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Relativistic plane-wave Born theory and its application to electron-impact excitation

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An exact treatment of the relativistic plane-wave Born (RPWB) cross section for electron-impact excitation is provided for an arbitrary atom or ion. This result represents an improvement over the cross section obtained from the widely used Bethe high-energy theory developed in the 1930s. The results obtained from this RPWB approach can be applied to a broad class of problems in fundamental electron-impact scattering theory. As an illustration, the approach is used to approximate the high-ℓ, partial-wave contribution in more accurate calculations of the excitation cross section, a problem which has been lacking a fully relativistic treatment for more than 20 years.

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The Bethe high-energy theory (BHET) for electron scattering from atoms and ions was put forth for nonrelativistic [1] and relativistic [2] systems during the 1930s. This work, along with a number of other topics, was summarized by Bethe in a monumental 1933 *Handbuch der Physik* paper [3]. The BHET approach begins with the standard, nonrelativistic plane-wave Born (PWB) or relativistic plane-wave Born (RPWB) expression for the cross section and employs a series of approximations, valid in the high-energy limit, to extract a remarkable amount of information from readily available, fundamental atomic physics quantities. During the intervening years this approach has been successfully applied to a wide range of practical and fundamental problems. For example, this approach was originally used in the determination of the stopping power of an arbitrary material from basic atomic data [3]. More fundamental applications have included a determination of the high-energy behavior of electron-impact ionization cross sections for neutral atoms [4], ions [5], and molecules [6].

A comprehensive review of the BHET has been written by Inokuti [7], providing further insight into the approximations used in this simple, yet powerful, method for obtaining solutions to a variety of electron scattering problems in the high-energy limit. This review is divided into a discussion of both the nonrelativistic and relativistic theories originally considered by Bethe and expanded upon by subsequent authors. While improvements to, and exact treatments of, the nonrelativistic theory are commonplace in the literature (see, for example, [8,9]), the relativistic approach (i.e., the use of plane waves that are four-vector solutions to the Dirac equation in free space) does not appear to have received much attention; this omission is most likely due to the fact that the relativistic approach is pertinent for heavy elements and relatively large electron energies that are not as commonly encountered in typical research applications. Furthermore, Bethe's relativistic approach included an additional simplification that was not germane to the nonrelativistic PWB theory: the assumption that the speed and energy of the incident and scattered electrons were equal eliminated the four-vector dependence of the plane waves from the scattering matrix elements. This additional simplification resulted in more tractable calculations, but further limited the range of validity of the relativistic BHET.

The purpose of the present work is to provide an exact treatment of the RPWB approach to electron-impact excitation of an arbitrary atom or ion. This formulation provides a framework for determining the RPWB excitation cross section for a variety of scattering problems of interest including excitations between fine-structure levels [10] or magnetic sublevels [11], as well as integrated or (angular) differential cross sections. In order to demonstrate the usefulness of this formulation, the expression for the integrated RPWB cross section for impact excitation between fine-structure levels is applied to the long-standing problem of computing a fully relativistic approximation of the high-ℓ (or "top-up") contribution [12] to a partial-wave summation of the excitation cross section. The example is presented within the relativistic distorted-wave (RDW) framework, but this method can also be applied to any higher-order theory that requires an accurate estimate of the top-up contribution, such as the relativistic R-matrix approach [13–15]. Values of the RDW cross sections are provided for He-like iron ions, which demonstrate the correct high-energy behavior when the RPWB top-up contribution is employed, as compared to the behavior obtained from previously available, quasirelativistic treatments.

In order to provide a concise description of our approach to obtaining the exact RPWB cross section for electron-impact excitation, we chose to work within the framework of the exact, nonrelativistic PWB treatment provided by Cowan [9]. The reader should consult that work for details that are not central to the relativistic description provided here. Working within this context also makes evident those terms which arise from strictly relativistic considerations. The convention will be to use Rydberg atomic units throughout, as in [9], except that relativistic expressions will be provided in an explicit form for clarity. The relevant RPWB, Coulomb matrix element for excitation between an initial magnetic sublevel $|\gamma JM\rangle$ and final sublevel $|\gamma' J' M'\rangle$ of an atom or ion with N bound electrons is given by

$$H_{\alpha\alpha'} = \left\langle \alpha \left| \sum_{q=1}^{N} \frac{2}{|\boldsymbol{r}_q - \boldsymbol{r}|} \right| \alpha' \right\rangle, \tag{1}$$

