Elastic scattering of fast electrons and positrons by atoms

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Elastic scattering of relativistic electrons and positrons by atoms is considered in the framework of the static field approximation. The scattering field is expressed as a sum of Yukawa terms to allow the use of various approximations. Accurate phase shifts have been computed by combining Bühring's power-series method with the WKB and Born approximations. This combined procedure allows the evaluation of differential cross sections for kinetic energies up to several tens of MeV. Numerical results are used to analyze the validity of several approximate methods, namely the first- and second-order Born approximations and the screened Mott formula, which are frequently adopted as the basis of multiple scattering theories and Monte Carlo simulations of electron and positron transport.

I. INTRODUCTION

An accurate description of elastic scattering of relativistic electrons and positrons by atoms is required in a number of fields (e.g, electron–γ-ray shower theory, electron microscopy, electron-probe microanalysis). The general theory of high-energy electron scattering has been reviewed by Walker.[1] For kinetic energies larger than a few keV, exchange and charge cloud polarization corrections are negligible[2,3] and the cross section can be computed by using the static field approximation. In this approximation, the differential cross section (DCS) is obtained by solving the partial wave expanded Dirac equation for the motion of the electron or positron in the central field of the atom. The convergence of the partial wave series slows down for increasing energy and, at the same time, the difficulty of obtaining the numerical solution of the radial equations for each phase shift also increases with energy. As a result of these difficulties, only a few systematic computations,[4,5] limited to energies up to a few hundred keV, have been reported to date.

In many practical circumstances electrons suffer multiple elastic collisions within the scattering medium. An accurate description of multiple scattering processes (including energy losses) may be obtained through Monte Carlo simulation.[6,7] Most of the high-energy Monte Carlo codes currently available use some form of the multiple scattering theory for infinite media together with approximate DCS's. An extensive compilation of approximate formulas for the DCS may be found in the review of Motz *et al.*[8] One class of Monte Carlo simulation procedures is based on the multiple scattering theory of Goudsmit and Saunderson[9] and Lewis[10] and incorporates the DCS's given by the first-order Born approximation or by the screened Mott formula (see below). Other simulation codes use the multiple scattering theory of Molière[11] which is based on the DCS derived from the eikonal approximation. This theory has been reformulated by Nigam *et al.*[12] who used the Dalitz cross section,[13] i.e., the DCS for a Yukawa field computed in the second-order Born approximation. The accuracy of the Monte Carlo simulation depends on the reliability of the DCS's underlying the adopted multiple scattering theory. Owing to the lack of data bases for elastic scattering at high energies, it is difficult to ascertain the range of validity of these approximate DCS's.[14]

In this paper we briefly describe a numerical procedure which allows the evaluation of DCS's for analytical fields expressed as a sum of Yukawa terms for energies up to a few tens of MeV. We present calculated total elastic cross sections and transport cross sections for electrons and positrons and for three elements (aluminum, silver, and gold). The particular form of the potential allows the easy evaluation of the DCS with three different approximations, which have been employed as the basis of several MC procedures, namely, the first-order and second-order Born approximations and the screened Mott formula. The quality of these approximations is analyzed on the basis of our numerical results.

We consider scattering fields of the form

$$V(r)=z\frac{Z}{r}\sum_{i=1}^{N}A_i\exp(-\alpha_i r)\ , \tag{1}$$

where Z is the atomic number and z is the projectile charge (equal to -1 for electrons and 1 for positrons). This expression is well suited to fit the numerical potentials obtained from self-consistent calculations.[15–17] The results reported below have been obtained by using the parameters given in Ref. 17. We use atomic Hartree units ($\hbar=m=e=1$) unless otherwise specified.

II. NUMERICAL CALCULATIONS

Scattering amplitudes for the potential (1) have been computed by summing the partial-wave series [Eqs. (15a) and (15b) of Ref. 1] with phase shifts δ_{la} (with $a=1$ and -1) evaluated numerically, or using the WKB and Born approximations where applicable. WKB phase shifts have been evaluated by applying the Langer method to the second-order Dirac equation (see Ref. 18, pp. 99, 227, and 228). Relativistic Born phase shifts were obtained from the Parzen formulas.[19] Similar calculations have al-

ready been performed for lower energies.[3,15,20] The extension to higher energies requires the use of more refined numerical methods to compute the first phase shifts, since the accuracy of the computed DCS's relies mainly on the quality of these phase shifts.

