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Matrix continuum distorted-wave approximation for electron capture

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Different aspects of relativistic distorted-wave models for electron capture in ion-atom collisions are analyzed. In particular, the nonrelativistic limit of the matrix continuum distorted-wave approximation is studied for reactions with or without change in the electron spin.

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I. INTRODUCTION

The use of different distorted-wave models to describe electron capture in relativistic ion-atom collisions has been a matter of interest in recent years. This has been associated with the development of great new accelerators which have allowed the obtention of beams of multicharged heavy ions at high velocities [1].

In our former works on the subject we have developed *distorted-wave approximations* where initial and final four-spinors representing the electronic clouds in the entry and exit channels, respectively, were distorted by scalar functions. These functions, which appeared multiplying the initial and final bound-state spinors, were first taken as ultrarelativistic projectile and target continuum factors, respectively. These scalar factors (which when multiplied by free-particle spinors are ultrarelativistic approximate solutions of the continuum in the second-order Dirac equations related to the projectile or target nucleus) were also interpreted as diagonal matrix distortions with identical elements [2]. This approximation, called the ultrarelativistic continuum distorted-wave (UCDW) approximation was thus expected to be valid only at ultrahigh relativistic energies ($\gamma \gg 1$ with $\gamma=[1-(v/c)^2]^{-1/2}$, where v is the impact velocity and c the speed of light). Moreover, in the nonrelativistic limit ($c \to \infty$), UCDW does not recover the nonrelativistic continuum distorted-wave (CDW) approximation [3]. In subsequent works [4,5] a relativistic symmetric eikonal (RSE) approximation was introduced, where the scalar continuum factors of UCDW were replaced by their asymptotic limits before or after the collision, given by eikonal phases. The RSE approximation, which could be considered as a symmetric version of the relativistic eikonal one (RE) [6], does not recover the nonrelativistic symmetric eikonal (SE) [7] approximation as $c \to \infty$. So, UCDW and RSE are not a relativistic extension of CDW and SE, respectively, even though they have been developed following the *philosophy* of these approximations, that is, distorting the bound states by scalar continuum factors or eikonal phases. A main goal in introducing the UCDW and RSE approximations was to describe the electron in the *simultaneous* presence of the fields of the projectile and target nuclei in both the entry and exit channels. In this *more realistic* representation, the electron bound to the target nucleus (projectile) is at the same time in a continuum state of the projectile (target nucleus) in the entry (exit) channel. Calculations developed by Deco and Rivarola [4] for high-velocity relativistic reactions showed that RSE underestimates existing experimental data. In addition, it was demonstrated [4] that when the impact velocity is reduced, charge exchange without (with) electron spin flip calculated in the RSE approximation gives total cross sections lower (larger) than in the relativistic target continuum distorted-wave approximation (RTCDW). In RTCDW only one channel is distorted, the final one, by a target continuum factor. Recently [8], this behavior of RSE was studied at the limit of low impact velocities ($\beta=v/c \to 0$), confirming our previous predictions for higher energies, but now in comparison with the one-channel distorted RE approximation [9].

In order to introduce a model which could represent the whole collision-energy range, we introduced [10] a matrix continuum distorted-wave approximation (MCDW). *Matrix operators* associated with the projectile-electron and target-nucleus-electron interactions were chosen to distort the initial and final bound-state spinors, respectively. As will be reexplained in this work, these matrix operators are constructed with relativistic continuum states of the electron in the potential of the projectile or target nucleus. This approximation reduces now to the nonrelativistic CDW as $c \to \infty$ and to UCDW as $\gamma \to \infty$ and can be thus considered as the relativistic version of the CDW model, including as particular cases the two limit models mentioned above. Moreover, to have a good representation of differential cross sections, the theoretical models must reproduce the Thomas's peak, characteristic of a two-step mechanism of electron capture. This is the case of MCDW but not for distorted models where only eikonal phases are used, such as the RE and RSE approximations.

Also, it must be noted that the use of symmetric models avoids post-prior discrepancies of the transition amplitudes. If only one channel is distorted, the loss of this property must be paid.