where

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$$\alpha \equiv |\gamma JM\rangle|e^{i\boldsymbol{k}\cdot\boldsymbol{r}},m_s\rangle, \quad \alpha' \equiv |\gamma' J' M'\rangle|e^{i\boldsymbol{k}'\cdot\boldsymbol{r}},m_s'\rangle \tag{2}$$

are direct products between the appropriate magnetic sublevel and a Dirac plane wave. The values m_s and m_s' represent the spin magnetic quantum numbers of the incident and scattered electrons, respectively, and have no analog in the nonrelativistic case. (In the present work, we consider only the Coulomb interaction between the bound and free electrons. Bethe's original relativistic approach also considered the effect of exchange of a transverse photon, represented by the Møller or Breit interactions [16], which becomes important for very high free- and bound-electron energies.)

While the matrix element in Eq. (1) is very similar in form to the nonrelativistic result, there are some key differences. First, the Coulomb operator is really a 4×4 diagonal matrix. Second, the bound and continuum wave functions represent four-component Dirac spinors. Third, the plane waves have a well-defined value for the spin magnetic quantum numbers m_s and m_s', which does not occur in the nonrelativistic case. Employing the relation $\boldsymbol{p}=\hbar\boldsymbol{k}$, the Dirac plane waves can be written as [17]

$$\psi_{\boldsymbol{k},m_s}(\boldsymbol{r}) = U(\boldsymbol{k},m_s)e^{i\boldsymbol{k}\cdot\boldsymbol{r}} = N_k\begin{pmatrix} \chi^{m_s} \\ \dfrac{c\boldsymbol{\sigma}\cdot\boldsymbol{p}}{E+mc^2}\chi^{m_s} \end{pmatrix} e^{i\boldsymbol{k}\cdot\boldsymbol{r}}, \tag{3}$$

where $\boldsymbol{\sigma}$ are the usual 2×2 Pauli matrices and χ^{m_s} are the eigenvectors of σ_z [17]. A value of $N_k=\sqrt{(E+mc^2)/2E}$, where $E=\sqrt{(pc)^2+(mc^2)^2}$ is the total energy, has been chosen such that the plane waves are orthonormal according to $\psi^\dagger_{\boldsymbol{k},m_s}\psi_{\boldsymbol{k},m_s'}=U^\dagger(\boldsymbol{k},m_s)U(\boldsymbol{k},m_s')=\delta_{m_sm_s'}$. More generally, when $\boldsymbol{k}'\neq\boldsymbol{k}$, the relativistic plane waves satisfy the more comprehensive orthonormality condition

$$\langle e^{i\boldsymbol{k}\cdot\boldsymbol{r}},m_s|e^{i\boldsymbol{k}'\cdot\boldsymbol{r}},m_s'\rangle = (2\pi)^3U^\dagger(\boldsymbol{k},m_s)U(\boldsymbol{k}',m_s')\delta(\boldsymbol{k}-\boldsymbol{k}'), \tag{4}$$

where

$$U^\dagger(\boldsymbol{k},m_s)U(\boldsymbol{k}',m_s') = N_kN_k'\left[\langle\chi^{m_s}|\chi^{m_s'}\rangle + \frac{c^2\langle\boldsymbol{\sigma}\cdot\boldsymbol{p}\chi^{m_s}|\boldsymbol{\sigma}\cdot\boldsymbol{p}'\chi^{m_s'}\rangle}{(E+mc^2)(E'+mc^2)}\right]. \tag{5}$$

Equation (5) represents the scalar product between the four-vector amplitudes of the incident and scattered plane waves, which has no analog in the nonrelativistic case. The term on the far right that contains the two dot products results from the small components of the incident and scattered plane waves. It is well known that the small component differs from the large component by a factor of $O(v/c)$, where $v=pc^2/E$ is the speed of the electron. Therefore, in the nonrelativistic limit the term containing the dot products can be ignored, the normalization constants N_k and N_k' can be approximated as 1, and the scalar product in Eq. (5) can be set to 1, provided that $m_s'=m_s$, or to 0 if $m_s'\neq m_s$.

