Eur. Phys. J. D **3**, 105–111 (1998)

THE EUROPEAN PHYSICAL JOURNAL D

On the continuity in energy of the free-bound one-photon cross-sections

V. Florescu[1,a] and R.H. Pratt[2]

[1] Faculty of Physics, University of Bucharest, P.O. Box 5211, Bucharest-Magurele, 76900, Romania
[2] Department of Physics and Astronomy, University of Pittsburgh, Pittsburgh, PA 15260, U.S.A.

Received: 13 February 1998 / Accepted: 14 May 1998

Abstract. For a charged particle in a central field of force we discuss the continuity in energy of the cross-sections for the related processes of ground state photoeffect and radiative capture. This continuity follows from general arguments, while for a Coulomb potential, where exact analytic expressions are available, the continuity can also be traced explicitly through the calculation. Our analysis allows us to identify an error in papers on radiative muon capture in the ground state which claim the existence of a discontinuity in the cross-section, occurring in hydrogen for muon energies in the neighbourhood of 2.8 keV. As a discontinuity in radiative capture would imply a discontinuity in atomic photoeffect, we note that in the latter case there are extensive experimental results in good qualitative agreement with the usual continuous result (Stobbe formula) for the cross-section.

PACS. 32.80.Fb Photoionization of atoms and ions

1 Introduction

We analyze the continuity in energy of the matrix element of the momentum operator between the ground state and a continuum energy eigenstate of *in* or *out* type for a particle in a central field of force. These matrix elements determine, respectively, the cross-section for ground state atomic photoelectric effect and for radiative capture to the ground state.

The continuity in energy of the cross-sections for these two related processes can be asserted on general grounds. In the particular case of a Coulomb potential, where exact analytic expressions are available, the continuity can be traced explicitly through the various versions and stages of the calculation. Our analysis here leads to the identification of an error present in two recent papers of Chatterjee *et al.* [1,2], which claim the existence of a discontinuity in the radiative *muon* capture cross-section, occurring in the nuclear Coulomb field of a proton, for muon energies in the neighbourhood of 2.8 keV. The same effect would also be present in radiative *electron* capture. As the authors have noted, this would also imply a discontinuity for the inverse process, *i.e.* in the electron case for atomic photoeffect. Chatterjee *et al.* assert that these discontinuities are confirmed in an examination of the relevant point Coulomb matrix elements, contrary to the generally accepted results for both photoeffect and radiative capture.

We begin in Section 2 by defining the relevant matrix elements and reviewing their properties which follow from general principles. In this section we restrict our discussion to the dipole approximation case, which is simpler, and for which the assertion of discontinuity was already made [1,2]. From a theorem of Poincaré [3] it follows that suitably normalized solutions of the Schrödinger equation are analytic in energy, and hence another well-established theorem [4,5] guarantees that reduced matrix element integrals over such a wave function are continuous functions of continuum energy.

In Section 3 we consider the Coulomb dipole case. An analytic expression for the non-relativistic Coulomb matrix element of photoeffect, even including retardation, has been known for a long time. It was obtained by Fischer and Sauter, who derived it independently [6]. The dipole approximation result follows directly from the Fischer-Sauter equation, or it can be obtained separately. The dipole result is associated with Stobbe [7]. (We give one of the possible alternative derivations of Stobbe's result in the Appendix.) We examine the derivation of the dipole result of Chatterjee *et al.* [1] in some detail, keeping in mind the continuity in energy and the circumstances in which various standard formulae are valid. In this way we demonstrate that the discontinuous expression obtained by Chatterjee *et al.* [1] results from a misapplication of a standard formula without considering its ranges of validity, and we demonstrate that the correct result is the Stobbe formula and, as required by the general theory, it is indeed continuous in energy: it does not have the discontinuity Chatterjee *et al.* [1] claim.

In Section 4 we discuss some further problems in the work of Chatterjee *et al.* [1,8], arising in their attempt

[a] e-mail: flor@barutu.fizica.unibuc.ro

to go beyond dipole approximation, which result from the use of an incorrect form for the full multipole matrix element.

Finally, in Section 5 we discuss to what extent experimental results for photoeffect show good agreement with the standard theoretical predictions and disagreement with the alternative of [1]. After some further discussion we present a summary of our comments and conclusions.

We use atomic units through all this paper.

