# Modified Sommerfeld-Maue wave function: Application to the pair-production process\*

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A solution of the Dirac equation for an electron in a point-Coulomb potential is given in the form of an expansion in the parameter 1/r. The main part of the solution is the Sommerfeld-Maue wave function. We introduce a correction term. All orders in  $\alpha Z$  are kept. The given solution (Sommerfeld-Maue plus correction term) contains the exact contributions of orders 0 and 1 in the expansion in 1/r. This modified Sommerfeld-Maue wave function is used to get the cross section for the pair-production process by  $\gamma$  rays in the field of a nucleus. The cross section is written in the form of the Fink-Pratt cross section plus a correction term. The formula is valid for all  $\alpha Z$ . The energetic relative accuracy should be of order  $1/E^2$ . The small-angle approximation is not introduced.

#### I. INTRODUCTION

Johnson and Mullin<sup>1</sup> have discussed the interest in an approximate solution of the Dirac equation for calculations of various electrodynamic processes such as electron scattering, bremsstrahlung, and pair production. They have given a relativistic Coulomb wave function which is valid to second order in  $\alpha Z$  for all electron velocities. This wave function has been used by Deck, Moroi, and Alling<sup>2</sup> to obtain bremsstrahlung and pair-production cross sections including a correction term to the Bethe-Heitler<sup>3</sup> formulas, of relative order  $\alpha Z$ . In addition, Borie<sup>4</sup> has performed a first-order calculation for the bremsstrahlung case. We have shown<sup>5</sup> that first-order corrections in  $\alpha Z$ seem not to be sufficient in the energy region from a few MeV to a few tens of MeV, for high values of Z. Furthermore, they do not give any contribution to the total cross section for pair production.

In previous bremsstrahlung and pair-production calculations,<sup>5,6</sup> we introduced a different way to compute higher-order Coulomb corrections to the cross sections obtained from the Sommerfeld-Maue wave function. The method starts with expansions both in powers of  $\alpha Z$  and in energy (or 1/r). In the bremsstrahlung case, the theoretical values have been found in good agreement with experimental results,<sup>5</sup> while in the pair-production case, Fink and Pratt<sup>7</sup> have shown that the correction is still too small for high Z values.

To improve our previous results, we have given, in a recent paper,<sup>8</sup> a general method to obtain the exact correction term to the Sommerfeld-Maue wave function. Nevertheless, it is possible that the corresponding numerical computations would be very difficult. Then, we come back to a search for an approximate correction term which might be more useful for numerical purposes. We introduce a wave function with only the expansion versus 1/r, all orders in  $\alpha Z$  being kept. In Sec. II, we shall deduce the wave function in the form of a correction term added to the Sommerfeld-Maue wave function. In Sec. III, this wave function will be applied to the pair-production process, the cross section being written in the form of the Fink-Pratt cross section<sup>7</sup> plus a correction term.

### II. THE MODIFIED SOMMERFELD-MAUE WAVE FUNCTION

#### A. Definition of the correction term

We look for a solution of the Dirac equation for an electron in the point-Coulomb potential of a nucleus:

$$(-i\vec{\alpha}\cdot\vec{\nabla}+\beta-\alpha Z/r-E)\Psi=0; \qquad (2.1)$$

 $\vec{\alpha}$  and  $\beta$  are Dirac matrices,  $\vec{r}$  is the electron's coordinate, *E* the total electron energy,  $\alpha$  the finestructure constant, and *Z* the charge number of the nucleus.<sup>9</sup>

The exact wave function  $\Psi$  is written

$$\Psi = \Psi_{\rm SM} + \Psi_c , \qquad (2.2)$$

with

$$\begin{split} \psi_{\mathbf{S}\mathbf{M}} &= \psi_a + \psi_b ,\\ \psi_a &= C e^{i\vec{\mathbf{y}}\cdot\vec{\mathbf{r}}} F u ,\\ \psi_b &= -(i/2E) C e^{i\vec{\mathbf{y}}\cdot\vec{\mathbf{r}}} \vec{\mathbf{q}}\cdot\vec{\nabla} F u ,\\ F &= {}_1F_1(i\nu; 1; ipr - i\vec{\mathbf{p}}\cdot\vec{\mathbf{r}}) , \end{split}$$
(2.3)

 $u = u(\mathbf{\tilde{p}})$  is the normalized Dirac spinor for a free electron of momentum  $\mathbf{\tilde{p}}$ ,  $_1F_1$  the confluent hypergeometric function, *C* a normalization constant, and  $\nu = \alpha ZE/p$ .

