistently, two theories were necessary, the theory of transition probability for scattering and quantum field theory of radiation, both of which were developed and published by Dirac during the period 1926–1927.

7.1 Dirac’s work. First, we look back this series of work by Dirac. Regarding the transition probability, Dirac developed time-dependent perturbation theory to treat the transition problem, and gave a formulation using an iterative approximation. (the last section of Ref. 30 (1926))

Then, in Ref. 31 (1927), he developed a theory that applied the second quantization to a general Boson system at first, and then to a photon system. This important work was a starting point of quantum field theory. The formulation in this work, however, was different from those of the generally used theory developed by Heisenberg and Pauli\(^{(32)}\) starting from the Lagrangian form. Hence, we survey here the main points of Dirac’s work.

First, we take a single-body system with a Hamiltonian given by $H_0 + V$, where $V$ denotes the interaction term. We then develop the wave function, $\psi$, of this system with the eigenfunction $\psi_r$ of $H_0$, such as $\psi = \sum b_r \psi_r$, where $|b_r|^2$ corresponds to the probability of this system being in the state $r$. If we consider a many body system consisting of a large assembly of the same single body system with no interaction with each other, then $|b_r|^2$ gives the number of particles in the state $r$, $N_r$. Hence, we can write $b_r$ as

$$b_r = e^{-i\theta_r} N_r^{1/2}, \quad b_r^* = N_r^{1/2} e^{i\theta_r} \quad \text{(7-1)}$$

The expressions of $\hat{b}_r$ and $i\hbar \hat{b}_r^*$ can be written in the form of the canonical equations of motion of which the Hamiltonian is $F = \sum_r b_r^* H_{rs} b_s$, as
The state of the whole system can be expressed by

The Hamiltonian

with frequency

energy is derived by considering the relation between the electron and an electromagnetic

dispersion theory using second-order perturbation

operators that express the creation and annihilation
down the vector potential

fi

electron and the electromagnetic

denotes the interaction term and \( \rho_f \) denotes the density of states. Taking \( (e/c)\hat{x} \cdot \mathbf{A} \) for \( v \), we can discuss the scattering of light accompanied by the transition of an electron inside of an atom (the dispersion).

This theory of dispersion by Dirac can be applied directly to Compton scattering with modifications on two points. One is to attach the factor \( e^{i\mathbf{k}\mathbf{r}} \), which expresses the space dependence to the vector potential, and the other is to rewrite the Hamiltonian of the electron into that of the Dirac equation as

\[
H = -e\rho_f \mathbf{\sigma} \cdot \mathbf{A} - \rho_0 mc^2.
\]

Here, the interaction term becomes \( -e\rho_f \mathbf{\sigma} \cdot \mathbf{A} \) and the state of the electron is expressed by the solution of the Dirac equation for a free electron. Then, the transition probability on the Compton scattering can be obtained by using Dirac’s theory of dispersion.

Naturally, Klein and Nishina should have known well about these works of Dirac concerning the quantization of an electromagnetic field, because Dirac wrote a paper on field quantization\(^{31}\) during his stay in Copenhagen and in the Nishina’s colloquium notes\(^{31}\) dated 26 Jan. and 28 Jan. 1927, Dirac’s lectures on this work are recorded. Dirac’s paper was received on 2nd Feb. 1927. Moreover, in autumn of 1927, Klein worked with Jordan\(^{34}\) to expand Dirac’s method of field quantization to a mutually interacting Bose system, so that he should be considerably interested in the problem of field quantization. In fact, on the introduction of the Klein–Nishina’s joint paper\(^{35}\) they commented on Dirac’s radiation theory as “Man wird erwarten, dass die eine Berücksichtigung der strahlungsämpfung erlaubt, in diesem Falle ein übereinstimmendes Resultat gibt, wenn es sich um die erste Nähe rung in bezug auf die Intensität der Primärstrahlung handelt.”\(^{32,47}\) (It will be expected that the radiation theory given by Dirac, which can afford to take radiation damping into account gives, in this case, the same result if the first-order approximation in the intensity of incident radiation is applied). Nevertheless, as far as Nishina’s source materials are concerned, we could not find any traces on their trials of adopting Dirac’s theory.