2 The nonrelativistic dipole matrix elements for radiative capture and photoeffect

In nonrelativistic theory and in dipole approximation (DA), the matrix element describing the radiative capture transition of a negatively charged particle of mass M (for example an electron or a muon) from a continuum state $\mid \mathbf{p}+\rangle$ of energy $E = p^2/2M > 0$ (taking $p > 0$) and asymptotic momentum $\mathbf{p}$ to the ground state $\mid 1s\rangle$, in an atomic central potential, neglecting spin, is

$$\mathcal{M}_{1s}^{rc,DA} = \boldsymbol{\epsilon}^* \cdot \langle 1s \mid \mathbf{P} \mid \mathbf{p}+\rangle, \tag{1}$$

where $\mathbf{P}$ is the momentum operator, and $\boldsymbol{\epsilon}$ is the polarization vector of the radiated photon. The continuum energy eigenstate $\mid \mathbf{p}+\rangle$ of the charged particle in the atomic field is characterized by its large distance behaviour as a superposition of a plane wave of momentum $\mathbf{p}$ and an outgoing spherical wave; it is normalized on the momentum scale, *i.e.*, $\langle \mathbf{p}+ \mid \mathbf{p}'+\rangle = \delta(\mathbf{p}-\mathbf{p}')$. Energy conservation requires

$$E = \omega + E_b, \tag{2}$$

with E_b the ground state energy (negative) and ω the photon energy.

In the same approximation the matrix element of the photoeffect, which corresponds to a transition from the ground state to the continuum, is

$$\mathcal{M}_{1s}^{ph,DA}(\mathbf{p}, \boldsymbol{\epsilon}) = \boldsymbol{\epsilon} \cdot \langle \mathbf{p}- \mid \mathbf{P} \mid 1s\rangle. \tag{3}$$

This matrix element involves the continuum energy eigenstate $\mid \mathbf{p}-\rangle$, with the large distance behaviour of a superposition of a plane wave of momentum $\mathbf{p}$ and an incoming spherical wave, again normalized on the momentum scale.

The relation between the matrix elements of photoeffect and radiative capture is

$$\mathcal{M}_{1s}^{rc,DA}(\mathbf{p}, \boldsymbol{\epsilon}) = -\mathcal{M}_{1s}^{ph,DA}(-\mathbf{p}, \boldsymbol{\epsilon}^*). \tag{4}$$

These matrix elements will be the main subject of our discussion.

We also note the expressions for the corresponding cross-sections, since these are the quantities that are to be considered in the end. In dipole approximation the differential cross-section for radiative capture, corresponding to the emission of a photon of polarization $\boldsymbol{\epsilon}$ in the solid angle $d\Omega_\gamma$, is

$$\frac{d\sigma_{rc}}{d\Omega_\gamma} = 4\pi^2\alpha^3 \frac{\omega}{Mp} \mid \langle 1s \mid \boldsymbol{\epsilon}^* \cdot \mathbf{P} \mid \mathbf{p}+\rangle \mid^2 , \tag{5}$$

with α the fine structure constant

For photoeffect the differential cross-section corresponding to absorption of photons of polarization $\boldsymbol{\epsilon}$ is

$$\frac{d\sigma_{ph}}{d\Omega_e} = 4\pi^2\alpha \frac{p}{M\omega} \mid \langle \mathbf{p}- \mid \boldsymbol{\epsilon} \cdot \mathbf{P} \mid 1s\rangle \mid^2 . \tag{6}$$

Here we will give some general arguments about the continuity in energy of the matrix element $\mathcal{M}_{1s}^{ph,DA}$ in equation (3). Due to equation (4) these also apply for the radiative capture case.

In the DA case, it is convenient (though not necessary) to express the dipole matrix element of the momentum operator in terms of the corresponding dipole matrix element of the position operator. Using the well-known identity

$$\mathbf{P} = iM[H, \mathbf{r}] , \tag{7}$$

one obtains the relation

$$\langle \mathbf{p}- \mid \mathbf{P} \mid 1s\rangle = M(E - E_b)\langle \mathbf{p}- \mid \mathbf{r} \mid 1s\rangle. \tag{8}$$

Except for the Coulomb case, analytic expressions are not available for the states $\mid \mathbf{p}\pm\rangle$. However, these dipole matrix elements may be reduced to a single radial matrix element, and as a consequence, it is common practice to work with their partial wave expansion. We consider a potential which may be described as the superposition of a short-range potential and a long range Coulomb potential of ionic charge Z_i. Due to the dipole approximation, and to the s-wave character of the ground state, only the continuum p partial waves contribute. The matrix element of $\mathbf{r}$ may be written as

$$\langle \mathbf{p}- \mid \mathbf{r} \mid 1s\rangle = -\frac{i}{\sqrt{2}\pi} \frac{\mathbf{p}}{p} \mathcal{R} \exp i(\sigma_1 + \delta_1), \tag{9}$$