Bethe and Maximon<sup>10</sup> have shown that  $\Psi_c$  satisfies the equation

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$$\begin{split} \left(\nabla^2 + p^2 + 2\frac{\alpha ZE}{r}\right)\Psi_c \\ &= i\alpha Z\vec{\alpha} \cdot \left(\vec{\nabla}\frac{1}{r}\right)\left(\Psi_b + \Psi_c\right) - \frac{\alpha^2 Z^2}{r^2}\left(\Psi_a + \Psi_b + \Psi_c\right). \end{split}$$

$$(2.4)$$

Looking for an expansion in 1/r, we notice that  $\Psi_a$  is of order 1 and  $\Psi_b$  of order 1/r. Then  $\Psi_c$  is also of order 1/r. Our approximate wave function, valid to order 1/r, will be

$$\Psi_{\rm app} = \Psi_{\rm SM} + \Psi_e \,, \tag{2.5}$$

where  $\Psi_e$  is a correction term defined by the following equation:

$$(\nabla^2 + p^2 + 2\alpha Z E/r)\Psi_e = -(\alpha^2 Z^2/r^2)\Psi_a.$$
 (2.6)

Putting

$$\Psi_a = C\chi_a u, \quad \Psi_e = \alpha^2 Z^2 C\chi_e u , \qquad (2.7)$$

we have

$$(\nabla^2 + p^2 + 2\alpha ZE/r)\chi_e = -(1/r^2)\chi_a.$$
 (2.8)

### B. Derivation of the correction term

We shall solve Eq. (2.8) using a form derived from the exact wave function given by Johnson and Deck.<sup>11</sup> This form is interesting in our case because it expresses the spin dependence in terms of the Dirac plane-wave spinor, just as is given the Sommerfeld-Maue wave function.

The Johnson and Deck wave function is

$$\Psi = [N + i\alpha ZM \,\vec{\alpha} \cdot (\hat{p} - \hat{r}) + L \,\vec{\alpha} \cdot (\hat{p} - \hat{r}) \vec{\alpha} \cdot \hat{p}] u .$$
(2.9)

Here  $\hat{p} = \vec{p}/p$  and  $\hat{r} = \vec{r}/r$ ; *N*, *M*, and *L* are functions of *Z*, *E*,  $\vec{p}$ , and  $\vec{r}$ . Because of the spin dependence of  $\chi_e$ , we shall be interested in the term *N* only. The explicit expression for *N* is

$$N = 2 \sum_{k=1}^{\infty} (-1)^{k} k \frac{\Gamma(\gamma - i\nu)}{\Gamma(2\gamma + 1)} e^{\nu \pi/2} x^{\gamma - 1} e^{-x/2} \\ \times {}_{1}F_{1}(\gamma - i\nu; 2\gamma + 1; x) (P'_{k-1} - P'_{k}), \quad (2.10)$$

with

$$\gamma = (k^2 - \alpha^2 Z^2)^{1/2}, \quad x = -2ipr,$$
 (2.11)

 $P_k$  is a Legendre polynomial of argument  $\cos \alpha = \hat{p} \cdot \hat{r}$ , and  $P'_k$  denotes the derivative with respect to the argument.

Johnson and Deck showed that the Sommerfeld-Maue wave function results from the approximation  $\gamma = k$ . Therefore, we shall try to solve (2.8) using

$$\alpha^{2}Z^{2}C\chi = N - N(\gamma = k) \approx (\gamma - k) \left(\frac{\partial N}{\partial \gamma}\right)_{\gamma = k}.$$
 (2.12)

We expand  $\gamma - k$  to first order in  $(\alpha Z/k)^2$ ,

$$\gamma - k \approx -\alpha^2 Z^2/2k ,$$

and notice that

$$C = \Gamma (1 - i\nu) e^{\nu \pi/2} \,. \tag{2.13}$$

Then

$$\chi_{a} = \sum_{k=1}^{\infty} (-1)^{k} \frac{2k\Gamma(k-i\nu)}{\Gamma(1-i\nu)\Gamma(2k+1)} x^{k-1} e^{-x/2} {}_{1}F_{1}(k-i\nu;2k+1;x)(P'_{k-1}-P'_{k}), \qquad (2.14a)$$

$$\chi = -\sum_{k=1}^{\infty} (-1)^k \left(\frac{\partial}{\partial \gamma}\right)_{\gamma=k} \frac{\Gamma(\gamma-i\nu)}{\Gamma(1-i\nu)\Gamma(2\gamma+1)} x^{\gamma-1} e^{-x/2} {}_1F_1(\gamma-i\nu; 2\gamma+1; x) (P'_{k-1}-P'_k) .$$
(2.14b)

Using

$$P'_{k-1} - P'_{k} = (-1)^{k-1} \sum_{l=0}^{k-1} (-1)^{l} (2l+1) P_{l},$$

reversing the order of summations, and performing the sum over k, the expression of  $\chi_a$  can be transformed into a form given by Gordon<sup>12</sup> (we have also changed the sign of the wave function):

$$\chi_{a} = \sum_{l=0}^{\infty} (-)^{l} (2l+1) P_{l}(\cos\alpha) e^{-x/2} \frac{\Gamma(l+1-i\nu)}{\Gamma(1-i\nu)\Gamma(2l+2)} x^{l}{}_{1}F_{1}(l+1-i\nu; 2l+2; x) .$$
(2.15)

