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Perturbation theory with arbitrary boundary conditions for charged-particle scattering: Application to $(e,2e)$ experiments in helium

J. H. Macek and J. Botero*

Department of Physics and Astronomy, University of Tennessee, Knoxville, Tennessee 37996 and Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831

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A perturbation series of the distorted-wave Born type is developed in such a way that the slow decrease of the Coulomb potential in which the incoming and scattered particles move plays no role. We apply this approach to triple-differential cross sections for electron-impact ionization of helium at low and intermediate energies, where we use Coulomb waves with an effective charge for the incoming, scattered, and ejected electron, and show that even though these wave functions are known to satisfy the wrong Coulomb boundary conditions at infinity, they give reasonably and unexpectedly good agreement with experiment.

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It is generally considered that perturbation expansions for charged-particle scattering are constrained to satisfy asymptotic boundary conditions that account for the slow decrease of the Coulomb field with distance [1-3]. This implies, for example, that the Coulomb Born approximation should never be used for electron scattering from neutral atoms despite the obvious practical value that this approximation may have for inner-shell excitation [4]. The Coulomb Born approximation is periodically proposed for neutral systems, but is based on invalid expressions for transition amplitudes [2,5]. In this report we show how one may simultaneously employ well-defined expressions for transition amplitudes, yet obtain first-order expressions where the wave functions are not constrained by the slow decrease of the Coulomb potential at large distances. This requires rewriting conventional perturbation theory recognizing that the solutions of the perturbation equations are not generally given by the conventional Green-function expressions universally used in formal scattering theory [6]. This can be done surprisingly simply, as we demonstrate here. Recent $(e,2e)$ measurements for He targets provide a test of this idea [7]. We find that the Coulomb Born approximation for this neutral system gives reasonably good agreement with experiments at energies as low as 50 eV, a case in which some important experimental features of the triple-differential cross section (TDCS) are reproduced by theory for the first time, where the usual Born approximation gives completely wrong results. Our new perturbation expansion has obvious implications for the computation of physically important quantities, such as the generalized oscillator strength, fundamental to the interaction of charged particles with matter [8]. Atomic units are used throughout.

Consider excitation or ionization of an $(N-1)$-electron ion with nuclear charge Z by a fast electron N. The Hamiltonian for the system is

$$H=H_0+V_T+V_{\rm int}\,, \tag{1}$$

where H_0 is the kinetic-energy operator for N electrons, V_T is the potential of the $N-1$ target electrons in the field of the nucleus, and $V_{\rm int}$ is the interaction potential of electron N with the target ion. As $r_N\rightarrow\infty$ we have $V_{\rm int}\rightarrow -Q/r_N$, where $Q=Z-N+1$ is the net charge of the ion in the initial state and r_N is the coordinate of electron N. Define $H(\lambda)$ according to

$$H(\lambda)=H_0+V_T+V_{\rm eff}+\lambda U+\lambda W\,, \tag{2}$$

where $V_{\rm eff}=-Z_{\rm eff}/r_N$, $U=(Z_{\rm eff}-Q)/r_N$, $W=V_{\rm int}+Q/r_N$, and $Z_{\rm eff}$ is arbitrary. Clearly, when $\lambda=1$ we recover the true Hamiltonian. When $\lambda=0$ we obtain the "initial" Hamiltonian of the $(N-1)$-electron target ion plus electron N in the field of a nucleus of charge $Z_{\rm eff}$. Our objective is to expand the T matrix $T(\lambda)$ in a power series in λ. To this end we define the Coulomb wave functions $\psi_{\mathbf{k}}^{\pm}(\lambda)$ for electron N which are eigenfunctions of the Hamiltonian

$$\mathcal{H}=K_0+V_{\rm eff}+\lambda U\,, \tag{3}$$

where K_0 is the kinetic-energy operator for electron N. The desired transition matrix element is

$$T_{fi}(\lambda)=\langle\psi_{\mathbf{k}}^{-}(\lambda)\Phi_f|\lambda W+\lambda^2 W G^{+}(\lambda)W|\psi_{\mathbf{k}}^{+}(\lambda)\Phi_i\rangle\,, \tag{4}$$

where Φ_i and Φ_f are initial i and final f target eigenstates, and $G^{+}(\lambda)=[E+i\eta-H(\lambda)]^{-1}$.

If the coefficients $\psi_{\mathbf{k}}^{(n)\pm}$ of λ^n in the expansion of the Coulomb waves were given by the usual Green-function expression

$$\psi_{\mathbf{k}}^{(n)\pm}=(E+i\eta-K_0-V_{\rm eff})^{-1}U\psi_{\mathbf{k}}^{(n-1)\pm}\,, \tag{5}$$

then the expansion of $T(\lambda)$ in powers of λ would just represent the usual distorted-wave Born expansion. However, it is known that the Coulomb waves cannot be expanded with coefficients given by Eq. (5), since the limit of the right-hand side of Eq. (5) as η goes to zero does not exist [2,3,9,10]. The standard response to this dilemma is to abandon [2,3,10] expansions in powers of λ. This allows no freedom to choose a $Z_{\rm eff}$ on physical grounds, rather the value of $Z_{\rm eff}$ is dictated by "boundary conditions" at infinite distance which should be physically unimportant.