where σ_1 is the Coulomb $l = 1$ ($p-$wave) phase shift,

$$\sigma_1 \equiv \arg\Gamma(2 - i\xi), \qquad \xi \equiv \eta/p \qquad \eta = MZ_i, \tag{10}$$

and δ_1 is the $p-$wave phase shift due to the short-range potential in the presence of the Coulomb potential of charge Z_i [9]. By $\mathcal{R}$ we denote the radial matrix element

$$\mathcal{R} = \int_0^\infty r^3 R_1(p; r) R_b(r) dr, \tag{11}$$

with $R_1(p; r)$ and $R_b(r)$ the radial wavefunctions (both real) associated with the continuum p wave of momentum p, and the ground state, respectively. The continuum p wave is normalized to have the asymptotic behaviour

$$R_1(p; r) \approx \frac{\sin(pr - \pi/2 + \xi ln(2pr) + \sigma_1 + \delta_1)}{pr} , \quad r \to \infty . \tag{12}$$

The radial function R_b is normalized by the condition $\int_0^\infty r^2 R_b^2 dr = 1$.

We also write, for its use in the appendix, the matrix element of the momentum operator, obtained directly from the partial wave expansion of the vector $\mid \mathbf{p}-\rangle$,

$$\langle \mathbf{p}- \mid \mathbf{P} \mid 1s\rangle = -\frac{i}{\sqrt{2}\pi} \frac{\mathbf{p}}{p} \mathcal{S} \exp i(\sigma_1 + \delta_1), \tag{13}$$

where

$$\mathcal{S} = \int_0^\infty r^2 R_1(p;r) \frac{d}{dr} R_b(r) dr. \quad (14)$$

The general relation (8) implies, for the case of an s bound state, the simple relation

$$i\mathcal{S} = M(E_b - E)\mathcal{R} \ , \quad (15)$$

with E_b the energy of the bound state.

The matrix element $\mathcal{R}$ is directly connected to a matrix element which has simple analytic properties [10,11], called the *reduced dipole matrix element*. We are interested here only in transitions involving a bound state, so we define

$$\mathcal{D}(E_b l, El') \equiv \int_0^\infty r \Phi_{E_b l}(r) \Phi_{El'}(r) \ dr, \quad (16)$$

where $\Phi_{El'}(r)$ and $\Phi_{E_b l}(r)$ are radial eigenfunctions respectively of eigenvalue $E = \frac{p^2}{2M} > 0$ and real bound eigenvalue $E_b < 0$ of the discrete spectrum. Both eigenfunctions are normalized by the condition

$$\lim_{r\to 0} r^{-l'-1} \Phi_{El'}(r) = \lim_{r\to 0} r^{-l-1} \Phi_{E_b l}(r) = 1. \quad (17)$$

From Poincaré's theorem [3] the solutions of the Schrödinger equation $\Phi_{El'}(r)$ normalized according to (17) are analytic functions of E; E and p need not be taken as real and positive. Similarly the reduced matrix element $\mathcal{D}$ may be defined by (16) whenever the integral exists, requiring $\sqrt{-2ME_b} > \pm \mathrm{Im}\, p$.

For real $E > 0$ and any bound state $E_{nl} < 0$, the connection between the two sets of radial wave functions is

$$rR_{l'}(p;r) = N_{l'}(p) \Phi_{El'}(r), \ rR_{nl} = N_{nl} \Phi_{E_{nl} l}(r) \ , \quad (18)$$

where $N_{l'}(p)$ and N_{nl} are real normalization constants defined for $E_{nl} < 0, E > 0$, so that (11) becomes

$$\mathcal{R} = N_1(p) N_{10} \mathcal{D}(E_b 0, E1) \ . \quad (19)$$

The ground state is labeled by (10), its energy by E_b, as in equation (2).

We may express the cross-sections (5) and (6) in terms of this *reduced* matrix element $\mathcal{D}(E_b 0, E1)$. For photoeffect we have

$$\frac{d\sigma^{ph}}{d\Omega_\gamma} = 2\alpha \frac{M\omega}{p} \mid \boldsymbol{\epsilon} \cdot \mathbf{p} \mid^2 N_{10}^2 N_1(p)^2 \mid \mathcal{D}(E_b 0, E1) \mid^2, \quad (20)$$

and for radiative capture

$$\frac{d\sigma^{rc}}{d\Omega_\gamma} = (\frac{\alpha\omega}{p})^2 \ \frac{d\sigma^{ph}}{d\Omega_e} \ . \quad (21)$$

The preceding relation can be derived directly from the time reversal invariance property of the electron-photon interaction.