7.2 Reasons for Klein and Nishina’s adoption of the semi-classical treatment. Here we consider why Klein and Nishina adopted the semi-classical way instead of the more consistent method based on
quantization of the radiation field. For this, we report three reasons, as described below:

The first reason: Klein was one of the founders of the semi-classical treatment. As noted in Sec. 1, Klein formulated in his paper\(^3\) (1927) the general method to treat the interaction between charged particles and an electromagnetic field on the basis of the semi-classical treatment; hence he should be called the founder of the semi-classical treatment (the Klein–Gordon equation was also derived here). In this paper, he also derived the conservation laws of energy and momentum upon Compton scattering on the basis of that method, while Gordon published his paper,\(^4\) in which the intensity of the Compton scattering was treated on the basis of the Klein–Gordon equation about two months before Klein's paper. Mentioning these former works, Klein wrote, in his private note (Ref. 15) "And naturally we had both of us been thinking how this effect would come out according to Dirac’s new theory.”

Thus it was not doubtful that Klein was attached to the semi-classical treatment, and he would like to adopt this method also in the case of the Dirac equation. Moreover, as noted in Sec. 1, Klein and Nishina intended to verify the validity of Dirac’s relativistic theory of the electron in their paper. For this purpose, it was certainly convenient to treat the problem on the basis of the semi-classical treatment using the Klein–Gordon equation and the Dirac equation, and to check the difference of the results.

The second reason: The problem of normalization. We discuss the normalization of the solution of the Dirac equation for a free electron. Klein wrote in his private note (Ref. 15), “I shall mention here one difficulty which now would seem trivial, namely that is not possible to include a Dirac electron in a box (and which led me later to a well-known paradoxon [sic]). Finally we decided on a procedure earlier used by Gordon on the advise of Pauli.” The passage “that is not possible to include a Dirac electron in a box” means that if we set \( \psi = 0 \) on a certain boundary surface, such a solution allowing \( \psi \neq 0 \) inside of the surface does not exist, because the Dirac equation is a first order differential equation. Because of this statement, Klein and Nishina seemed to think that for a Dirac electron such normalization could not be allowed as to produce a discrete wave number \( k \) of the \( e^{ikr} \) type solution expressing the eigenstate of the momentum. There are two kinds of procedures to normalize the \( e^{ikr} \) type solution: One is the box normalization, which claims for an eigenfunction \( \psi_k(r) = L^{-3/2}e^{ikr} \) in a finite volume, \( L^3 \)

\[
\int \int \psi_k^*(r)\psi_k(r)dr = L^{-3} \int \int e^{-ikr}e^{ikr}rdr = \delta_{kk'} \quad [7-10]
\]

In this case, when the periodic boundary condition is applied, \( k \) takes the discrete value \( (2\pi/L)n_1, (2\pi/L)n_2, (2\pi/L)n_3 \). The other is the \( \delta \)-function-type normalization, which claims for continuous values of \( k \) in an infinite space that

\[
\psi_k(r) = (2\pi)^{-3/2}e^{ikr}r
\]

\[
\int \int \psi_k^*(r)\psi_k(r)dr = (2\pi)^{-3} \int \int e^{-ikr}e^{ikr}rdr = \delta(k - k') \quad [7-11]
\]

In Gordon’s paper on Compton scattering,\(^5\) as stated in Sec. 2.2, the \( \delta \)-function type normalization is adopted, while in Dirac’s quantization of electromagnetic field, it is necessary to make the wave number \( k \) of radiation field discrete: When both electron and radiation fields are taken into consideration, the consistency of the concept of space is spoiled unless the wave vectors of the wave function of electron are treated as being discrete under the same boundary condition as that for radiation. For that purpose, the periodic boundary condition for a Dirac electron should be adopted, as is usually done today. However, the concept of the periodic boundary condition might not be well understood when Klein and Nishina were working on the Compton scattering, because it was an artificial device made up for mathematical convenience. The other method to make wave vectors discrete is a standing-wave-type boundary condition that claims the value of the wave function to be zero at a boundary surface. This method has a definite physical meaning. Note that the density of states assigned by the set of discrete wavenumbers is the same for the standing-wave-type and periodic boundary conditions. This is probably the reason to accept the periodic boundary condition even though the physical meaning was not clear. However, the standing-wave-type boundary condition could not be adopted for a Dirac electron because of the reason stated above. Hence, the grounds for accepting the periodic boundary condition became infirm. Namely, the validity for taking discrete wave vectors was ambiguous. Klein might have meant this situation when he mentioned “one difficulty”. Here, we add some remarks concerning the acceptance of the periodic boundary condition. Born and Dirac adopted this early in their studies on quantum mechanics. In fact, Born devised the
periodic boundary condition before quantum mechanics appeared. He introduced it to calculate the density of states in Ref. 35 dealing with the classical treatment of lattice vibration. This might be the origin of the periodic boundary condition. He used it to discuss the probability interpretation of quantum mechanics (Ref. 36), particularly in the calculation of the density of states. Dirac also claimed the validity of the periodic boundary condition in Ref. 30 to express functions defined in the finite region in terms of a Fourier series. On the other hand, in the paper (Ref. 37) arguing the Klein’s paradox, Klein stated that in the case of the Dirac equation, the standing-wave-type boundary condition could not be applied without mentioning the periodic boundary condition, which probably was not in his mind.