The first phase shifts ($l=0,1,\ldots$) have been determined by solving the radial Dirac equation using the Bühring power series method[1,21] as described elsewhere.[22] The function $rV(r)$ has been replaced by the natural cubic spline which interpolates the values of this function for a grid of points dense enough to ensure that interpolation errors in the potential have a negligible effect on the computed phase shifts. The Bühring method has two important advantages in comparison with the more conventional numerical procedures such as the Numerov,[23] Runge-Kutta,[24] and Milne methods[25] usually adopted to solve the radial equations. First, truncation errors are completely avoided and, therefore, the radial functions are only affected by unavoidable round-off errors. Second, the spacing of the grid of points where $V(r)$ is tabulated has no effect on the accuracy of the numerical procedure (provided the interpolating spline do approach the actual field). We note in passing that conventional numerical methods require the use of grids dense enough to keep the effect of truncation errors below some reasonable limit and, therefore, the density of the grid should be increased for increasing energies to maintain the truncation error constant. The only disadvantage of the Bühring method is its higher cost in computer time.

The algorithm to compute the phase shifts proceeds as follows. First, Born phase shifts are evaluated for all orders l up to a value of the orbital angular momentum $l=L$ large enough to guarantee the convergence of the partial wave series. Numerical and WKB phase shifts are then computed for increasing orders; the relative difference between these phase shifts decreases with the order and for a certain order $l=L_1$ it becomes smaller than a given value ϵ ($=5\times10^{-4}$ in the present calculations). The evaluation of numerical shifts is then discontinued. For $l>L_1$, the phase shifts are approximated by the WKB phase shifts which are computed up to an order $l=L_2$ for which the relative differences between the WKB and Born phase shifts become smaller than ϵ. For $l>L_2$, the Born phase shifts are used. The accuracy of this scheme is mainly limited by ϵ. Of course, the ϵ value has to be at least larger than the relative uncertainty due to round-off errors in the numerical phase shift; otherwise, the computation of exact shifts could never stop. Our computer code generates up to 4000 Born phase shifts, which ensure the convergence of the partial wave series for energies up to about 20 MeV for all the elements. The DCS, $d\sigma/d\Omega$, has been evaluated by direct summation of the partial wave series.

The total elastic cross section σ and the transport (or momentum transfer) cross section σ_{tr} are given by

$$\sigma\equiv 2\pi\int_0^{\pi}\frac{d\sigma}{d\Omega}\sin\theta\, d\theta \tag{2}$$

and

$$\sigma_{tr}\equiv 2\pi\int_0^{\pi}(1-\cos\theta)\frac{d\sigma}{d\Omega}\sin\theta\, d\theta\ . \tag{3}$$

It is well known[11,26] that the angular distribution after increasingly multiple elastic scattering becomes strongly influenced by the value of σ_{tr} and it is practically insensitive to other details of the single scattering DCS.

III. APPROXIMATE CROSS SECTIONS

The field (1) leads to analytical expressions for the DCS in the first-order and second-order Born approximations.[8] The first-order Born cross section for electrons or positrons of momentum p may be written in the form

$$\frac{d\sigma^{(B)}}{d\Omega}=[1-F(q)]^2\frac{d\sigma^{(R)}}{d\Omega}\ , \tag{4}$$

where

$$F(q)=\sum_{i=1}^{N}A_i\frac{\alpha_i^2}{\alpha_i^2+q^2} \tag{5}$$

is the atomic form factor [normalized so that $F(0)=1$]

$$\frac{d\sigma^{(R)}}{d\Omega}=\frac{4Z^2}{q^4}\frac{1-\beta^2\sin^2(\theta/2)}{1-\beta^2} \tag{6}$$

is the Mott-Born cross section,[8] i.e., the first-order Born DCS for the unscreened Coulomb field. Here $q=2p\sin(\theta/2)$ is the momentum transfer and β is the electron velocity in units of the speed of light. The second-order Born cross section is given by the Gorshkov formula—Eq. (A108) in Ref. 8. It is worth noticing that the potential parameters used here, see Table I, were determined in such a way that the form factor (5) for small momentum transfers coincides with the form factor computed from the Dirac-Hartree-Fock-Slater atomic electron density and, therefore, the first-order Born DCS (4) practically coincides with the one computed from the numerical self-consistent field.

TABLE I. Parameters of the analytical potential (1) used in the present calculations (Ref. 17). For aluminum, the potential has only two terms.