The *total* cross-section for photoeffect, integrated over electron directions, in the case of unpolarized photons is

$$\sigma^{ph}_{unpol} = \frac{8\pi\alpha}{3} M\omega p N_{10}^2 N_1(p)^2 \mid \mathcal{D}(E_b 0, E1) \mid^2 . \quad (22)$$

The *total* cross-section for radiative capture is obtained by summing over photon polarizations and integrating over the photon direction. This leads to the relation

$$\sigma^{rc} = 2 \ (\frac{\alpha\omega}{p})^2 \ \sigma^{ph}_{unpol} \ . \quad (23)$$

Features of the reduced matrix element (16) have been discussed by Oh and Pratt [12]. For our purposes here the key fact is that this matrix element is a continuous function of E. This follows from two mathematical theorems:

i) A theorem due to Poincaré [3] guarantees that for complex E and p the function Φ_{El} is an entire function of the parameter $p \equiv \sqrt{2ME}$, in the complex plane of p, because it satisfies the radial Schrödinger equation, in which the coefficients are analytic in p (simply E), with a boundary condition (17) in which the parameter p does not appear.

ii) Another theorem [4,5] states that if an integrand is analytic in a parameter, the integral, if uniformly convergent, is an analytic function of the parameter. This may be used to deduce the analyticity of the reduced matrix element (16) in p. The integrand is an analytic function of p in the complex p plane for every value of the integration variable r. So, whenever it is convergent, the integral is an analytic function of the parameter p. Thus whenever $(\pm \mathrm{Im}\, p) - \sqrt{-2ME_b} < 0$, D is a convergent integral, as can seen from the asymptotic behaviour of the two wavefunctions: $\Phi_{E_b 0}(r)$ goes exponentially to zero and bounds $\Phi_{El'}(r)$. Hence, for real E the integral is continuous for $E - E_b > 0$.

In the case of potentials which are Coulombic at large distances, Dillon and Inokuti [13] have analyzed in detail the reduced matrix element (16) and have shown that it is a continuous function of the real transition energy $E - E_b$, except for zero transition energy. In our case of a continuum-bound transition the transition energy does not vanish, so the reduced matrix element is continuous for all $E > 0$ (actually for $E > E_b$, with $E_b < 0$).

Coming back to equations (8), (9) and (19), since the reduced matrix-element is continuous, the matrix element $\langle \mathbf{p}- \mid \mathbf{P} \mid 1s \rangle$ will be a continuous function of the energy E if the normalization constant $N_1(p)$ and the phase-shift $\sigma_1 + \delta_1$ are also continuous functions for real $E > 0$; the cross-sections (20)-(21) are in fact independent of this phase shift. The normalization constants are such functions. For justification we refer to Section 6.5 of Goldberger and Watson [14], giving the connection between the normalization constant and the Jost function [Chapter VI, Eq. (237)]. For the behaviour of the phase-shift we use its relation to the element of the S-matrix [Chapter VI, Eq. (57)] to see that it may be taken as continouus. The needed analytic properties of the Jost function and the S-matrix elements have been established for a class of short-range potentials (see [15]); they may also

be extended to the Coulomb potential and, presumably, to potentials with long range Coulomb tails considered as limits of short range potentials. As already noted, all the cross-sections considered here are independent of the phase-shift.

In the next section we will verify the continuity in energy of the matrix-element $\langle \mathbf{p}- \mid \mathbf{P} \mid 1s\rangle$ in the the Coulomb case, tracing through the analytic expressions for the different steps of the calculation.

3 The matrix element in the Coulomb case: Dipole approximation

In the Coulomb case all the conditions required to ensure the continuity of the continuum-bound matrix elements of $\mathbf{r}$ or $\mathbf{p}$ are satisfied, as can also be seen from the explicit equations written below. The regular solution of the radial Schrödinger equation is an analytic function of p,

$$\Phi_{El}(r) = \exp(-ipr)r^{l+1} \times {}_1F_1(l+1+i\xi, 2l+2; 2ipr), \qquad (24)$$

where ${}_1F_1$ denotes the Kummer series [16], and $\xi = MZ_i/p$ as defined in equation (10), even for complex p. The normalization constant $N_l(p)$, determined from equations (12) and (18) for real p, and the phase-shift σ_l of the l-th partial-wave are given by continuous functions of p, for real $p > 0$:

$$N_l(p) = \frac{(2p)^l}{(2l+1)!} e^{\pi\xi/2} \mid \Gamma(i\xi + l + 1) \mid, \qquad (25)$$

$$\sigma_l = \arg\Gamma(-i\xi + l + 1).$$

As mentioned in the introduction, in the Coulomb case the photoeffect matrix element can be expressed analytically (by the Fischer-Sauter equation if retardation is included, by the Stobbe formula in dipole approximation). Derivations of these results can be found in the book of Sommerfeld [6], or in [17]. In this section we continue to consider the dipole approximation case, for which Chatterjee *et al.* have already asserted the existence of a discontinuity. As we would expect from our previous discussion, Stobbe's result is a continuous function of energy. We will therefore examine the derivation which Chatterjee *et al.* [1,2] present, in obtaining an analytic expression of the momentum operator matrix element (3) between a continuum "in" state and the ground state, in dipole approximation.

