Nonperturbative electron-ion-scattering theory incorporating the Møller interaction

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Relativistic distorted-wave studies by Fontes *et al.* [Phys. Rev. A **47**, 1009 (1993)] demonstrated that the generalized Breit interaction (equivalently, the Møller interaction) can affect electron-impact excitation cross sections of hydrogenlike U^{91+} by more that 50% in comparison to calculations that employ the Coulomb interaction alone. We present calculations that investigate the effects of both the Møller interaction and close coupling in the calculation of electron-impact excitation cross sections. Electron scattering from U^{91+} is used as a test case. The relativistic convergent close-coupling (RCCC) method is nonperturbative and we emphasize the restrictions and subsequent limitations associated with employing the Møller interaction in the RCCC method.

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I. INTRODUCTION

The first-order relativistic distorted-wave calculations of electron-impact excitation of highly charged ions by Walker [1], Fontes *et al.* [2], and Moores and Pindzola [3] have shown that the generalized Breit interaction (equivalently, the Møller interaction) can significantly affect cross sections by up to 50% in comparison to Coulomb-only interaction calculations. For the case of electron-impact ionization, experiment [4] has confirmed the theoretical predictions that the Møller interaction can increase cross sections by up to 50% [5,6]. Recent years have seen further demonstration of the importance of Møller interaction effects in reconciling experimental results and theory in dielectronic recombination in highly charged ions [7–9], and in the polarization of x rays emitted by highly charged ions excited by electron impact [10,11].

An important consideration that remains to be investigated is the incorporation of the Møller interaction in close-coupling scattering calculations. Close-coupling (nonperturbative) calculations are required to resolve resonance features in electron-impact excitation cross sections; resonant features are absent in first-order perturbative calculations and yet such resonances can provide a significant contribution to effective collision strengths obtained by integrating over Maxwellian distributions of electron velocities corresponding to temperatures found in astrophysical and torrential fusion plasmas [12,13].

The early quantum electrodynamics research of the Nobel-prize-winning physicist Nambu [14] indicated that employing the Møller interaction beyond a first-order calculation is fraught with conceptual difficulties, and that the concept of a potential as a whole begins to lose its meaning in a fully covariant quantum field theory. In the next section, we outline some of the historical and conceptual aspects associated with the use of the Møller interaction in quantum electrodynamics and its use beyond first order. In Sec. III, we provide an overview of the relativistic convergent close-coupling (RCCC) method and the approximations that have been made in employing the Møller interaction in the RCCC method. Section IV contains results for electron-impact excitation cross sections of U^{91+} that exhibit resonant features obtained with the close-coupling formalism.

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II. THE MØLLER AND GENERALIZED BREIT INTERACTIONS

In 1929, Breit [15–17] used classical arguments to include relativistic corrections to the Coulomb potential for helium fine-structure calculations. In the Coulomb gauge, the Breit interaction between two electrons (denoted 1 and 2) is of the form

$$V_{12}^{\mathrm{B}} = \frac{e^2}{r_{12}}\left[-\boldsymbol{\alpha}_1\cdot\boldsymbol{\alpha}_2 + \frac{1}{2}(\boldsymbol{\alpha}_1\cdot\boldsymbol{\nabla}_1)(\boldsymbol{\alpha}_2\cdot\boldsymbol{\nabla}_2)r_{12}^2\right], \quad (1)$$

and must be *added* to the Coulomb potential. In 1931, Møller [18] performed a first-order time-dependent perturbation-theory calculation applied to the relativistic scattering of two electrons. Møller utilized an *unquantized* electromagnetic field A_μ in the Lorenz gauge (often incorrectly referred to as the Lorentz gauge) to obtain an interaction potential:

$$V_{12}^{\mathrm{Møller}} = \frac{e^2}{r_{12}}(1-\boldsymbol{\alpha}_1\cdot\boldsymbol{\alpha}_2)\mathrm{e}^{iKr_{12}}, \quad (2)$$

where $K = |E-E'|/\hbar c$, and E and E' denote the initial and final energies, respectively, of one of the electrons. The Møller interaction *includes* the Coulomb interaction. Moiseiwitsch [19] provided an English translation of Møller's original derivation.