Element	Z	A_1	A_2	α_1	α_2	α_3
Al	13	0.6002	0.3998	5.1405	1.0153	
Ag	47	0.2562	0.6505	15.588	2.7412	1.1408
Au	79	0.2289	0.6114	22.864	3.6914	1.4886

The Mott DCS,[18,27,28] i.e., the exact DCS for an unscreened Coulomb field, provides an alternative approach to the cross section for an atom. In the calculations, we have used the algorithm described by Vande Putte.[29] Actually, in the limit of large-momentum transfers, screening effects vanish and the Mott cross section should be very accurate. However Mott's DCS, as well as the Mott-Born DCS (6), diverges for small scattering angles. To obtain a finite total cross section it is then necessary to account for the screening by the atomic electrons. This effect can be introduced approximately by considering the screened Mott DCS defined as[6]

$$\frac{d\sigma^{(\mathrm{SM})}}{d\Omega}=[1-F(q)]^2\frac{d\sigma^{(\mathrm{M})}}{d\Omega}\ , \tag{7}$$

where $d\sigma^{(\mathrm{M})}/d\Omega$ stands for the Mott DCS [cf. Eq. (4)]. A related procedure has been described by Zeitler and Ol-

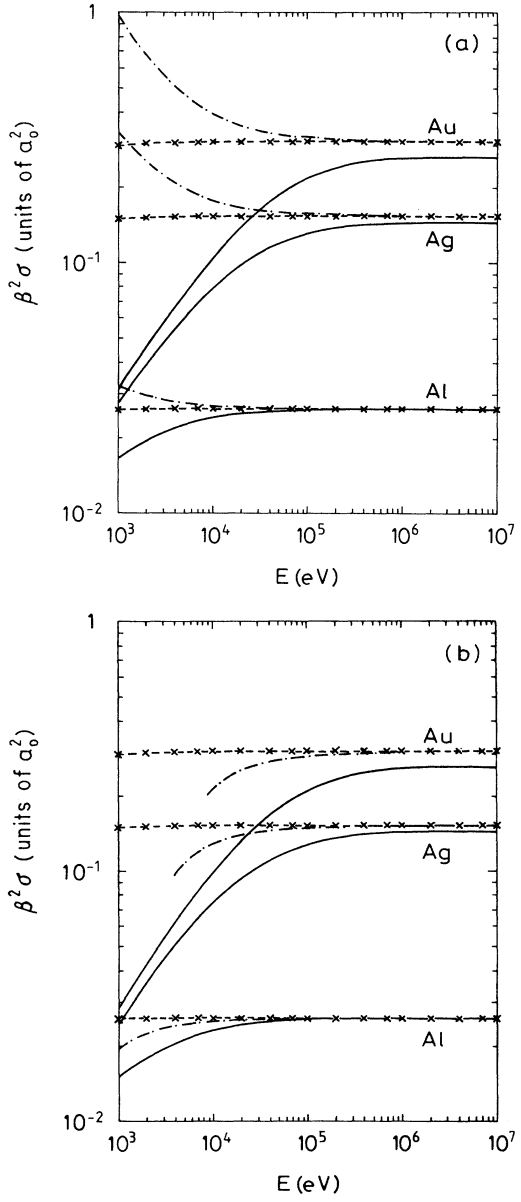

FIG. 1. Total elastic cross sections for (a) electrons and (b) positrons scattered by Al ($Z=13$), Ag ($Z=47$), and Au ($Z=79$) obtained from the three-term potentials given in Table I. The quantity plotted is $\beta^2\sigma$, with $\beta^2\equiv(\gamma^2-1)/\gamma^2$ and $\gamma=1+E/c^2$, in units of a_0^2 (atomic units) vs kinetic energy E. The continuous curves are the results of the present calculations. Dashed and dotted-dashed lines correspond to the screened Mott (7) and Gorshkov cross sections, respectively. The first-order Born cross sections (4) are indicated by crosses.