Finally, we remark that the RSE, UCDW, and MCDW approximations have been developed satisfying appropri-

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ate boundary conditions. This means that the information corresponding to the long-range Coulombic behavior of perturbative potentials is contained in the respective initial and final distorted wave functions.

In this work, we show that MCDW not only goes asymptotically (as $c\to\infty$) on the nonrelativistic CDW but also that, for the spin-flip reaction, MCDW gives cross sections that are negligible compared with the case without spin flip as the energy of the collision decreases to the nonrelativistic domain. This will serve to clarify some criticism made by other authors [8]. Atomic units will be used throughout except where otherwise stated.

II. THE LOW ASYMPTOTIC LIMIT OF THE MATRIX CONTINUUM DISTORTED-WAVE APPROXIMATION

Let us consider for simplicity a bare heavy ion of nuclear charge Z_P impacting on a monoelectronic ion (atom) target of nuclear charge Z_T. Reference frames S and S' are fixed on the projectile and target nucleus, respectively, and the straight-line version of the impact-parameter approximation is used. Exact initial and final bound-state functions Φ_i and Φ_f, representing the electron moving around the target nucleus and projectile, respectively, satisfy the Dirac equations:

$$(H_i-i\partial_t)\Phi_i=(-ic\alpha\cdot\nabla_{\mathbf{r}_T}+\beta c^2+V_T-i\partial_t)\Phi_i=0\ , \qquad (1a)$$

$$(H_f'-i\partial_{t'})\Phi_f'=(-ic\alpha\cdot\nabla_{\mathbf{r}_P'}+\beta c^2+V_P'-i\partial_{t'})\Phi_f'=0\ , \qquad (1b)$$

where α and β are the Dirac matrices, $\mathbf{r}_T$ ($\mathbf{r}_P'$) and t (t') are the electron position vector relative to the target nucleus (projectile) and time as measured from S (S'), respectively. Also, V_T is the electron–target-nucleus potential with respect to S, and V_P' is the electron-projectile potential with respect to S'.

Initial and final four-spinors Φ_i and Φ_f' are distorted by matrix operators $\mathcal{L}_i$ and $\mathcal{L}_f'$, so that distorted initial and final wave functions (seen from S and S', respectively) result in the following:

$$\chi_i=\mathcal{L}_i\Phi_i\ , \qquad (2a)$$

$$\chi_f'=\mathcal{L}_f'\Phi_f'\ . \qquad (2b)$$

If with H we denote the Dirac total Hamiltonian as described from S, we have

$$H=-ic\alpha\cdot\nabla_{\mathbf{r}_T}+\beta c^2+V_T+LV_P'\ , \qquad (3)$$

where L is the matrix operator which transforms the scalar potential V_P' to the scalar and vector potentials referred to S. Then the initial perturbative potential W_i (associated with χ_i) can be obtained using Eq. (1a) in the total Dirac equation [10], so that

$$(H-i\partial_t)\chi_i=W_i\chi_i=[-ic\alpha\cdot\nabla_{\mathbf{r}_T}\mathcal{L}_i+LV_P'\mathcal{L}_i-c^2\mathcal{L}_i+c^2\beta\mathcal{L}_i\beta-i\partial_t\mathcal{L}_i]\Phi_i$$
$$+[-ic(\alpha\mathcal{L}_i-\mathcal{L}_i\alpha)\cdot\nabla_{\mathbf{r}_T}\Phi_i+c^2(\beta\mathcal{L}_i-\mathcal{L}_i\beta+\mathcal{L}_i-\beta\mathcal{L}_i\beta)\Phi_i]\ . \qquad (4)$$

$\mathcal{L}_i$ is now chosen to make zero the first term of the right-hand side (rhs) of Eq. (4), that is,

$$[-ic\alpha\cdot\nabla_{\mathbf{r}_T}\mathcal{L}_i+LV_P'\mathcal{L}_i-c^2\mathcal{L}_i+c^2\beta\mathcal{L}_i\beta-i\partial_t\mathcal{L}_i]=0\ . \qquad (5)$$