The correct result for this matrix element is (for real $p \geq 0$)

$$\langle \mathbf{p}- \mid \mathbf{P} \mid 1s\rangle = 2\sqrt{2}(\eta)^{5/2} \frac{\mathbf{p}}{(p^2+\eta^2)^2} \Gamma(2 - i\xi) \times \exp(\pi\xi/2) \left(\frac{i\xi - 1}{i\xi + 1}\right)^{i\xi}, \qquad (26)$$

where the argument of $\dfrac{i\xi - 1}{i\xi + 1}$ is to be taken in the range $(-\pi, \pi)$, as follows from the corresponding choice of argument in the integral representation of Φ in equation (24). This will be make clear in the following, and also in a simpler version of the derivation of (26) which is presented in the Appendix.

Then in equation (26) one can write

$$\frac{i\xi - 1}{i\xi + 1} = \exp(-i\tau)\ , \qquad (27)$$

with the angle τ defined by

$$\sin\tau = -\frac{2\xi}{1+\xi^2}\ , \qquad \cos\tau = \frac{\xi^2 - 1}{1+\xi^2}\ , \qquad (28)$$

and τ in the range $(-\pi, \pi)$. But since $\xi \geq 0$, sin $\tau \leq 0$ and therefore the range of τ is $(-\pi, 0)$. Then from the expression for cos τ we see that

$$-\frac{\pi}{2} < \tau < 0 \quad \text{for} \quad p < \eta \quad (\xi > 1)\ , \qquad (29)$$

$$-\pi < \tau < -\frac{\pi}{2} \quad \text{for} \quad p > \eta \quad (\xi < 1)\ . \qquad (30)$$

At $p = 0$ the angle τ is zero, at $p = \eta$ it is equal to $-\pi/2$, and for very large values of p the angle τ approaches $-\pi$. We note that the error of Chatterjee *et al.* results from an incorrect assignment of the ranges of τ. We mention that τ is the notation used by Sommerfeld in the calculation including retardation [18]; it reduces in dipole approximation to the angle described here.

Inserting the expression (26) for the matrix element in equation (5), we get the final expression for the *total* radiative capture cross-section,

$$\sigma_{rc} = \frac{256\pi^2}{3}\alpha^3 \frac{\xi^6}{(1+\xi^2)^4} \frac{\exp(2\xi\tau)}{1 - \exp(-2\pi\xi)}\ . \qquad (31)$$

We also write the corresponding expression for the total K-shell photoeffect cross-section (integrated over the electron direction), for unpolarized photons [17],

$$\sigma_{ph} = \frac{1024\pi^2}{3}\alpha \frac{1}{p^2} \frac{\xi^6}{(1+\xi^2)^4} \frac{\exp(2\xi\tau)}{1 - \exp(-2\pi\xi)}\ . \qquad (32)$$

Before proceeding, we mention the more common way [17, 19] of writing the expression (27),

$$\left(\frac{i\xi - 1}{i\xi + 1}\right)^{i\xi} = \exp(-2\xi\ \cot^{-1}\xi)\ , \qquad (33)$$

which emphasises the negative value of the exponent, and implies that the angle ϕ (we use the notation in [1]) defined by

$$\phi/2 \equiv \cot^{-1}\xi = \tan^{-1} p/\eta \equiv -\tau/2 \qquad (34)$$

is in the range $(0, \pi)$. This angle takes the value 0 for $p = 0$, the value $\pi/2$ for $p = \eta$, and approaches the value π for very large values of p. There is nothing ambiguous in the expression (26), if written in terms of this angle ϕ, once its range is defined, for which equation (34) is not enough. The matrix element (26) is a continuous function of the real electron momentum p. The result, however, reported

in [1] is the same as that in equation (31) for $p < \eta$, but larger by a factor of $e^{2\pi\xi}$ for $p > \eta$. This comes from a different range which is attributed to the angle ϕ.