In the expression for  $\chi$ , the sum over k cannot be reduced. We obtain

$$\chi = -\sum_{l=0}^{\infty} (-1)^{l} (2l+1) P_{l}(\cos\alpha) e^{-x/2} \left[ \left( \frac{\partial}{\partial \gamma} \right)_{\gamma=l} \frac{\Gamma(\gamma+1-i\nu)}{\Gamma(1-i\nu)\Gamma(2\gamma+3)} x^{\gamma}{}_{1}F_{1}(\gamma+1-i\nu; 2\gamma+2; x) -2\sum_{k=l}^{\infty} \left( \frac{\partial}{\partial \gamma} \right)_{\gamma=k} \frac{\Gamma(\gamma+2-i\nu)}{(2\gamma+2)\Gamma(1-i\nu)\Gamma(2\gamma+5)} x^{\gamma+1}{}_{1}F_{1}(\gamma+2-i\nu; 2\gamma+4; x) \right].$$

$$(2.16)$$

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Let us recall that we are looking for a solution of (2.8) and that  $\chi_e$  is of order 1/r. Then, in Eq. (2.16), we are led to investigate the limit  $|x| \rightarrow \infty$ . We have

$$\frac{\Gamma(\gamma+1-i\nu)}{\Gamma(2\gamma+2)}x^{\gamma}{}_{1}F_{1}(\gamma+1-i\nu;\,2\gamma+2;\,x)\sim\frac{\Gamma(\gamma+2-i\nu)}{\Gamma(2\gamma+4)}x^{\gamma+1}{}_{1}F_{1}(\gamma+2-i\nu;\,2\gamma+4;\,x)\sim\frac{1}{x}$$

As a result of the factors in the denominator, the last sum in Eq. (2.16) may be omitted. Next, we compute  $(\nabla^2 + p^2 + 2\alpha ZE/r)\chi$ , with

$$\chi = -\sum_{l=0}^{\infty} (-1)^{l} (2l+1) P_{l}(\cos\alpha) e^{-x/2} \left(\frac{\partial}{\partial\gamma}\right)_{\gamma = l} \frac{\Gamma(\gamma+1-i\nu)}{\Gamma(1-i\nu)\Gamma(2\gamma+3)} x^{\gamma}_{1} F_{1}(\gamma+1-i\nu; 2\gamma+2; x) .$$

$$(2.17)$$

We get (see the Appendix)

$$\left(\nabla^{2} + p^{2} + \frac{2\alpha ZE}{r}\right)\chi = -\frac{1}{r^{2}}\sum_{l=0}^{\infty} (-1)^{l}(2+1)P_{l}(\cos\alpha)e^{-x/2}\frac{(2l+1)\Gamma(l+1-i\nu)}{\Gamma(2l+3)\Gamma(1-i\nu)}x^{l}{}_{1}F_{1}(l+1-i\nu;2l+2;x).$$
(2.18)

Comparison with expression (2.15) shows that (2.17) would be a solution of (2.8) if we had  $1/\Gamma(2l+2)$  instead of  $(2l+1)/\Gamma(2l+3)$  in (2.18). Then, it follows that, changing  $(2l+1)/\Gamma(2\gamma+3)$  to  $1/\Gamma(2\gamma+2)$  in (2.17), we get the solution of Eq. (2.8) (see Appendix). We have

$$\chi_{e} = -\sum_{l=0}^{\infty} (-1)^{l} P_{l}(\cos\alpha) e^{-x/2} \left(\frac{\partial}{\partial\gamma}\right)_{\gamma=l} \frac{\Gamma(\gamma+1-i\nu)}{\Gamma(1-i\nu)\Gamma(2\gamma+2)} x^{\gamma} {}_{1}F_{1}(\gamma+1-i\nu; 2\gamma+2; x) .$$

$$(2.19)$$

The interest in the derivation from the Johnson and Deck expression is that we get directly the right asymptotic behavior for the correction term. It is important to point out that the correction term  $\chi_e$  contains only outgoing spherical waves.

## C. Expression for the modified Sommerfeld –Maue wave function

For the asymptotic behavior of a plane wave plus outgoing spherical waves, the modified Sommerfeld-Maue wave function is then given by

$$\Psi = \Psi_{\rm SM} + \Psi_e + O(1/r^2) , \qquad (2.20)$$

where  $\Psi_{\rm SM}$  is defined by Eqs. (2.3) and (2.13),  $\Psi_e$  by (2.7), (2.13), and (2.19).

A function  $\Psi'$  with the asymptotic form of a plane wave plus incoming spherical waves can be obtained via time reversal. The adjoint of the function  $\Psi'$  can be written

$$\Psi'^{\dagger} = \Psi_{\rm SM}'^{\dagger} + \Psi_e'^{\dagger} + O(1/r^2) , \qquad (2.21)$$

with

$$\begin{split} \Psi_{\rm S\,M}^{\prime \dagger} &= \Psi_{a}^{\prime \dagger} + \Psi_{b}^{\prime \dagger} , \\ \Psi_{a}^{\prime \dagger} &= C^{\prime \ast} e^{-i\vec{y}\cdot\vec{\tau}} u^{\dagger} F^{\prime \ast} , \\ \Psi_{b}^{\prime \dagger} &= (i/2E) C^{\prime \ast} e^{-i\vec{y}\cdot\vec{\tau}} u^{\dagger} \vec{\alpha} \cdot \vec{\nabla} F^{\prime \ast} , \\ F^{\prime \ast} &= {}_{1}F_{1}(i\nu; 1; ipr + i\vec{p}\cdot\vec{r}) , \\ C^{\prime \ast} &\equiv C \quad [\text{cf. Eq. (1.13)}]; \\ \Psi_{e}^{\prime \dagger} &= \alpha^{2} Z^{2} C^{\prime \ast} \chi_{e}^{\prime \ast} u^{\dagger} , \end{split}$$
(2.22)

$$\chi_{e}^{\prime *} = -\sum_{l=0}^{\infty} P_{l}(\cos\alpha) e^{-x/2} \left(\frac{\partial}{\partial\gamma}\right)_{\gamma=l} \frac{\Gamma(\gamma+1-i\nu)}{\Gamma(1-i\nu)\Gamma(2\gamma+2)} x^{\gamma} \times_{1} F_{1}(\gamma+1-i\nu; 2\gamma+2; x) .$$
(2.23)