In the high-energy limit considered by Bethe, $\boldsymbol{k}'\approx\boldsymbol{k}$ and the scalar product can also be set to 1 due to the orthonormalization condition, again provided that $m_s'=m_s$ (otherwise the result is zero). If the spin polarization for the incident and scattered electrons is not of interest, then the resulting scalar product obtained after performing the appropriate averaging and sums over the spin quantum numbers (see details below) can also be approximated as 1 in both the nonrelativistic and high-energy limits. Approximations of this latter type have been used, for example, in Eq. (52.23) of Ref. [3] and Eq. (13) of Ref. [18].

To determine an expression for the RPWB cross section for electron-impact excitation, the manipulation of the matrix element in Eq. (1) can proceed similarly to that described by Cowan. In particular, the square of the matrix element can be written in the form

$$|H_{\alpha\alpha'}|^2 = \frac{64\pi^2}{K^4}|U^\dagger(\boldsymbol{k},m_s)U(\boldsymbol{k}',m_s')|^2 \times\left|\langle\gamma JM|\sum_m e^{i\boldsymbol{K}\cdot\boldsymbol{r}_m}|\gamma' J' M'\rangle\right|^2, \tag{6}$$

where $\boldsymbol{K}=\boldsymbol{k}'-\boldsymbol{k}$ is the momentum transfer. The above expression is formally identical to its nonrelativistic counterpart, except for the extra factor containing the square of the scalar product of the four-vector amplitudes. In the present work, we wish to determine an expression for the excitation cross section between fine-structure levels ($\gamma J\rightarrow\gamma' J'$). Therefore, Eq. (6) must be averaged over M and summed over M' values. The relevant double sum can be performed in a manner that is formally identical to that applied in the nonrelativistic case (since the scalar product is independent of M and M'), and the reader is referred to [9] for details.

If the spin orientation of the incident and scattered electrons is not of interest (i.e., the free electrons are unpolarized), an averaging over m_s and summing over m_s' must also be performed. The manipulations apply only to the square of the scalar product in Eq. (6). A convenient expression that is suitable for computational purposes can be obtained after repeated applications of the relationship

$$(\boldsymbol{\sigma}\cdot\boldsymbol{p})(\boldsymbol{\sigma}\cdot\boldsymbol{p}') = \boldsymbol{p}\cdot\boldsymbol{p}' + i\boldsymbol{\sigma}\cdot(\boldsymbol{p}\times\boldsymbol{p}') \tag{7}$$

or via applications of the more elegant trace theorems associated with the Dirac matrices (e.g., [17]). We present the final result in the compact form

$$\frac{1}{2}\sum_{m_s,m_s'}|U^\dagger(\boldsymbol{k},m_s)U(\boldsymbol{k}',m_s')|^2 = (N_kN_k')^2\left[\left(1+\frac{c^2}{D}\boldsymbol{p}\cdot\boldsymbol{p}'\right)^2+\frac{c^4}{D^2}(\boldsymbol{p}\times\boldsymbol{p}')^2\right], \tag{8}$$

where $D\equiv(E+mc^2)(E'+mc^2)$.

Equation (8) is a key result of this work as it normally appears in the electron scattering literature for the simpler case of Mott (elastic) scattering for which $E=E'$ and $p=p'$ (see, for example, [17,19,20]). This expression clearly displays the additional angular dependence that will eventually appear in the (angular) differential cross section due to relativistic effects since $\boldsymbol{p}\cdot\boldsymbol{p}'=pp'\cos\theta$ and $|\boldsymbol{p}\times\boldsymbol{p}'|=pp'\sin\theta$, where θ is the angle between the incident and scattered momentum vectors. From Eq. (8) it is easy to see that, in the

limit of small velocities, this expression reduces to 1, as previously stated. With a modicum of manipulation it can be shown that Eq. (8) also reduces to 1 in the high-energy ($\boldsymbol{p}' \to \boldsymbol{p}$) limit.