Let us analyze now the calculation in Sections 4 to 6 of [1]. The calculation is based on the expression of an integral $\mathbf{I}$, defined in their equation (3), which for $\kappa = 0$ is, up to a factor, the matrix element (1). The authors evaluate this matrix element, directly, utilizing the analytic expression of the full three dimensional Coulomb continuum energy eigenstate,

$$\langle \mathbf{r} \mid \mathbf{p}- \rangle = \frac{\exp(\pi\xi/2)}{(2\pi)^{3/2}}\, \Gamma(1+i\xi)\, \exp(i\mathbf{p}\cdot\mathbf{r}) \times {}_1F_1(-i\xi, 1; -i(pr + \mathbf{p}\cdot\mathbf{r}), \tag{35}$$

and using explicitly a result for integration over such functions derived by Nordsieck [Ref. [20], Eq. (1)]. The derivation of Nordsieck is based on the use of an integral representation for the hypergeometric function in the full-continuum state, equation (35). There is no ambiguity in the definition of the complex power of complex argument, appearing first in the integral representation, which enters the integrand, and then in the final result. Equation (4) of [1] would be correct (only a factor π is missing), if the principal value for the argument of the complex power in

$$f \equiv 2^{i\xi} e^{-\pi\xi} (p^2 - \eta^2 + 2i\eta p)^{-i\xi} \tag{36}$$

was used. With the notation (28) used previously, one finds this way

$$f = (\frac{p^2+\eta^2}{2})^{-i\xi} e^{\tau\xi}, \tag{37}$$

which leads to the relation

$$\theta = \tau + \pi, \tag{38}$$

between the angle τ in equation (28) and the angle θ, used in [1]. The range of θ should therefore be $(0, \pi)$. However the authors of [1] write an expression for θ in terms of its tangent, assuming the range is $(-\pi/2, \pi/2)$, rather than considering the full definition of θ which follows from the calculation.

We mention that the correct result for their integral $\mathbf{I}$ can also be found in reference [19]. The expression for $\mid \mathbf{I} \mid^2$ given in equation (6) of [1] (from which a factor 16 is missing) is based on the assumption that the range of θ is $(-\pi/2, \pi/2)$, and so it is not correct. If the proper range $(0, \pi)$ is used for θ, the equation becomes correct.

The important quantity for the discussion in [1] is the function defined after their equation (6):

$$F = \mid f \mid^2 = \exp[\, 2\xi(\theta - \pi)] = \exp(-2\xi\phi). \tag{39}$$

(In fact they write $F = f^2$, presumably a misprint, since f is not real). With this expression, Chatterjee *et al.* introduce the angle $\phi = \pi - \theta$, which we defined before in (34), but specifying that ϕ is in the range $(0, \pi)$; one has, as already noted, $\phi = -\tau$. However, instead of giving values to ϕ in the range $(0, \pi)$, they assign to it values between $-\pi/2$ and $\pi/2$. For $p < \eta$ this is correctly given as $\phi \in (0, \pi/2)$, but for $p > \eta$ instead of continuing from $\pi/2$ to π, they give for ϕ the range $(-\pi/2, 0)$. This causes the incorrect jump at $p = \eta$ of the matrix element. The correct value of F at $p = \eta$ is $F = \exp(-\pi)$. In fact, the correct angle ϕ here is identical with the angle which Chatterjee *et al.* denoted by ϕ' in [1]. If they had used their ϕ' in the analytic equations, everything would have been correct, and no jump would have been predicted.

The argument of the authors, based on the values of the tangent function for the angles they manipulate, is not justified: the proper branch of the tangent function is determined by the original integral. A numerical evaluation of F, using the correct phases in the integrand coming from the representation of the hypergeometric function, confirms the dotted curve in Figure 4 of [1], not the erroneous discontinuity of the full curve.

4 The matrix element with retardation

The retarded matrix element for radiative capture in an atomic field is

$$\mathcal{M}^{rc}_{1s}(\boldsymbol{\kappa}, \mathbf{p}, \boldsymbol{\epsilon}) = \boldsymbol{\epsilon}^* \cdot \langle 1s \mid \exp(-i\boldsymbol{\kappa}\cdot\mathbf{r})\mathbf{P} \mid \mathbf{p}+ \rangle, \tag{40}$$

where we have used the same notations as in Section 2. The retardation effects are due to the factor $\exp(-i\boldsymbol{\kappa}\cdot\mathbf{r})$, where $\boldsymbol{\kappa}$ is the photon momentum. In the usual dipole approximation this exponential is simply replaced by 1, which is equivalent to taking $\boldsymbol{\kappa} = 0$, but equation (2) remains unchanged. The matrix element (1) is obtained in this way.