For applications, the partial-wave expansion of the Sommerfeld-Maue function can be of interest.  $\Psi_a$  can be expressed using (2.7), (2.13), and (2.15). For  $\Psi_a^{\dagger \dagger}$ , we have

$$\begin{split} \Psi_{a}^{\prime \dagger} &= C^{\prime *} \chi_{a}^{\prime *} u^{\dagger} ,\\ \chi_{a}^{\prime *} &= \sum_{l=0}^{\infty} (2l+1) P_{l} (\cos \alpha) e^{-x/2} \frac{\Gamma(l+1-i\nu)}{\Gamma(1-i\nu) \Gamma(2l+2)} x^{l} \\ &\times {}_{1} F_{1} (l+1-i\nu; 2l+2; x) . \end{split}$$

 $\Psi_b$  and  $\Psi_b^{\prime \dagger}$  can be deduced from the work of Johnson and Deck:

$$\begin{split} \Psi_{b} &= i \alpha Z M (\gamma = k) \overrightarrow{\alpha} \cdot (\overrightarrow{p} - \overrightarrow{r}) u , \\ \Psi_{b}^{\prime \dagger} &= i \alpha Z M^{\prime} (\gamma = k) u^{\dagger} \overrightarrow{\alpha} \cdot (\overrightarrow{p} + \overrightarrow{r}) , \end{split}$$
(2.25)

M and M' being given by Eqs. (32) and (44) of Ref. 11.

# III. APPLICATION TO THE PAIR – PRODUCTION PROCESS A. Matrix element

The matrix element including the Coulomb correction, but neglecting the atomic electron screening effect, is

$$M = \int d^{3}r \, \Psi_{2}^{\dagger}(\vec{\alpha} \cdot \vec{\epsilon}) e^{i\vec{\kappa} \cdot \vec{r}} \, \Psi_{1} , \qquad (3.1)$$

where the  $\Psi$ 's are solutions of the Dirac equation (2.1). In the expression of M, indices 1 and 2 refer to the positron and the electron, respectively;  $\overline{k}$ 

and  $\bar{\epsilon}$  are momentum and unit polarization vectors of the photon.

Writing each  $\Psi$  in the form  $\Psi = \Psi_a + \Psi_b + \Psi_c$ , we are led to an expansion of the matrix element in nine terms. Our aim is to compute the main correction term  $M_c$  to the Bethe-Maximon matrix element  $M_{\rm BM}, {}^{6,10}$ 

$$M_{\rm BM} = M_{2a,1a} + M_{2a,1b} + M_{2b,1a} , \qquad (3.2)$$

$$M_c = M_{2a,1e} + M_{2e,1a} \,, \tag{3.3}$$

using the  $\Psi_a$  functions obtained above.

From (2.7), (2.13), (2.15), (2.19), (2.23), and (2.24), we have

$$M_{c} = \alpha^{2} Z^{2} C_{2}^{*} C_{1} \langle u_{2} | \overrightarrow{\alpha \cdot \epsilon} | u_{1} \rangle I_{4} , \qquad (3.4)$$

(3.5)

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$$\chi_{1a} = \sum_{l_{1}=0}^{\infty} (2l_{1}+1) P_{l_{1}}(\cos\alpha_{1}) e^{-x_{1}/2} \frac{\Gamma(l_{1}+1+i\nu_{1})}{\Gamma(1+i\nu_{1})\Gamma(2l_{1}+2)} x_{1}^{l_{1}} F_{1}(l_{1}+1+i\nu_{1};2l_{1}+2;x_{1}) , \qquad (3.6)$$

$$\chi_{1e} = -\sum_{l_1=0}^{\infty} P_{l_1}(\cos\alpha_1) e^{-x_1/2} \left(\frac{\partial}{\partial\gamma}\right)_{\gamma=l_1} \frac{\Gamma(\gamma+1+i\nu_1)}{\Gamma(1+i\nu_1)\Gamma(2\gamma+2)} x_{11}^{\gamma} F_1(\gamma+1+i\nu_1;2\gamma-2;x_1) , \qquad (3.7)$$

$$C_1 = \Gamma(1 + i\nu_1)e^{-\pi\nu_1/2} ,$$

 $I_4 = \int d^{3} r \, e^{\, i \vec{\mathbf{k}} \cdot \vec{\mathbf{r}}} (\chi_{2a}^* \chi_{1e} + \chi_{2e}^* \chi_{1a}) \; , \label{eq:I4}$ 

and similar expressions for  $\chi_{2a}^*$ ,  $\chi_{2e}^*$ ,  $C_2^*$ , i.e.,  $l_2$ ,  $\nu_2$ ,  $x_2$ ,  $\cos \alpha_2$  instead of  $l_1$ ,  $-\nu_1$ ,  $x_1$ ,  $\cos \alpha_1$ .