To recover the freedom to employ arbitrary Z_{eff} some authors [11] screen the real potentials with a large screening radius R_0. The T matrix is then multiplied by large phase factors $\exp[iv(\lambda)\ln(2kR_0)]$, where $v(\lambda)=[(1-\lambda)Z_{\text{eff}}+\lambda Q]/k$, which also precludes expansions in powers of λ. This lack of flexibility emerges only when higher-order terms are computed, thus it has not completely deterred the use of effective charges in practical calculations [4]. It has always been troublesome, however, that the higher-order terms are known to diverge. Here we propose a simple alternative to abandoning the expansion of T, namely, compute $\psi_{\mathbf{k}}^{(n)\pm}$ directly from the known Coulomb functions [6]. We then easily verify that this immediately gives us lowest-order terms with the desired Z_{eff}, but at the same time gives finite, well-defined expressions for all orders.

For the zeroth order we have as usual $T^{(0)}=0$ and for the first order we obtain

$$T^{(1)}=\langle\psi_{\mathbf{k}'}^{-}(0)\Phi_f|V_{\text{int}}|\psi_{\mathbf{k}}^{+}(0)\Phi_i\rangle\,, \tag{6}$$

where the orthogonality of initial and final target eigenstates has been used to eliminate Q/r_N. This is just the desired expression since the distorted waves are Coulomb waves in an attractive potential with the arbitrary strength parameter Z_{eff}.

The second-order term is not the conventional result of distorted-wave theory; rather, we have

$$T^{(2)}=\frac{\partial}{\partial\lambda}\langle\psi_{\mathbf{k}'}^{-}(\lambda)\Phi_f|V_{\text{int}}|\psi_{\mathbf{k}}^{+}(\lambda)\Phi_i\rangle\Big|_{\lambda=0}$$
$$+\langle\psi_{\mathbf{k}'}^{-}(0)\Phi_f|WG^{+}(0)W|\psi_{\mathbf{k}}^{+}(0)\Phi_i\rangle\,. \tag{7}$$

Since the derivatives of the Coulomb functions are well defined, and since $W\to 0$ as $r_N\to\infty$ faster than $1/r_N$, it is easily seen that $T^{(2)}$ is finite and well defined. Alternatively, if Eq. (5) with $n=1$ is erroneously used to compute the derivatives of the Coulomb functions with respect to the expansion parameter λ, then one obtains the usual expression

$$T^{(2)}=\langle\psi_{\mathbf{k}'}^{-}(0)\Phi_f|(V_{\text{int}}-V_{\text{eff}})G^{+}(0)(V_{\text{int}}-V_{\text{eff}})|\psi_{\mathbf{k}}^{+}(0)\Phi_i\rangle\,, \tag{8}$$

which diverges unless $Z_{\text{eff}}=Q$. In contrast, our perturbation series allows complete freedom in choosing Z_{eff} and thereby extends the Coulomb Born approximation to scattering from neutral systems as proposed in Ref. [5].

This freedom is useful for analysis of atomic collisions at high and moderately high energies. For example, excitation cross sections at large momentum transfer $\mathbf{q}$ correspond to close collisions where $Z_{\text{eff}}=Z$. In the Born approximation the cross sections decrease as q^{-12}, while in the Coulomb Born approximation [Eq. (6)] the cross sections decrease as q^{-4}, i.e., they behave as Rutherford cross sections for large q.

As a more detailed test of these expansions, we consider the ionization of He by electron impact, since much high-quality data is available from $(e,2e)$ experiments. We have used a model in which the correlation between the two atomic electrons is neglected, and therefore we approximated the bound-state wave function by a simple hydrogenic wave function $\varphi_{1s}(r)=Z_T^{3/2}\pi^{-1/2}e^{-Z_T r}$, with Z_T equal to the screened charge chosen such that it gives the binding energy of the $1s$ electron, and an effective charge $Z_{\text{eff}}=1.6$ in the Coulomb waves. The T matrix is computed using Eq. (6).