In the Tamm’s paper,38 which is discussed later, the periodic boundary condition was adopted for the Dirac electron. However, he added an annotation explaining Born’s idea of a periodic lattice. Since this paper was published in 1930, the periodic boundary condition did not seem to be so broadly accepted, even then.

The third reason: Question on negative energy states. As noted in Sec. 3, there are two solutions of the Dirac equation for a given momentum value: one with the positive energy eigenvalue \( \sqrt{m^2c^4 + c^2p^2} \) and the other with the negative energy eigenvalue \(-\sqrt{m^2c^4 + c^2p^2}\). When Dirac’s relativistic electron theory6 appeared, this negative energy state was not interpreted validly, and it was generally regarded as being physically meaningless. In fact, we can find the words “den physikalisch nicht sinnvollen negativen Energiewerten” (physically meaningless negative energy values) in the Klein–Nishina’s joint paper (Ref. 8, p. 856). It was surely inevitable that in 1928, the above view was generally accepted, because in 1930 Dirac presented his hole theory40 which was verified in 1932 by discovery of the positron. If Klein and Nishina had taken up Dirac’s scattering theory as the basis, they should have taken into account all of the possible states as intermediate states. Then, was it possible for them to exclude the negative energy states at this stage? They seemed to avoid Dirac’s scattering theory because of this question. The answer to this question was given by Waller41 and Tamm,38 as described below.

7.3 Treatments based on field quantization. In 1930 Waller41 and Tamm38 independently carried out calculations for Compton scattering on the basis of field quantization and scattering theory, and reproduced the Klein–Nishina formula. Their analyses differed in the following points: Tamm adopted the quantization of an electron field as well as an electromagnetic field relying on Heisenberg–Pauli’s paper,32 while Waller adopted a method in which the electron field was not quantized. Both Waller and Tamm emphasized that it was essentially necessary to take the negative energy states into account as intermediate states.12,47 They stated that especially in the limit of \( \hbar \nu \ll mc^2 \), the contributions to the intensity of the scattered wave were given exclusively by these negative energy intermediate states, and as a result the classical Thomson-scattering formula was obtained. This indicates that negative energy states must be considered as physically meaningful states. The necessity of the negative energy states in this manner was regarded as a paradox at that time, called “Waller’s paradox”. Another paradox was “Klein’s paradox”37: when an electron with a positive energy entered into a step-type potential barrier, the part of the electron invading inside of the barrier tended to have a negative energy state if the potential barrier was sufficiently high. Klein mentioned this point in his private note,15 as sited in Sec. 7.2, in regard to the second reason. There are two letters from Waller to Nishina in the Sangokan Nishina Source: One was dated 17 May 1929,42 in which Waller wrote “I have been working chiefly on the scattering theory”. The other was dated 25 Jan. 1930,43 in which Waller wrote on the negative energy states “I have recently been doing some things on scattering which tends to be my hobby. It will perhaps interest you to hear that the Dirac scattering theory gives for free electron just your and Klein’s formula, if states of negative energy are properly taken into account”. And in the margin of this letter Nishina wrote a draft44 of a reply in English, and referred to Waller’s work as follows: “I am very much interested to hear about your results on the scattering, and anxious to see the details of your work. From Heisenberg’s lecture at Copenhagen I also thought that the states of negative energy must be taken into account in order to get the correct result but I did not expect that you would obtain the same formula as ours. I am looking forward to your paper.” Waller made a note on Heisenberg’s lecture in the footnote of his paper (Ref. 41, p. 844) “In einer nicht veröffentlichten Untersuchung hat Prof. W. Heisenberg schon gefunden, dass in dem Grenzfall, wo \( \hbar \nu/mc^2 \) gegen eins vernachlässigt wird, die klassische Streuformel wegen der Zwischenzustände negativer Energie erhalten wird” (In an unreleased work Prof. W. Heisenberg had already found that in the limiting case of \( \hbar \nu/mc^2 \) negligibly smaller than
unity, the classical scattering formula is obtained by the negative energy intermediate states). It must be before October 1928 that Nishina listened to this Heisenberg’s lecture in Copenhagen, and therefore this Heisenberg’s foreknowledge must have been obtained at rather an earlier time point.