We shall compute  $I_4$  by expanding  $e^{i\vec{k}\cdot\vec{r}}$  in partial waves:

$$e^{i\vec{k}\cdot\vec{r}} = \sum_{l=0}^{\infty} (2l+1)P_{l}(\cos\alpha)i^{l}j_{l}(kr) .$$
 (3.9)

Here,  $\cos \alpha = \vec{\mathbf{k}} \cdot \vec{\mathbf{r}} / kr$  and  $j_i$  is a spherical Bessel function of the first kind. The angular and radial integrals separate:

$$I_4 = \sum_{l_1, l_1, l_2} A_{l_1, l_1, l_2} R_{l_1, l_1, l_2}.$$
(3.10)

The angular integration is easy to perform. We get

$$A = (2l+1) \int d\Omega P_{l}(\cos\alpha) P_{l_{1}}(\cos\alpha_{1}) P_{l_{2}}(\cos\alpha_{2})$$
$$= \frac{16\pi^{2}}{[(2l_{1}+1)(2l_{2}+1)]^{1/2}} \sum_{m} Y_{l_{2},-m}(\theta_{2},\phi_{2}) Y_{l_{1},m}(\theta_{1},\phi_{1})$$
$$\times T(l,l_{1},l_{2};m). \qquad (3.11)$$

 $\vec{k}$  is taken along the polar z axis.  $\theta_1, \phi_1$  and  $\theta_2, \phi_2$ define, respectively, the momentum directions of the positron and the electron. The  $Y_{l,m}$  are spherical harmonics and T contains the Wigner 3-j symbols<sup>13</sup>:

$$T(l, l_1, l_2; m) = (2l+1) \begin{pmatrix} l & l_1 & l_2 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l & l_1 & l_2 \\ 0 & m & -m \end{pmatrix} \cdot (3.12)$$

The radial integration is more difficult. It involves integrals of the type:

$$\int_{0}^{\infty} d\gamma \, r^{2+l_{1}+r} e^{i(p_{1}+p_{2})r} j_{l}(kr) \, _{1}F_{1}\left(l_{1}+1+i\nu_{1};2l_{1}+2;-2ip_{1}r\right) \, _{1}F_{1}\left(\gamma+1-i\nu_{2};2\gamma+2;-2ip_{2}r\right) \, .$$

Similar calculations have been discussed and performed by Øverb $\emptyset^{,14}$  After computing the derivatives  $(\partial/\partial\gamma)_{\gamma=l_1}$  and  $(\partial/\partial\gamma)_{\gamma=l_2}$ , we finally obtain

$$\begin{split} R = & \frac{z_1^{l_1} z_2^{l_2}}{(2k)^3 z^2} \frac{\Gamma(b_1)}{\Gamma(1+i\nu_1)\Gamma(c_1)} \frac{\Gamma(b_2)}{\Gamma(1-i\nu_2)\Gamma(c_2)} \sum_{n=0}^{l} \frac{(l+n)!}{n! \, (l-n)!} \, \Gamma(a) z^n \left\{ (2l_1+1) [2C_A \operatorname{Im}(F_A) + 2\operatorname{Im}(F_A') - \pi F_A^*] \right. \\ & \left. + (2l_2+1) [2C_B \operatorname{Im}(F_B) + 2\operatorname{Im}(F_B') - \pi F_B^*] \right\}, \end{split}$$

with

(3.8)

$$\begin{split} z &= \frac{k + p_1 + p_2}{2k}, \quad z_1 = \frac{2p_1}{k + p_1 + p_2}, \quad z_2 = \frac{2p_2}{k + p_1 + p_2}, \\ a &= l_1 + l_2 - n + 2, \\ b_1 &= l_1 + 1 + i\nu_1, \quad c_1 = 2l_1 + 2, \\ b_2 &= l_2 + 1 - i\nu_2, \quad c_2 = 2l_2 + 2, \\ C_A &= \Psi(a) + \Psi(b_2) - 2\Psi(c_2) + \ln z_2, \\ C_B &= \Psi(a) + \Psi(b_1) - 2\Psi(c_1) + \ln z_1, \\ F_A &\equiv F_B = F_2(a; \ b_1, b_2; \ c_1, c_2; \ z_1, z_2), \\ F'_A &= \frac{\partial}{\partial l_2} F_A, \quad F'_B &= \frac{\partial}{\partial l_1} F_B. \end{split}$$

Here,  $\Psi$  is the logarithmic derivative of the  $\Gamma$  function and  $F_2$  is the Appell function.

### B. Cross section

The Bethe-Maximon matrix element, Eq. (3.2), can be written

$$M_{\rm BM} = C_2^* C_1 \langle u_2 \mid \vec{\alpha} \circ \vec{\epsilon} I_1 + \vec{\alpha} \cdot \vec{\epsilon} \vec{\alpha} \circ \vec{I}_2 + \vec{\alpha} \cdot \vec{I}_3 \vec{\alpha} \circ \vec{\epsilon} \mid u_1 \rangle.$$
(3.15)

[See Ref. 10, Eq. (6.2).] Taking into account Eq.