The TDCS corresponding to ejection of an atomic $1s$ electron with momentum $\mathbf{k}_s$ into the solid angle $d\Omega_s$, and to scattering of the incident electron in the direction (θ',ϕ') into the solid angle $d\Omega'$ is then given by

$$\frac{d^5\sigma}{d\Omega' d\Omega_s d^3\mathbf{k}_s}=(2\pi)^4\frac{2k'}{k}|T_{fi}|^2\,. \tag{9}$$

Figure 1 shows the TDCS for He corresponding to an energy of the incoming electron of 256 eV, energy of the ejected electron of 3 eV, and a scattering angle of $\theta'=4°$. The experimental results are from Ref. [7]. Even though both experiment and theory give absolute values of the TDCS, we have multiplied the experimental results by 0.703 for comparison purposes. This overall multiplicative factor is in agreement with other calculations [12] using correlated three-body continuum final wave functions and has been the subject of previous studies [13]. Notice that the ratio between the binary and recoil peaks is reproduced by the theory, as well as the angular position of the peaks, whereas the plane-wave Born approximation, given by the dashed line, does not reproduce these features of the TDCS. Several theoretical calculations, such as a much more elaborate distorted-wave calculation of Madison, Calhoun, and Shelton [14] and a second Born calculation of Mota Furtado, and O'Mahony [15] (for a recent

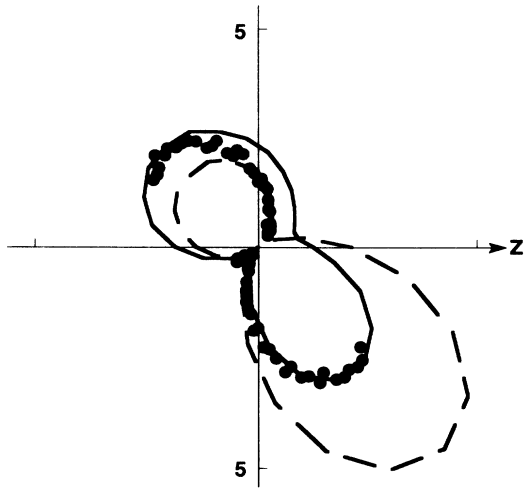

FIG. 1. TDCS for He corresponding to an energy of the incoming electron of 256 eV moving parallel to the Z axis, energy of the ejected electron of 3 eV, and a scattering angle of 4°. The solid line is the present calculation, the dashed line is a plane-wave Born calculation, and the solid dots are the experimental results from Ref. [7].

review see Ref. [16]), have reproduced these results.

Figure 2 shows the TDCS for He for an energy of the incoming electron of 50 eV, energy of the ejected electron of 10.5 eV, and a scattering angle of 7°. Notice that even though these results are not in perfect agreement with the experiment, some of the important features are reproduced by theory for the first time, such as a double peak at negative angles, a small cross section in the forward direction, and a larger cross section in the backward direction. The dashed line shows the results of a plane-wave Born calculation, which gives a completely wrong angular distribution, with most of the intensity in the forward direction.

We have presented a perturbation series that allows one to use Coulomb waves with arbitrary Z_{eff} in the calculation of cross sections for inelastic scattering of charged particles from neutral atoms. We have shown that, by writing the perturbation series for the T matrix in a particular way, the boundary condition of the zeroth-order wave function becomes irrelevant. We applied this method to calculate the triple-differential cross section for electron-impact ionization of He at intermediate and low energies and found that even using a simple model for both the ground state and the ejected electron wave functions the theory reproduces reasonably well most of the experimental features of the cross section. It is indeed a great improvement over the plane-wave Born approximation, which, as pointed out above, does not reproduce the ratio between the binary and recoil peaks at 256 eV and gives completely wrong results at 50 eV. This method should prove particularly useful for the investigation of inner-shell excitation [17] and for the computation of generalized oscillator strengths. A more comprehensive study of the method and its applications to $(e,2e)$ cross sections in electron scattering from atomic hydrogen is now under way, and the results will be published elsewhere.

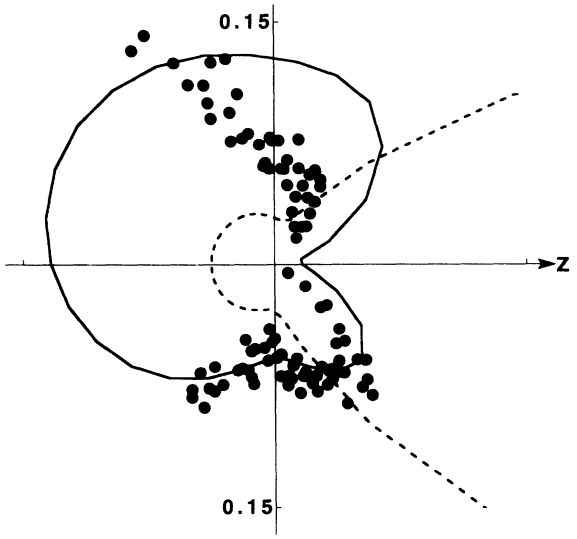

FIG. 2. TDCS for He corresponding to an energy of the incoming electron of 50 eV moving parallel to the Z axis, energy of the ejected electron of 10.5 eV, and a scattering angle of 7°. The solid line is the present calculation, the dashed line is a plane-wave Born calculation, and the solid dots are the experimental results from Ref. [7], normalized to the present calculation.

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*On leave from Escuela Colombiana de Ingeniería, Bogotá, Colombia.

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