As for the problem of normalization, which was a worrying matter for Klein and Nishina, Waller did not seem to worry and used the \(\delta\)-function type normalization for the electron, while he dealt with the wave vector of the electromagnetic field as being discrete. Tamm, on the other hand, used the periodic boundary condition for both the electron and the electromagnetic field, and thus treated space consistently.

Here, we examine how Waller and Tamm dealt with the problem of choosing the final state of an electron that Klein and Nishina worried about most. First, Waller adopted four independent final states of an electron with a given momentum as four solutions of the same type as those of Klein and Nishina, namely one of \(\psi_1, \psi_2, \psi_3, \psi_4\) being equal to zero, and used these in actual calculations. He clearly stated that the orthogonality condition was necessary for choosing four final states, and moreover, added at the end that the intensity of the scattered wave did not depend on the concrete form of the four final states as long as they satisfied the orthonormal condition. On the other hand, Tamm established a calculation method, which was capable of obtaining the intensity of the scattered wave using orthonormality alone, and did not use any concrete forms of the four independent states. However, he also mentioned an example of concrete forms, which was the same as that used by Waller, namely four solutions, each one of which had one of \(\psi_1, \psi_2, \psi_3, \psi_4\) equal to zero (Klein–Nishina–type solutions).

Waller and Tamm might have reached the orthogonality condition because they used Dirac’s scattering theory (time-dependent perturbation theory). Nevertheless, the following general viewpoint Tamm stated in his paper (Ref. 38, p. 549) would not have been established at the time of point Tamm stated in his paper (Ref. 38, p. 549) Waller, himself, stated on this matter in the footnote of Ref. 41 and Dirac did also the same in Ref. 40.

From the above arguments it became clear that the Klein–Nishina formula can be reproduced by using field quantization or hole theory. It was already stated in Sec. 1 that this formula played an important role to support of the Dirac equation and, moreover, Waller’s theory and Tamm’s theory should be recognized as having reinforced that role.

8. The equivalence between the Klein–Nishina’s theory and the theory based on the field quantization

In Klein–Nishina’s theory, the negative energy solutions of the Dirac equation were not taken into account. On the contrary, it is already noted that in the theory based on the field quantization (see for instance, W. Heitler\(^{45}\) 3rd ed. Chap. V, §22, pp. 211–224), the negative energy states play a very important role as intermediate states. Nevertheless, both theories give the same result for the scattering cross section of a photon as the Klein–Nishina formula. To clarify this seemingly paradoxical matter, we rewrite here Klein–Nishina’s theory into the form in which the intermediate states appear, and thus reveal the equivalence between both theories.

At first, in Eq. [KN-36], which gives the vector potential \(A(p, p')\) of the scattered wave (where \(p\) and \(p'\) are the momentum of the electron in the initial and final states, respectively), we rewrite as follows: \(u(p) \rightarrow u'(p), f(p) \rightarrow \tilde{g}(p), \nu(p) \rightarrow u(l, p, \rho, \sigma \rightarrow \alpha, \nu \rightarrow \omega).\) We then obtain

\[
A'(p \rightarrow p') \propto e^{-i(\omega t - \mathbf{k} \cdot \mathbf{r})} u(p)[\alpha g(p') + \tilde{g}(p)\alpha]u(p'), \tag{8-1}
\]