(3.4), our matrix element  $M = M_{BM} + M_c$  is

$$M = C_2^* C_1 \langle u_2 | \vec{\alpha} \cdot \vec{\epsilon} (I_1 + \alpha^2 Z^2 I_4) + \vec{\alpha} \cdot \vec{\epsilon} \vec{\alpha} \cdot \vec{I}_2 + \vec{\alpha} \cdot \vec{I}_3 \vec{\alpha} \cdot \vec{\epsilon} | u_1 \rangle.$$
(3.16)

Then, the differential cross section  $d^{3}\sigma$  can be obtained directly from previous results [Eq. (6.26), Ref. 10 or Eq. (1.45), Ref. 15] through the substitution  $I_1$  by  $I_1 + \alpha^2 Z^2 I_4$ . In a second step, we separate the contribution of  $I_4$ , which yields

$$d^{3}\sigma = d^{3}\sigma_{\text{main}} + d^{3}\sigma_{c}. \qquad (3.17)$$

 $d\,{}^3\sigma_{\rm main}$  is the main term, while  $d\,{}^3\sigma_c$  is the correction term due to  $I_4.$ 

For  $d^{3}\sigma_{\text{main}}$ , we can take our previous result [Eq. (1.45), Ref. 15] or the more sophisticated expression derived by Fink and Pratt [Eq. (2.5), Ref. 7].

For  $d^{3}\sigma_{c}$ , we write

$$d^{3}\sigma_{c} = d^{3}\sigma_{c_{1}} + d^{3}\sigma_{c_{2}}, \qquad (3.18)$$

 $d \, {}^{3}\sigma_{c_{1}}$  being computed from  $2 \operatorname{Re}(M_{\text{BM}}^{*}M_{c})$  and  $d \, {}^{3}\sigma_{c_{2}}$  from  $|M_{c}|^{2}$ . We get

$$d^{3}\sigma_{c_{1}} = dE_{1} d\Omega_{1} d\Omega_{2} \frac{Z^{2} e^{6}}{8\pi^{4}} \frac{p_{1} p_{2}}{k} \left| C_{1} C_{2} \right|^{2} \sum_{\nu=1}^{2} I_{4\nu} \left[ I_{1\nu} (E_{1} E_{2} + 1 - p_{1z} p_{2z}) + E_{2} (\vec{p}_{1} \cdot \vec{I}_{2\nu} - p_{1z} I_{3z\nu} + E_{1} (\vec{p}_{2} \cdot \vec{I}_{3\nu} - p_{2z} I_{2z\nu}) \right],$$

$$(3.19)$$

$$d^{3}\sigma_{c_{2}} = dE_{1} d\Omega_{1} d\Omega_{2} \frac{Z^{2} e^{6}}{16\pi^{4}} \frac{p_{1} p_{2}}{k} |C_{1} C_{2}|^{2} (\alpha Z)^{2} |I_{4}|^{2} (E_{1} E_{2} + 1 - p_{1z} p_{2z}).$$
(3.20)

Here,  $\nu = 1$  and  $\nu = 2$  refer to the real and imaginary parts, respectively.  $I_4$  is given by Eqs. (3.10)-(3.14). For  $I_1$ ,  $\overline{I}_2$ , and  $\overline{I}_3$ , see the work by Bethe and Maximon [Eq. (6.23), Ref. 10]. The z axis is taken along  $\overline{k}$ ;  $d\Omega_1$  and  $d\Omega_2$  are the elements of solid angles in the directions of  $\overline{p}_1$  and  $\overline{p}_2$ 

$$|C_1 C_2|^2 = \frac{4\pi^2 \nu_1 \nu_2}{(e^{2\pi\nu_1} - 1)(1 - e^{-2\pi\nu_2})} , \qquad (3.21)$$

with

 $v_1 = \alpha Z E_1 / p_1, \quad v_2 = \alpha Z E_2 / p_2.$ 

C. Correction term in first approximation in  $\alpha Z$ 

As a check of the expression (2.20) for the correction term to the Sommerfeld-Maue wave function, we perform a first-order calculation of the integral  $I_4$ , Eq. (3.5). In fact, we give the derivation for the first part of  $I_4$ , i.e.,

$$I'_{4} = \int d^{3}r \, e^{\,i\vec{k}\cdot\vec{r}} \, \chi^{*}_{2a}\chi_{1e} \,. \tag{3.22}$$

To zero order in  $\alpha Z$ , we have

$$\chi_{2a}^* = e^{-i\vec{p}_2\cdot\vec{r}}$$
,

$$\chi_{1e} = -\sum_{l_1=0}^{\infty} P_{l_1}(\cos\alpha_1) \left(\frac{\partial}{\partial\gamma}\right)_{\gamma=l_1} (-i)^{\gamma} j_{\gamma}(p_1\gamma) .$$
(3.23)

Expanding  $e^{i(\vec{k} - \vec{p}_2) \cdot \vec{r}}$  in partial waves, the angular and radial integrals in  $I'_4$  separate. Putting

$$\vec{s}_1 = \vec{k} - \vec{p}_2, \quad \cos\omega_1 = \vec{s}_1 \cdot \vec{p}_1 / s_1 p_1, \quad (3.24)$$

we get

$$I'_{4} = \sum_{l_{1}=0}^{\infty} A'_{l_{1}} R'_{l_{1}}$$
(3.25)

with

$$A' = 4\pi P_{I_1}(\cos\omega_1) ,$$
  

$$R' = \frac{\pi}{2s_1} \frac{(p_1/s_1)^{I_1}}{s_1^2 - p_1^2} .$$
(3.26)