Chatterjee *et al.* [1] have also presented results for the pure Coulomb case, including retardation. At the end of Section 6 of [1], we find a complicated result for the nonrelativistic total cross-section of radiative capture with retardation included. This is surprising, since the well-known Fischer-Sauter equation [17] is completely different. Looking back at the paper [8], which gives more details, we notice that the quantity presented as the differential cross-section is already very different. Instead of the rather simple Fischer-Sauter result,

$$\mid \mathcal{M}^{rc}_{1s} \mid^2 = \frac{16}{\pi}\eta^5 \frac{\xi^2(1+\xi^2)}{1-\exp(-2\pi\xi)} \frac{\mid \boldsymbol{\epsilon}\cdot\mathbf{p} \mid^2}{\mathcal{A}^4} \exp(2\xi\tau), \tag{41}$$

where

$$\mathcal{A} = (\mathbf{p} - \boldsymbol{\kappa})^2 + \eta^2, \tag{42}$$

and

$$\tan\tau = \frac{-2\eta p}{\kappa^2 - p^2 + \eta^2}\ , \tag{43}$$

with the condition $-\pi < \tau < 0$, which results from considerations very similar to those presented in Section 3, a very complicated expression is given. Note that equation (41)

is identical with the dipole result except for setting $\kappa = 0$ in (42) and (43).

We can see that equation (9) of [8] is so different because the integral evaluated there, defined in equation (6) of [8], is not the right quantity. An error is made in the beginning: the simple replacement of the momentum operator by the position operator (with a factor) is possible only in the dipole approximation, which is not the case now under consideration. The replacement of the operator $\mathbf{P}$, using the identity (7), leads to additional terms in comparison to the DA case, due to the presence of the factor $\exp(-i\boldsymbol{\kappa}\cdot\mathbf{r})$ in the matrix element equation (40). These terms are ignored in [8]. Note that although Akhiezer and Beresteskii [19] are cited for this form of matrix element, in fact they are only obtaining this form when they make the dipole approximation.

5 Further discussion and conclusions

Finally, we refer to photoeffect, and we invoke experimental data in favor of the theoretical result contained in equation (32). We consider K shell photoionization cross-sections at high energies, where screening effects are not important and the Coulomb cross-section is measured directly. Generally excellent agreement is found between theory and experiment. For example, one may consider the exhaustive comparisons for all elements of experimental and theoretical X-ray attenuation coefficients between 0.1–100 keV due to Saloman and Hubbell [21]. The alleged discontinuity in the photoeffect cross-section would occur at twice the K shell threshold energy. At this energy total attenuation is dominated by K shell photoeffect. This region is shown in Salomon and Hubbell's tabulation for $Z < 60$, and for most elements there is substantial experimental data. There is no evidence of a discontinuity, and there is generally very good agreement between experiment and standard theory.

We mention the existence of a paper on radiative muon capture in light atoms [22], which makes use of Stobbe's result (32) in the correct way. In fact, Stobbe's result was used in many calculations of electron capture in ion-atom collisions, whenever the impulse approximation was adopted [23]. Good agreement is found with experiments, and there is no evidence for a discontinuity. For a recent review, see McCann *et al.* [24]. See also the papers of Ichimaru *et al.* [25] and references therein.

In conclusion, in this paper we have argued that there is no discontinuity in the energy dependence of continuum-bound transitions in an atomic field. In Section 2 we have used general arguments based on the continuity in energy of the reduced matrix element, a property which can be rigorously proven [3,5,12], based on theorems of Poincaré and Titchmarsh. In the Coulomb case, discussed in Section 3, we have identified the error in [1], coming from a misapplication of Nordsieck's result [20]. The retarded results of [8] further suffer from an incorrect treatment of the matrix element of the momentum operator $\mathbf{P}$ in the presence of retardation.

This work is a continuation of cooperative work of the authors in the framework of a National Research Council Romanian Twinning Program, whose support is warmly acknowledged. It has also been partly supported under NSF Grant PHY9601752.

Appendix

We present here a very direct derivation of equation (26). This allows us to verify once more the correctness of the value assigned to τ in equations (28) and (27). The derivation starts from equation (13), and it is based on the evaluation of the integral $\mathcal{S}$ in (14). With the explicit expressions for the continuum p wave [Eq. (24) with $l = 1$] and for the ground state radial wavefunction, one has

$$\mathcal{S} = -2(\eta)^{5/2} N_1(p) S_0, \tag{44}$$

with

$$S_0 \equiv \int_0^\infty r^3 \exp(-ipr - \eta r)_1F_1(2 + i\xi, 4; 2ipr)dr\ . \tag{45}$$

The quantities p and ξ are real. Up to a factor the integral is a function of the parameter ξ only, as it can be rewritten as

$$S_0 = \frac{1}{16p^4} \int_0^\infty \rho^3 \exp[-\frac{1}{2}(\xi + i)\rho]_1F_1(2 + i\xi, 4; i\rho)d\rho\ . \tag{46}$$