Before discussing excitation cross sections it is convenient to first define the relativistic generalized oscillator strength (GOS) according to

$$gf_{JJ'}(K) \equiv \frac{\Delta E}{K^2} \sum_{M,M'} \left| \left\langle \gamma JM \middle| \sum_m e^{i\boldsymbol{K}\cdot\boldsymbol{r}_m} \middle| \gamma' J' M' \right\rangle \right|^2 = \frac{\Delta E}{K^2} \sum_t (2t+1) \left\langle \gamma J \middle\| \sum_m j_t(Kr_m) \boldsymbol{C}_m^{(t)} \middle\| \gamma' J' \right\rangle^2, \tag{9}$$

where $g=2J+1$ is the statistical weight of the level γJ and ΔE is the energy associated with the transition $\gamma J \to \gamma' J'$. This expression agrees formally with the nonrelativistic result except that the reduced matrix element is treated relativistically, so that the small component of the target wave functions is also considered. As in the nonrelativistic case, Eq. (9) has the desired property that it reduces to the length form of the relativistic dipole oscillator strength, $gf_{JJ'}$, in the limit $K \to 0$.

Moving along to a determination of the excitation cross section, the relativistic angular differential cross section can be written as

$$I_{aa'}(\theta) = \frac{1}{16\pi^3} \left(\frac{EE'}{m^2c^4} \right) \frac{k'}{k} |H_{\alpha\alpha'}|^2, \tag{10}$$

where $a \equiv |\gamma JM; m_s\rangle$, $a' \equiv |\gamma' J' M'; m_s'\rangle$, $|H_{\alpha\alpha'}|^2$ is the squared matrix element appearing in Eq. (6), and the cross section is in units of πa_0^2/sr. The substitution

$$\frac{k'}{k} \to \left(\frac{EE'}{m^2c^4} \right) \frac{k'}{k} \tag{11}$$

has been performed in order to take into account the kinematic effect due to the relativistic relationship between the velocity and the momentum [7], $\boldsymbol{v}=\boldsymbol{p}c^2/E$, for the incident and scattered electrons.

The integrated cross section is given by

$$Q_{aa'} = 2\pi \int_0^\pi I_{aa'}(\theta) \sin\theta d\theta, \tag{12}$$

and the integration over θ can be converted to an integration over K using standard techniques. The total cross section between fine-structure levels, $Q_{JJ'}$ (in units of πa_0^2), is then obtained by summing $Q_{aa'}$ over M', m_s' and averaging over M, m_s. Substituting the results from Eqs. (8) and (9) and employing the relativistic expression for the (dimensionless) collision strength [10] $\Omega_{JJ'}$ yields

$$\Omega_{JJ'}(\varepsilon) \equiv k^2 g Q_{JJ'}(\varepsilon) = \frac{8}{\Delta E} \int_{K_{\min}}^{K_{\max}} F_{\rm rel}(K) gf_{JJ'}(K) d(\ln K), \tag{13}$$

where $\varepsilon = E - mc^2$ is the kinetic energy of the incident electron, ΔE is expressed in Rydbergs, k is in atomic units, and the relativistic limits of integration are obtained from standard relationships [7]. Formally, the only difference between Eq. (13) above and the usual nonrelativistic PWB cross section is the appearance of the relativistic correction factor $F_{\rm rel}(K)$ which consists of the product of Eq. (8) and the right-hand side of Eq. (11), expressed as a function of K.

Equation (13) is the main result of this work. It presents an exact expression for the RPWB excitation cross section for an arbitrary fine-structure transition in an atom or ion. An evaluation of this expression simply requires numerical values for the relativistic GOS and transition energy, both of which can be readily obtained from a relativistic atomic structure code (see, for example, [21]), and also a numerical integration over the appropriate range of K values.

For comparison, we note that the BHET cross section can be obtained from Eq. (13) with the two approximations

$$F_{\rm rel}(K) \to \frac{E^2}{m^2c^4}, \quad f_{JJ'}(K) \to f_{JJ'}, \tag{14}$$

where $f_{JJ'}$ is the dipole oscillator strength, and also a determination of a suitable cutoff value to replace $K_{\max}$. Some obvious shortcomings of this approach are that it holds only for dipole-allowed transitions, the incident electron energy must be large enough so that the first approximation in Eq. (14) is valid, and a value for the cutoff replacement for $K_{\max}$ must be determined, which is not straightforward in a general sense. On the other hand, an evaluation of Eq. (13) is straightforward and the result is an exact value of the RPWB excitation cross section.