The summation over  $l_{+}$  yields

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$$\left(1 - 2\frac{p_1}{s_1}\cos\omega_1 + \frac{p_1^2}{s_1^2}\right)^{-1/2} = \frac{s_1}{\left|\bar{s}_1 - \bar{p}_1\right|} \ .$$

We have

 $\vec{s}_1 - \vec{p}_1 = \vec{k} - \vec{p}_2 - \vec{p}_1 = \vec{q}$ ,

where  $\mathbf{\tilde{q}}$  is the recoil momentum of the nucleus, and

$$s_1^2 - p_1^2 = 2k(E_2 - p_{2z}) = D_2.$$
(3.27)

Then

$$I_4' = 2\pi^2/qD_2, \qquad (3.28)$$

which is in agreement with our previous approximate result [Eq. (9.1), Ref. 6].

### D. First numerical results

We have performed a numerical calculation of the cross section  $d\sigma/dE_1$  in the following particular case:

 $E_1 = E_2 = k/2, \quad Z = 82,$ 

for k = 2.1, 2.6, 3.5, and 5.2 ( $mc^2$  units).

Table I gives the contribution of the terms  $d\sigma_{c_1}$ ,  $d\sigma_{c_2}$ ,  $d\sigma_c = d\sigma_{c_1} + d\sigma_{c_2}$ , and  $d\sigma_{main} = d\sigma_{FP}$  (Fink and Pratt<sup>7</sup>). It is seen that  $d\sigma_{main}$  is still smaller than  $d\sigma_c$  at k = 5.2. However, for this photon energy,  $d\sigma_{FPRJ} = d\sigma_{main} + d\sigma_c$  approaches the exact value  $d\sigma_{OMO}$  of Øverbø *et al.*<sup>16</sup> within 1%. Also, it is interesting to point out that  $d\sigma_{c_1}$  is much smaller

TABLE I. Numerical results. The cross sections are given in  $b/mc^2$ . The calculation has been performed for Z = 82 and  $E_1 = E_2 = k/2$ .

Ref.	k	2.1	2.6	3.5	5.2
a	$\frac{1}{Z^2} \frac{d\sigma_{c_1}}{dE_1}$	~10 <sup>-10</sup>	3×10 <sup>-6</sup>	8×10 <sup>-6</sup>	1×10 <sup>-6</sup>
b	$\frac{1}{Z^2}\frac{d\sigma_{c_2}}{dE_1}$	$0.06 \times 10^{-6}$	35×10 <sup>-6</sup>	$107 \times 10^{-6}$	109×10 <sup>-6</sup>
с	$\frac{1}{Z^2}\frac{d\sigma_c}{dE_1}$	$0.06 \times 10^{-6}$	$38 \times 10^{-6}$	115×10 <sup>-6</sup>	110×10 <sup>-6</sup>
d	$\frac{1}{Z^2}\frac{d\sigma_{\rm FP}}{dE_1}$	0.05×10 <sup>-6</sup>	$7 \times 10^{-6}$	45×10 <sup>-6</sup>	95×10 <sup>-6</sup>
е	$\frac{1}{Z^2}\frac{d\sigma_{\rm FPRJ}}{dE_1}$	0.065×10 <sup>-6</sup>	45×10 <sup>-6</sup>	160×10 <sup>-6</sup>	205×10 <sup>-6</sup>
f	$\frac{1}{Z^2}\frac{d\sigma_{\rm OMO}}{dE_1}$	$0.125 \times 10^{-6}$	62×10 <sup>-6</sup>	$172 \times 10^{-6}$	$207 \times 10^{-6}$
g	$R = \frac{d\sigma_{\rm FPRJ}}{d\sigma_{\rm OMO}}$	0.52	0.73	0.93	0.99

<sup>a</sup> First correction term [Eq. (3.19)] integrated over the angles. <sup>b</sup> Second correction term [Eq. (3.20)] integrated over the angles.

Total correction term  $d\sigma_c = d\sigma_{c_1} + d\sigma_{c_2}$ 

<sup>d</sup>Fink and Pratt cross section integrated over the angles  $d\sigma_{\rm FP}$  (from Ref. 7).

<sup>e</sup>Our approximate result  $d\sigma_{\rm FPRJ} = d\sigma_{\rm FP} + d\sigma_{\rm c}$ .

<sup>f</sup> Exact differential cross section  $d\sigma_{OMO}$  computed by Øverbø *et al.* (Ref. 16).

<sup>g</sup>Ratio  $R = d\sigma_{\rm FPRJ}/d\sigma_{\rm OMO}$ .

than  $d\sigma_{c_2}$ ; at higher photon energies, it is supposed to be negligible.

Figure 1 gives the relative error between  $d\sigma_{\rm FPRJ}$ and  $d\sigma_{\rm OMO}$ . For *k* higher than 3 MeV, our calculation method should be correct with an accuracy better than 1%.