The integral is convergent for $\xi > 0$, which is the case here, and it is given by the simple elementary expression [see Appendix f of [26], Eq. (f.3)]

$$S_0 = \frac{6}{p^4(1 + \xi^2)^2} \left(\frac{i\xi - 1}{i\xi + 1}\right)^{i\xi}\ , \tag{47}$$

where again, as stated in [26], the phase of the term in parenthesis is to be taken in the range $(-\pi, \pi)$. Using the angle τ (47) becomes

$$S_0 = \frac{6}{p^4(1 + \xi^2)^2} \exp(\xi\tau). \tag{48}$$

The correct choice for the complex power follows from the calculation and can be seen by tracing it through the Landau and Lifschitz [26] derivation. The expression one gets in this way for the matrix element (3) is identical with equation (26). The result (26) is, in agreement with our general discussion, a continuous function of the electron energy.

References

1. L. Chatterjee, G. Das, R. Goswami, Z. Phys. D **32**, 73 (1994).
2. L. Chatterjee *et al.*, Hadron. J. **7**, 75 (1992).
3. L. Schiff, *Quantum Mechanics*, 3rd edn. (McGraw Hill, New York, 1968).

4. E. Goursat, *Cours d'Analyse Mathematique*, 4th edn., Ch. XVII (Gauthiers-Villars, Paris, 1924).
5. E.C. Titchmarsh, *The Theory of Functions*, 2nd edn., Ch. II (Oxford University Press, Oxford, 1939).
6. A. Sommerfeld, *Atombau und Spektrallinien* Vol. 2, Ch. VI, §5, (Braunschweig, Vieweg, 1939).
7. M. Stobbe, Ann. Phys. (Leipzig) **7**, 661 (1930).
8. L. Chatterjee, G. Das, A. Chakrovorty, Europhys. Lett. **18**, 145 (1992).
9. P.G. Burke, C.J. Joachain, *Theory of Electron-Atom Collisions, Part 1, Potential Scattering* (Plenum Press, 1994).
10. L. Infeld, T.E. Hull, Rev. Mod. Phys. **23**, 21 (1951).
11. S.D. Oh, R.H. Pratt, Phys. Rev. A **34**, 2486 (1986).
12. S.D. Oh, R.H. Pratt, Comments. At. Mol. Phys. **22**, 363 (1996).
13. M.A. Dillon, M. Inokuti, J. Chem. Phys. **74**, 6271 (1981).
14. M.L. Goldberger, K.M. Watson, *Collision Theory* (John Wiley, New York, 1964).
15. R.G. Newton, *Scattering theory of waves and particles* (McGraw Hill, New York, 1966).
16. A. Erdelyi, W. Magnus, F. Oberhettinger, F. Tricomi, *Higher Transcendental Functions*, Vol. 1 (McGraw-Hill, New York, 1953).
17. H.A. Bethe, E.E. Salpeter, *Quantum Mechanics of One- and Two-Electron Atoms* (Springer, Berlin, 1957).
18. Ref. [6], Eq. (4.19b), Chapter VI.
19. A.I. Akhiezer, V.B. Beresteskii, *Quantum Electrodynamics* (Interscience, New York, 1965).
20. A. Nordsieck, Phys. Rev. **93**, 785 (1954).
21. E.B. Salomon, J.H. Hubbell, Report NBSIR 86-3431, "X-Ray Attenuation Coefficients (Total Cross Sections): Comparison of the Experimental Data Base with the Recommended Values of Henke and the Theoretical Values of Scofield for Energies Between 0.1−100 keV", National Bureau of Standards, U. S. Department of Commerce, Gaithersburg, MD (July 1986).
22. G. Soff, J. Rafelski, Z. Phys. D - Atoms, Molecules and Clusters **14**, 187 (1989).
23. M. Kleber, D.H. Jakubasa, Nucl. Phys. A **252**, 152 (1975).
24. J.F. McCann, J.T. Glass, D.S.F. Crothers, *The Physics of Electronic and Atomic Collisions 19th International Conference, Whistler, Canada 1995*, edited by J.L. Dube, J.B.A. Mitchell, J.W. McConkey, C.E. Brion, AIP Conference Proceedings 360 (AIP Press, American Institute of Physics, Woodbury, New York, 1966), p. 857.
25. A. Ichihara, T. Shirai, J. Eichler, Phys. Rev. A. **54**, 4954 (1996).
26. L.D. Landau, E.M. Lifschitz E.M., *Quantum Mechanics. Nonrelativistic Theory* (Pergamon, Oxford, 1978).