In 1932, Fermi [20] taught a generation of physicists how to perform quantum electrodynamic calculations in the Coulomb gauge. Using the Coulomb gauge techniques presented in Fermi's 1932 paper, Bethe and Fermi [21] in the same year derived a first-order expression for the interaction between electrons in which the electromagnetic field A_μ is quantized. Bethe and Fermi [21] worked in momentum space and the corresponding coordinate space representation of the interaction takes the form

$$V_{12}^{\mathrm{GBI}} = -\frac{e^2}{r_{12}}\boldsymbol{\alpha}_1\cdot\boldsymbol{\alpha}_2\mathrm{e}^{iKr_{12}} + e^2\left(\boldsymbol{\alpha}_1\cdot\boldsymbol{\nabla}_{r_{12}}\right)\left(\boldsymbol{\alpha}_2\cdot\boldsymbol{\nabla}_{r_{12}}\right) \times \frac{e^{ir_{12}K}-1}{K^2 r_{12}}. \quad (3)$$

Following a trend set by Mann and Johnson [22], Eq. (3) is often referred to as the generalized Breit interaction (GBI). In the limit of low-energy photons transferred between electrons ($cK = \omega \to 0$), it can be shown [23] that the generalized Breit interaction reduces to the Breit interaction given by

Eq. (1). Furthermore, Hata and Grant [24] have shown that the Møller [Eq. (2)] and generalized Breit [Eq. (3)] forms for the interaction have equivalent matrix elements provided that the wave functions used in the calculations are derived from a local potential.

The use of the Møller interaction (or GBI) in first-order perturbation techniques is warranted because the interaction was originally derived by Møller using first-order time-dependent perturbation theory, but what is the quantum electrodynamic potential between two electrons for higher-order terms? The first thorough analysis of the problem using the manifestly covariant quantum-field-theory techniques of Tomonaga [25] and Schwinger [26,27] was performed by Nambu [14] in an important paper titled "Force potentials in quantum theory." Nambu derived the Breit and Møller interactions (i.e., first-order interactions) from covariant quantum-field-theory techniques, but when analyzing higher-order terms in this covariant framework, he came to the following conclusion: "We may say that the concept of potential cannot enjoy a wide and practical extension beyond the classical and nonrelativistic form" [14].

In the introduction to their treatise on quantum electrodynamics, Berestetskii *et al.* [28] reinforce the conceptual tensions that arise when translating concepts from nonrelativistic quantum mechanics to quantum field theory: "At first sight one might expect that the change to a relativistic theory is possible by a fairly direct generalization of the formalism of nonrelativistic quantum mechanics. But further consideration shows that a logically complete relativistic theory cannot be constructed without invoking new physical principles."

This holds relevance for the relativistic convergent close-coupling method [29], which is an attempt at a relativistic generalization of the successful nonrelativistic CCC method [30]. The RCCC method involves solving a relativistic version of the Lippmann-Schwinger equation [31] based on the Dirac equation, and therefore since it is nonperturbative involves *all* orders of interaction between the electron. Bethe and Salpeter [32], Mann and Johnson [22], and Sucher [33] have reiterated the now "ancient" (as Sucher phrases it) caveat that the use of the Breit (or Møller) interaction beyond first order in atomic physics calculations can lead to problems due to matrix elements taken between the positive- and negative-energy states that appear in the solution of the Dirac equation. Sucher [33] advocates working in the no-virtual-pair approximation. Despite receiving criticism in the literature [34], it is in this approximation that we work when employing the RCCC method. It does not vindicate the use of the first-order Møller interaction in the nonperturbative RCCC method; however, we do so in the spirit encouraged by Dirac in his 1966 lectures on quantum field theory [35] in which he stated, "The systems of approximations I shall use will be somewhat similar to the approximations that engineers use in their calculations. Engineers have to get results and there are so many factors occurring in their problems that they have to neglect an awful lot of them; they don't have time to study everything seriously and they develop a sort of feeling as to what can be neglected and what can't. I believe that physicists working in QFT will have to develop a similar sort of feeling as to what can be neglected and what can't. The final test is whether the resulting theory is coherent and in reasonable agreement with experiment."