where \(g(p)\) and \(\tilde{g}(p)\) are modified parts of the solutions for a free electron interacting with the field of the incident wave, as given in [KN-23]. The scattered wave propagating in the direction \(n'\) has two directions of polarization. Denoting one of them as \(e'\), we obtain the intensity of the scattered radiation of polarization, \(e'\), as

\[
I = \frac{\omega^2}{4\pi e^2} |A'(p \rightarrow p') \cdot e'|^2
\]

\[
\propto e^2 |u(p)[(\alpha \cdot e')g(p') + \tilde{g}(p)(\alpha \cdot e')]u(p')|^2
\]

\[
= e^2 |u'(p)[g(p')(\alpha \cdot e') + (\alpha \cdot e')\tilde{g}(p)]u(p')|^2. \tag{8-2}
\]

Determining \( g(p) \) and \( \bar{g}(p) \) as below, we will show that the quantity in \( |\psi|^2 \) in Eq. [8-2] is just equal to the transition matrix element in the Heitler–like method.

We first rewrite the fundamental equations appearing in Sec. 2. The Dirac equation is given by

\[
\left[ i\hbar \frac{\partial}{\partial t} - (H_0 - e\alpha \cdot A) \right] \psi_0(p) + \psi_1(p) = 0
\]

\[
H_0 = e\alpha \cdot \left( -i\hbar \frac{\partial}{\partial p} - \frac{e}{c} A \right),
\]

where \( A \) denotes the vector potential of the incident wave

\[
A = a_0 \left[ e^{i\omega(t - \frac{2\pi}{c})} + e^{-i\omega(t - \frac{2\pi}{c})} \right]
\]

and \( \psi_0(p) \) denotes the solution that expresses the initial state of the electron as

\[
\psi_0(p) = u(p)e^{i\omega(p - E(p)t)}
\]

\[
H_0(p)u(p) \equiv (e\alpha \cdot p + \beta mc^2) u(p) = E(p)u(p)
\]

\[
E(p) = \sqrt{c^2p^2 + m^2c^4} > 0
\]

Using [8-4] for \( A \), in the first-order approximation in parameter \( \alpha \), Eq. [8-3] can be reduced to

\[
\left[ i\hbar \frac{\partial}{\partial t} - H_0 \right] \psi_1(p) = -e\alpha \cdot A \psi_0(p)
\]

Setting \( \psi_1(p) \) in the following form

\[
\psi_1(p) = [g(p)e^{i\omega(t - \frac{2\pi}{c})} + \bar{g}(p)e^{-i\omega(t - \frac{2\pi}{c})}]\psi_0(p),
\]

then \( g(p) \) and \( \bar{g}(p) \) are determined according to [8-4], [8-5], [8-6], and [8-7] as

\[
g(p) = \frac{1}{(E(p) - \hbar\omega) - H_0 \left( \frac{p - \hbar\omega}{e} n \right)} (-e\alpha \cdot e_0)\alpha
\]

\[
\bar{g}(p) = \frac{1}{(E(p) + \hbar\omega) - H_0 \left( \frac{p + \hbar\omega}{e} n \right)} (-e\alpha \cdot e_0)\alpha
\]

In the Klein–Nishina’s joint paper, they rewrote the linear order Eq. [8-3] into the quadratic equation as

\[
\left[ i\hbar \frac{\partial}{\partial t} - H \right] \left( i\hbar \frac{\partial}{\partial t} - H \right) \psi = 0
\]

and determined \( g \), \( \bar{g} \) using Eq. [8-9] instead of Eq. [8-3]. They thus obtained \( g(p) \) and \( \bar{g}(p) \) instead of Eq. [8-8] as

\[
g(p) = \frac{1}{[(E(p) - \hbar\omega) - H_0(p - \frac{\hbar\omega}{e} n)](E(p) - \hbar\omega) + H_0(p - \frac{\hbar\omega}{e} n)]}
\]