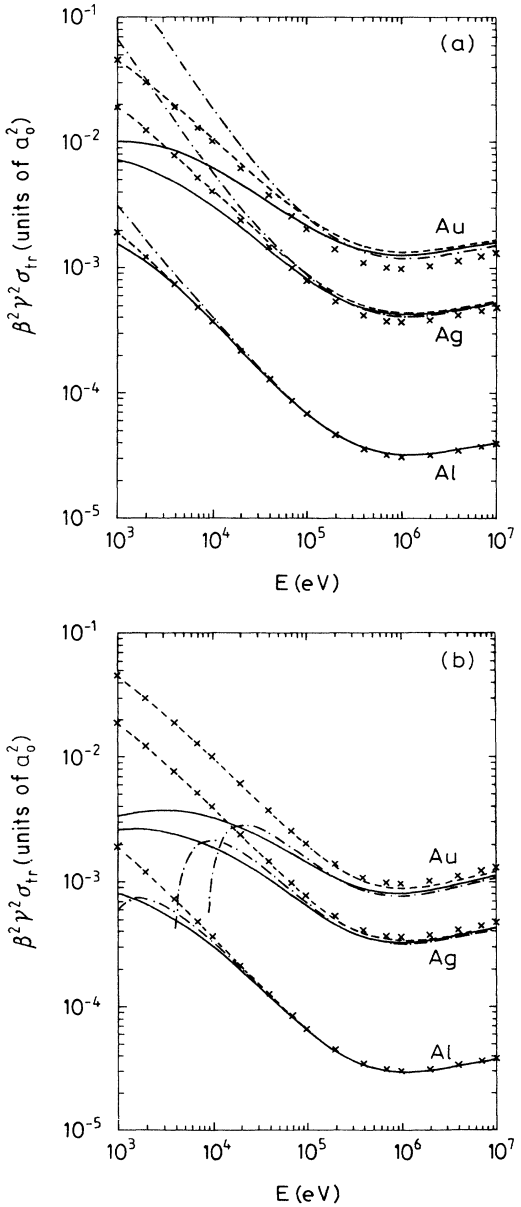

FIG. 2. Transport or momentum transfer cross sections for (a) electrons and (b) positrons scattered by Al ($Z=13$), Ag ($Z=47$), and Au ($Z=79$) obtained from the three-term potentials given in Table I. The quantity plotted is $\beta^2\gamma^2\sigma_{tr}$ in atomic units. Details are the same as in Fig. 1.

sen[30] who used the eikonal approximation instead of the Born approximation to evaluate the screening correction factor. This last method leads to better results than Eq. (7) at the expense of a considerable numerical effort that makes it virtually useless for high energies.

In order to get a clear indication of the accuracy of these approximation methods we consider the corresponding total cross section and transport cross section, which are plotted in Figs. 1 and 2 for electrons and positrons scattered by aluminum, silver, and gold atoms as functions of the kinetic energy E. These figures include the present numerical results, the (first-order) Born formula (4), the screened Mott formula (7), and the Gorshkov formula[8] calculated for the *same* analytical field.

Owing to the fact that the DCS for high energies is a rapidly decreasing function of θ, the major contributions to the integral (2) originate from small scattering angles where the three approximate formulas practically coincide. Hence these formulas lead to nearly the same total cross section (at high enough energies). The effect of the second-order Born correction becomes prominent for low energies. The relative differences between the numerical and approximate total cross sections increase for decreasing energies and for increasing atomic numbers. It is worth noticing that for high energies these differences attain a constant value, rather than decreasing with energy as it could be naively expected. This is a direct consequence of the failure of these approximations to adequately describe the screening effect. It is also seen that the Born and screened Mott total cross sections practically coincide since the ratio of Mott to Mott-Born DCS's for unscreened Coulomb fields approaches unity for $\theta \rightarrow 0$ irrespective of the energy.

The reliability of the approximate formulas when used in Monte Carlo simulations of electron and positron transport may be stated in terms of the transport cross section [Figs. 2(a) and 2(b)] which is the parameter which has the dominant influence in the multiple scattering angular distribution. The limitations of the first-order Born approximation are clearly evidenced in these figures: it leads to important errors except for low atomic numbers and moderately high energies. The improvement introduced by the second-order Born correction is effective for high energies, albeit for low energies the Gorshkov formula may be worse than the first-order Born approximation. For high energies, the screened Mott transport cross section is slightly less accurate than the Gorshkov one but considerably more reliable than the first-order Born transport cross section. For high energies, the Gorshkov and screened Mott cross sections lead to relative errors in the transport cross section which are of similar magnitude and opposite signs. In the case of gold and at an energy as high as 10 MeV these errors are of the order of 5%. Hence, at least for high atomic numbers, Monte Carlo simulations of electron and positron transport should be based on cross sections more accurate than those given by the aforesaid approximations. The present calculation method may be useful for this particular purpose.[31]

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