We note that the present calculations for electron scattering on U^{91+} are in the low-energy region just above the excitation thresholds, which is well below the threshold for pair production ($\approx$1 MeV). In order to accommodate variation in particle numbers during scattering (due to electron-positron pair creation), formal quantum-field-theory techniques must be employed. Dyson's 1951 lecture notes on quantum electrodynamics [36] provide an excellent introduction to techniques developed by Tomonaga [25], Schwinger [26,27], and Feynman [37–39] which provide the suitable frameworks. Dyson's lectures also explicitly highlight the issues associated with the Dirac equation and associated hole theory. The Appendix A contains further information pertaining to the conceptual inconsistencies associated with hole theory that can only be circumvented with quantum field theory.

III. THE RCCC METHOD

A complete description of the RCCC method, including the incorporation of the Breit and Møller interaction matrix elements, can be found in Ref. [40], and only a brief overview is provided in this section. There are two main parts to the RCCC method for electron scattering on hydrogenlike targets:

(1) The Dirac Hamiltonian for the target is diagonalized using a Dirac L spinor basis [41].

(2) The target states generated are then used in the formulation of a relativistic Lippmann-Schwinger equation for the T-matrix elements of the electron-target scattering system.

In this latter step, the relativistic Lippmann-Schwinger equation has the following partial-wave form:

$$T_{fi}^{\Pi J}(k_f\kappa_f,k_i\kappa_i) = V_{fi}^{\Pi J}(k_f\kappa_f,k_i\kappa_i) + \sum_n \sum_\kappa \int\!\!\!\!\!\!\diagup dk \frac{V_{fn}^{\Pi J}(k_f\kappa_f,k\kappa) T_{ni}^{\Pi J}(k\kappa,k_i\kappa_i)}{E-\epsilon_n^N-\epsilon_{k'}+i0}. \quad (4)$$

The notation in Eq. (4), the matrix elements, and the method of solution using a hybrid open-multiprocessing–message-passing-interface (OpenMP-MPI) parallelization suitable for high-performance supercomputing architectures is given in Ref. [40]. The T-matrix elements obtained from the solution of the relativistic Lippmann-Schwinger equation are then used to calculate differential cross sections and other observables of interest.

For the off-shell matrix elements of the Møller interaction, we follow the method adopted by Fontes *et al.* [2] and use the operator derived by Mittleman [42–44],

$$V_{12}^{\text{Møller}} = 1/2\left[V_{12}^{\text{Møller}}(K_{AC}) + V_{12}^{\text{Møller}}(K_{BD})\right], \quad (5)$$

where $K_{AC} = |E_C - E_A|/c$ and $K_{BD} = |E_D - E_B|/c$. Fontes *et al.* [2] have performed calculations that show that the effect of dropping the imaginary part in (5) is negligible and is of the order of 2–3% for $1s$–$2s$, $1s$–$2p_{1/2}$, and $1s$–$2p_{3/2}$ excitation cross sections for a very highly charged $Z = 100$ hydrogenlike target. Thus, only the real part of the Møller interaction is used in the calculations.

Several other approximations are employed: the uranium nucleus is treated as a point nucleus and therefore the finite size and large quadrupole moment of the nucleus [45] are

TABLE I. Calculated energy thresholds for U^{91+}.

State	Energy (keV)
$1s_{1/2}$	0.000
$2s_{1/2}$	98.065
$2p_{1/2}$	98.065
$2p_{3/2}$	102.630
$3s_{1/2}$	117.612
$3p_{1/2}$	117.612
$3p_{3/2}$	118.973
$3d_{3/2}$	118.973
$3d_{5/2}$	119.321

neglected. Furthermore, radiative correction terms, such as electron self-energy, vacuum polarization, and vertex corrections, are neglected in the RCCC method. The Lamb shift for the U^{91+} ground state is of the order of 500 eV [46], which is not insignificant, but is only a fraction of a percent compared to the magnitude of the 132 keV ground-state energy. Electron energy losses due to Bremsstrahlung are also neglected; however, these are negligible for the projectile energies considered [47]. Finally, as discussed in the previous section, we also neglect the negative-energy states that appear in the diagonalization of the hydrogenlike target and work in the no-virtual-pair approximation [33].

A nine-state RCCC calculation was used for electron scattering on U^{91+} in order to compare with the nine-state Dirac *R*-matrix calculation of Kisielius *et al.* [13]. The results of Kisielius *et al.* [13] pertain only to the Coulomb interaction, and not the Møller interaction. The energy levels of the states used in the RCCC calculation are indicated in Table I.