Finally, let us point out that, for k = 5.2, we need six partial waves for each particle (positron and electron), while the exact calculation requires 17 partial waves for each particle to get  $d\sigma_{\rm OMO}$  within 1%.

### **IV. CONCLUSION**

We think that the modified Sommerfeld-Maue wave function of Johnson and Mullin<sup>1</sup> and the present one complement each other. The Johnson and Mullin function is valid for all 1/r but limited to first order in  $\alpha Z$ . The present one is valid for all  $\alpha Z$  but limited to first order in 1/r. They have different interests. The Johnson and Mullin function should be preferable for low  $\alpha Z$  and low energies, while ours has to be chosen at higher  $\alpha Z$  and energy values.

If neither of these two approximations are accurate enough, the exact correction calculation method which has been investigated elsewhere<sup>8</sup> can be applied.

The main interest of the approximate wave function given here should be for a total cross-section calculation of the pair-production process in the intermediate energy region, from a few MeV to a



FIG. 1. The ratio  $Y = (d\sigma_{OMO} - d\sigma_{IPRJ})/d\sigma_{OMO}$  versus the photon energy value k expressed in  $mc^2$  units.

few tens of MeV, because a first-order correction in  $\alpha Z$  yields no contribution. The next step of our study will be this calculation.

The cross section involved here includes the Coulomb correction only. At high energies and small angles, the atomic electron screening effect has to be introduced.

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### APPENDIX; COMPUTATION OF $Y = (\nabla^2 + p^2 + 2\alpha ZE/r)\chi$

We write

$$\chi = -\sum_{l=0}^{\infty} (-1)^{l} P_{l}(\cos\alpha) L_{l}(r) ,$$

with

$$L_{l}(\gamma) = e^{-x/2} \left(\frac{\partial}{\partial \gamma}\right)_{\gamma=l} G x^{\gamma} {}_{1}F_{1}(\gamma+1-i\nu; 2\gamma+2; x) \ . \label{eq:Ll}$$

In Eq. (2.17),

$$G = \frac{(2l+1)\Gamma(\gamma+1-i\nu)}{\Gamma(1-i\nu)\Gamma(2\gamma+3)} .$$
 (A1)

In Eq. (2.19),

$$G = \frac{\Gamma(\gamma + 1 - i\nu)}{\Gamma(1 - i\nu)\Gamma(2\gamma + 2)}.$$
 (A2)

We take

$$\nabla^2 = \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin \alpha} \frac{\partial}{\partial \alpha} \left( \sin \alpha \frac{\partial}{\partial \alpha} \right) \,.$$

Applying the angular operator to  $P_1$ , we get

$$\frac{1}{\sin\alpha}\frac{\partial}{\partial\alpha}\left(\sin\alpha\frac{\partial P_l}{\partial\alpha}\right) = -l(l+1)P_l.$$

Then we have

$$\begin{split} Y &= -\frac{1}{r^2} \sum_{l=0}^{\infty} (-1)^l P_l(\cos\alpha) \\ & \times \left( \frac{\partial}{\partial x} x^2 \frac{\partial}{\partial x} - \frac{x^2}{4} + i\nu x - l(l+1) \right) L_l(x) \,. \end{split}$$

The derivation with respect to x yields

$$Z = \left(\frac{\partial}{\partial x}x^{2}\frac{\partial}{\partial x} - \frac{x^{2}}{4} + i\nu x - l(l+1)\right)L_{l}(x)$$
$$= e^{-x/2}\left(\frac{\partial}{\partial \gamma}\right)_{\gamma=l}Gx^{\gamma}\left\{x^{2}F'' + xF'(2\gamma+2-x) + F\left[-x(\gamma+1-i\nu) + \gamma(\gamma+1) - l(l+1)\right]\right\}$$

with

$$F = {}_{1}F_{1}(\gamma + 1 - i\nu, 2\gamma + 2, x)$$
$$F' = \frac{\partial F}{\partial x}, \quad F'' = \frac{\partial^{2}F}{\partial x^{2}}.$$

Taking into account Kummer's equation,

$$xF'' + (2\gamma + 2 - x)F' - (\gamma + 1 - i\nu)F = 0,$$

Z is written

$$Z = e^{-x/2} \left(\frac{\partial}{\partial \gamma}\right)_{\gamma=l} G x^{\gamma} F[\gamma(\gamma+1) - l(l+1)] .$$

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Finally, computation of the derivative with respect to  $\gamma$  yields

$$Z = e^{-x/2}G(l)x^{l}F(l)(2l+1),$$

$$\begin{split} Y &= -\frac{1}{r^2} \sum_{l=0}^{\infty} (-1)^l (2l+1) P_l(\cos \alpha) e^{-x/2} G(l) x^l \\ & \times_1 F_1(l+1-i\nu; \ 2l+2; \ x) \; . \end{split}$$

If we take for G the expression (A1), we get Eq. (2.18), while the value of (A2) yields Eq. (2.8).

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- <sup>9</sup>Throughout the paper, unless otherwise stated, we use the system of units where  $\hbar = m = c = 1$ . Then,  $\alpha = e^2 = \frac{1}{137}$ . In this system, energies, momenta, and cross sections are expressed in  $mc^2$ , mc, and  $(r_0/\alpha)^2$  units,
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