Using the properties of matrix \( \alpha \), the denominator in Eq. [8-10] is reduced to the c-number \( |E(p) - \hbar\omega|^2 - |E(p - \hbar\omega/c)\alpha|^2 \), and thus we need not find the inverse matrix. This was the reason why Klein and Nishina used the quadratic Eq. [8-9] instead of Eq. [8-3]. However, to reveal the equivalence to the Heitler–like method, it is rather convenient to adopt Eq. [8-8] without change. Substituting Eq. [8-8] into Eq. [8-2], we obtain

\[
|\psi|^2 = c^2\alpha^4 \left[ \frac{1}{(E(p') - \hbar\omega) - H_0(p' - \frac{\hbar\omega}{c} n)}(\alpha \cdot e')^2 \right.
\]

\[
+ \left. (\alpha \cdot e' E(p' + \hbar\omega) - H_0(p + \frac{\hbar\omega}{c} n)(\alpha \cdot e_0)\right] u(p)|^2
\]

Generally, in the eigenstate \( |n\rangle \) of \( H_0(p) |n\rangle = E(p)|n\rangle \), there are two kinds of states: one belongs to the positive energy value \( E(p) = \sqrt{c^2p^2 + m^2c^4} \) and the other belongs to the negative energy value \( E(p) = -\sqrt{c^2p^2 + m^2c^4} \). For each kind of states, there are two mutually independent states in terms of the spin direction. These four eigenstates span a complete system. Therefore, denoting \( \sum_n \) as the summation over these four eigenstates for a given \( p \) following Heitler,\(^{45}\) we can insert \( \sum_{p'} - (\hbar\omega/c)\alpha|n\rangle \langle n| \) for the first term in Eq. [8-11] and \( \sum_{p'} (\hbar\omega/c)\alpha|n\rangle \langle n| \) for the second term after \( 1/(E - H_0) \). Thus \( |\psi|^2 \) in the right-hand side of Eq. [8-11] reduces to

\[
\sum_{\langle n |} \frac{(u_1(p') \langle \alpha \cdot e_0 | u_0(p') \langle \alpha \cdot e' | u(p))}{(E(p') - \hbar\omega) - E_n(p' - \frac{h\omega}{e} n)}
\]

\[
+ \sum_{\langle n |} \frac{(u_1(p') \langle \alpha \cdot e' | u_0(p) \langle \alpha \cdot e_0 | u(p))}{(E(p) + \hbar\omega) - E_n(p + \frac{h\omega}{e} n)}
\]

By the conservation laws

\[
p' + \frac{h\omega}{e} n' = p + \frac{h\omega}{e} n,
\]

\[
E(p') + \hbar\omega' = E(p) + \hbar\omega
\]

we obtain \( p' - (\hbar\omega/c) n = p - (\hbar\omega'/c) n' \), \( E(p') - \hbar\omega = E(p) - \hbar\omega' \).

Using above, we rewrite the denominator of the first term of Eq. [8-12] as \( E(p) + \hbar\omega - [E(p) - (\hbar\omega'/c) n') + \hbar\omega + \hbar\omega'] \). We then recognize that the first term of Eq. [8-12] coincides with the transition matrix element in the Heitler theory,\(^{45}\) where the intermediate state corresponds to the emission of a photon at the final state at first and the electron having momentum \( p' - (\hbar\omega'/c) n' \). Likewise, the second term of Eq. [8-12] coincides with the transition matrix element in which the intermediate state corresponds to the absorption of a
photon of the initial state at first and an electron having momentum $p + (\hbar \omega / c) \mathbf{n}$. We can thus show that Eq. [8-12] just coincides with the transition matrix element in the Heitler theory, namely the Eq. [H-18] (Equation (18) in Ref. 45, p. 215) given by

$$d\phi = e^4 \frac{E k^2}{\mu k_0^3} \sum \left( \frac{u^* \alpha \alpha' u' (u^* \alpha \alpha' u)}{\mu + k_0 - E'} \right) + \left( \frac{u^* \alpha \alpha' u' (u^* \alpha \alpha' u)}{\mu - k - E''} \right)^2, \quad [H-18]$$

where $d\phi$ denotes the differential cross section of a photon scattered by an electron initially at rest and $\mu = mc^2$, $k_0 = \hbar \omega$, and $k = \hbar \omega'$. The reason why no negative energy states appeared explicitly in Klein–Nishina’s theory was that they adopted a quadratic Eq. [8-9] to find the wave function of an electron modified by the incident wave, and thus reducing the denominator of Eq. [8-10] to a c-number. As a result, in the calculation of matrix elements, it became possible to use only the initial and final states having positive energies only for the bras $| \rangle$ and kets $\langle |$.}

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**References**


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