IV. RESULTS

In Figs. 1–3, we present the electron-impact excitation cross sections for the $1s_{1/2} \rightarrow 2s_{1/2}$, $1s_{1/2} \rightarrow 2p_{1/2}$, and $1s_{1/2} \rightarrow 2p_{3/2}$ transitions in hydrogenlike U^{91+} in the ≈20 keV region above the thresholds. Also shown are the Dirac *R*-matrix close-coupling calculations of Kisielius *et al.* [13], which included only the Coulomb interaction, and the first-order relativistic distorted-wave calculations of Fontes *et al.* [2]. Several pieces of information can be gleaned from the data. First, the main effect of the close coupling is to superimpose a sequence of resonant peaks (associated with the formation of temporarily bound resonant states) on top of a smooth background. As expected, the magnitude of the smooth background can be determined very accurately from first-order calculations. The second important point is that the Møller interaction affects the optically forbidden $1s_{1/2} \rightarrow 2s_{1/2}$ transition by a significant amount, i.e., on the order of 50%. For optically allowed transitions, the effect of the Møller interaction is approximately 15% in the energy range considered.

A comparison of our Coulomb-only results in the three figures indicates that some of the resonance peaks align well with those in the data of Kisielius *et al.* [13]; however, there are also differences in the position and magnitude of the Coulomb-only results for the two theories. The calculations

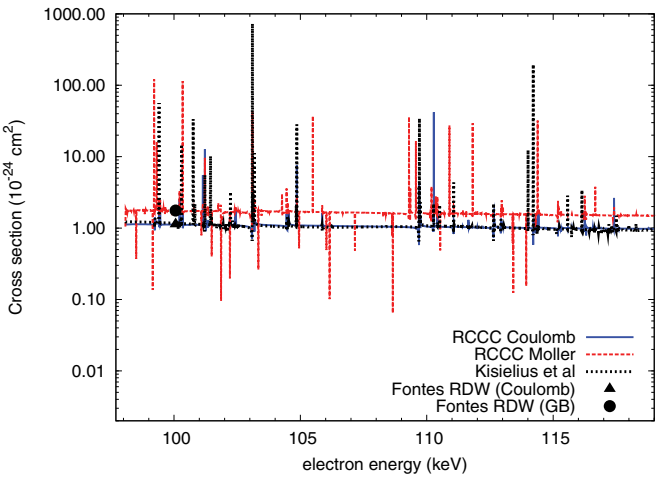

FIG. 1. (Color online) $1s_{1/2} \rightarrow 2s_{1/2}$ electron-impact excitation RCCC-calculated cross section (solid blue line: Coulomb interaction; dashed red line: Møller interaction) compared with the *R*-matrix nine-state calculation of Kisielius *et al.* [13] (dotted black line) and the first-order relativistic distorted-wave calculations of Fontes *et al.* [2] (black triangle: Coulomb interaction; black circle: GB interaction).

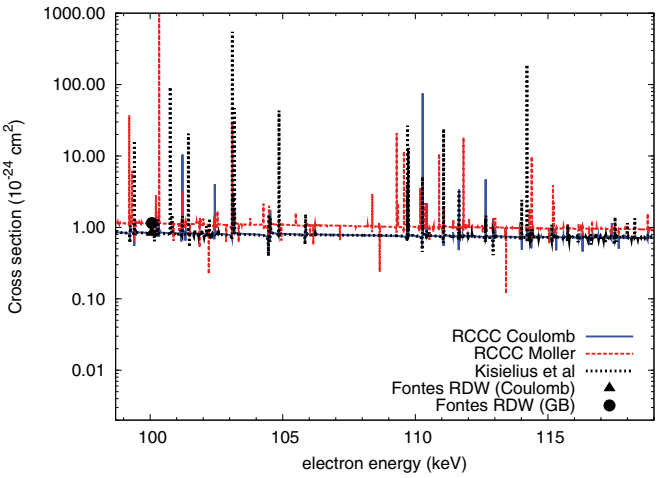

FIG. 2. (Color online) $1s_{1/2} \rightarrow 2p_{1/2}$ electron-impact excitation: see Fig. 1 for description of results.