As an application of Eq. (13), we consider its use in approximating the high-ℓ contribution in a RDW calculation of the collision strength. In practice, the infinite sum over incident and scattered partial-wave contributions (denoted by ℓ and ℓ', respectively) to the RDW collision strength must be truncated at finite values (denoted by $\ell_{\max}$, $\ell'_{\max}$). The remainder of that sum (the top-up contribution) can be approximated by the corresponding RPWB partial-wave contribution. With this prescription the RDW collision strength can be computed according to the Kummer transformation [22,23]

$$\Omega^{\rm RDW} \approx \Omega^{\rm RPWB} + \sum_{\ell,\ell'=0}^{\ell_{\max},\ell'_{\max}} (\Omega^{\rm RDW}_{\ell,\ell'} - \Omega^{\rm RPWB}_{\ell,\ell'}), \tag{15}$$

where the values for $\ell_{\max}$ and $\ell'_{\max}$ are chosen such that the distorted waves can be reasonably approximated by plane waves beyond this point. For convenience the JJ' subscripts and ε dependences have been omitted from Eq. (15), but they are implied with each occurrence of Ω.

Nonrelativistic [23] and quasirelativistic (i.e., the bound electrons are treated relativistically, but the free electrons are treated nonrelativistically) [24] forms of Eq. (15) have been applied to the calculation of distorted-wave collision strengths with good success for relatively low-energy collisions. The fully relativistic version has been implemented in the RDW code described in [10] and the resulting collision strength for the $(1s2s)_{J=1} \to (1s2p_{1/2})_{J=1}$ transition in He-like iron is presented in Fig. 1. For this calculation, values of

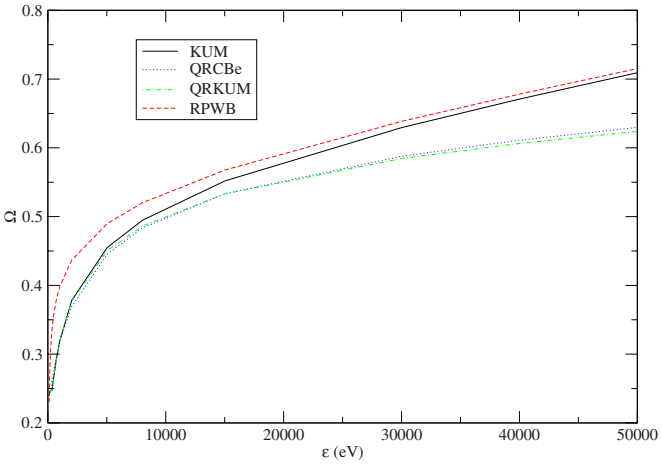

FIG. 1. (Color online) Collision strengths obtained via different top-up methods as a function of impact energy for the $(1s2s)_{J=1} \rightarrow (1s2p_{1/2})_{J=1}$ transition in He-like iron. Solid curve: relativistic (Kummer) top-up contribution from Eq. (15). Dotted curve: quasirelativistic, Coulomb-Bethe top-up contribution [10]. Dot-dashed curve: quasirelativistic, Kummer top-up contribution [24]. The RPWB collision strength obtained from Eq. (13) is also provided (dashed curve).

$\ell_{\max}=73$ and $\ell'_{\max}=69$ were used at the highest impact energies in Eq. (15). The resulting RDW collision strength (labeled "KUM") merges nicely into the RPWB result at high energies, as expected. For comparison, the RDW collision strength obtained via two traditional quasirelativistic (QR) top-up methods is also provided: the QR Coulomb-Bethe (QRCBe) [10] and the QR Kummer (QRKUM) [24] approaches. As can be seen from the figure, the two QR methods start to separate from the Kummer result at an energy of ~5 keV and develop different trends by 50 keV. A strong divergence continues beyond this energy, but the plot is terminated at that point because the exchange of a transverse photon, mentioned previously in connection with Eq. (1), is expected to become important beyond this range. However, within the range of validity, Eq. (15) provides a convenient prescription for obtaining an accurate estimate of the top-up contribution for any transition that is described by a nonzero RPWB collision strength.

In conclusion, an exact expression has been provided for the relativistic plane-wave Born collision strength for electron-impact excitation between arbitrary fine-structure levels. The result was applied to the problem of computing the top-up contribution to RDW collision strengths for He-like iron ions, producing the correct behavior in the high-energy region. This example demonstrates an improvement in the accuracy of atomic data for heavier systems that are employed in applications such as astrophysical modeling and line diagnostics. The development and application of the RPWB approach for other fundamental excitation cross sections, such as angular-differential and magnetic-sublevel results, is planned for future investigations.

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