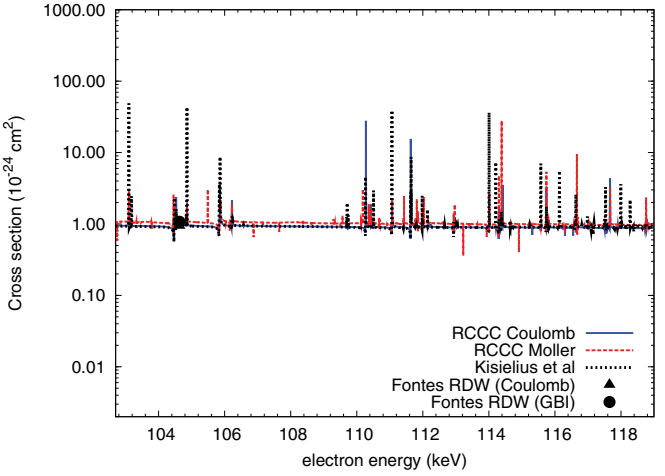

FIG. 3. (Color online) $1s_{1/2} \rightarrow 2p_{3/2}$ electron-impact excitation: see Fig. 1 for description of results.

were performed with same energy mesh grid as that used by Kisielius *et al.* [13]. The important feature of the Møller interaction results is that the overall magnitude of the cross section is determined by the first-order calculation, and the effect of close coupling with the Møller interaction is simply to introduce very sharp resonance peaks on top of the background. We find that generally the resonance peaks obtained with the Møller interaction coincide with those obtained employing the Coulomb interaction.

V. CONCLUSION

We have highlighted some of the conceptual issues that surround the use of Møller interaction in a nonperturbative quantum theory. In the theme of Dirac's "engineering approach" required to obtain practical results, we have incorporated the Møller interaction in a relativistic close-coupling scattering formalism, as it is only within a close-coupling formalism that resonant features in electron-excitation cross sections can be obtained. The Møller interaction can have a significant effect on electron-impact excitation cross sections. We have found that the effects of close coupling are simply to introduce sharp resonances on top of an overall background cross section, the magnitude of which can be obtained with a first-order calculation. Therefore, the dominant rise in the cross section due to the Møller interaction can be obtained with a first-order calculation. Application of the present method to larger energies, particularly where pair creation becomes an important reaction channel, does not look internally consistent within the framework of the RCCC method. In this case, a formulation based on quantum field theory should be invoked.

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APPENDIX: INTERNAL INCONSISTENCIES WITH HOLE THEORY

Problems arise in theories based on the Dirac equation and associated hole theory, as opposed to the full apparatus of relativistic quantum field theory. It is well known that the Dirac-Coulomb Hamiltonian for two or more electrons suffers from "problems" associated with "continuum dissolution" [48]; any positive-energy bound state of a two-electron system is degenerate with the state in which one electron is in a high-lying positive-energy continuum state and the other electron is in a negative-energy continuum state. Switching on the interaction between the electrons can lead to the bound state making a transition to the continuum state described. Sucher [33] highlights that working in the no-virtual-pair approximation is a means to implement the boundary condition of a filled sea of negative-energy states. Surrounding the Dirac-Coulomb Hamiltonian with projection operators for free-particle positive-energy states can enforce this boundary condition. Interestingly, Heully *et al.* [49] highlight that the use of unsuitable projection operators can actually introduce negative-energy states into the Hamiltonian of interest rather than remove them. Johnson [50] discusses the care that must be exercised when projection operators are employed.

Broyles [51] has indicated how the problems can be averted with the aid of Feynman's propagator approach to QED. Dyson [36] outlines how more formal quantum-field-theory techniques can be employed to address the issues with Dirac's hole theory. The conceptual problems underlying hole theory are clearly highlighted by Weinberg [52] in his treatise on quantum field theory: "How can we interpret the antiparticles of charged *bosons*, such as the $\pi^{\pm}$ mesons or $W^{\pm}$ particles, as holes in a sea of negative-energy states? For particles quantized according to Bose-Einstein statistics, there is no exclusion principle, and hence nothing to keep positive-energy particles from falling down into the negative-energy continuum states, occupied or not. And if the hole theory does not work for bosonic antiparticles, why should we believe it for fermions?"

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