Transforming Eq. (5) into the reference frame S', we have the resulting simpler equation [11]:

$$[-ic\alpha\cdot\nabla_{\mathbf{r}_P'}\mathcal{L}_i+V_P'-i\partial_{t'}]\mathcal{L}_i'+c^2\beta\mathcal{L}_i'\beta=0\ , \qquad (6)$$

with

$$\mathcal{L}_i'=T^{-1}\exp(-ic^2t)\mathcal{L}_i \qquad (7)$$

and where T is the operator which transforms the spinors seen from the reference frame S' into the frame S. Except by the last matrix β appearing in the last term of Eq. (6), this equation corresponds to the Dirac one associated only with the electron-projectile interaction. Our interest is in describing the electron in a bound state of the target but at the same time also in a continuum state of the projectile in the entry channel. Let us try to construct the matrix $\mathcal{L}_i'$ with *exact* relativistic continuum vectors of the electron in the presence of the projectile. It can be easily shown that a solution of Eq. (6) is given by a matrix $\mathcal{L}_i'$ where the two first columns represent exact continuum four-spinors of the electron-projectile interaction. The third and fourth columns which complete the determination of $\mathcal{L}_i'$ are obtained exchanging the two upper components with the two lower components of the first and second columns, respectively. Then the perturbative potential is the result:

$$W_i\chi_i=-ic(\alpha\mathcal{L}_i-\mathcal{L}_i\alpha)\cdot\nabla_{\mathbf{r}_T}\Phi_i$$
$$+c^2(\beta\mathcal{L}_i-\mathcal{L}_i\beta+\mathcal{L}_i-\beta\mathcal{L}_i\beta)\Phi_i\ . \qquad (8)$$

Up to this point, no approximations have been used and W_i is in exact correspondence with χ_i. In a similar way we can proceed with the exit channel. However, instead of working with numerical *exact* continuum wave functions, we use an analytical approximate solution of Eq. (6). This approximation avoids tedious and complicated calculations associated with the utilization of numerical wave functions and also allows one to go deeper into the physical interpretation of the distortion used. The solution is constructed by using the Furry matrix [12] Ω_i and is expressed in the form

$$\mathcal{L}_i'=\exp(-i\gamma c^2t-i\gamma\mathbf{v}\cdot\mathbf{r}_P')\Omega_iT^{-1}\ , \qquad (9)$$

with

$$\Omega_i = \exp(\pi Z_p/2v)\Gamma(1-iZ_P/v)[\underline{1}-(i/2\gamma c)\alpha\cdot\nabla_{\mathbf{r}'_P}] \times {}_1F_1(iZ_P/v;1;i\gamma(vr'_P+\mathbf{v}\cdot\mathbf{r}'_P)) , \tag{10}$$

where $\underline{1}$ is the identity matrix. The matrix Ω_i, when acting on a plane-wave spinor, generates relativistic continuum-state solutions of the Dirac-Coulomb equation, describing the electron as moving in the field of the projectile as seen from S'. This is the case when Ω_i is applied separately to each one of the two first columns of T^{-1}. If this result is multiplied by the exponential factor given by (9), we obtain appropriate relativistic continuum states of the electron moving with velocity $-\mathbf{v}$ with respect to the projectile.

Then, the initial distorted-wave function is the result

$$\chi_i \cong (T\Omega_i T^{-1})\Phi_i . \tag{11}$$

Equation (11) can be interpreted in the following way: The initial bound spinor as seen from S is translated to the frame S' through the application of the operator T^{-1}; then, the operator Ω_i, instead of being applied to a plane-wave spinor, acts as a distortion of the initial bound state; and finally, the operator T acts to translate the initial wave function to S again.

Proceeding in a similar way with the distorted final wave function, we obtain the approximate solution

$$\chi'_f \cong (T^{-1}\Omega_f T)\Phi'_f , \tag{12}$$

where Ω_f is the Furry operator

$$\Omega_f = \exp(\pi Z_T/2v)\Gamma(1+iZ_T/v)[\underline{1}-(i/2\gamma c)\alpha\cdot\nabla_{\mathbf{r}_T}] \times {}_1F_1(iZ_T/v;1;-i\gamma(vr_T+\mathbf{v}\cdot\mathbf{r}_T)) , \tag{13}$$

which, when applied to plane-wave spinors, will give continuum states of the electron as moving in the presence of the target nucleus and observed from S. It is obvious that when the distortion $\mathcal{L}_i = T\Omega_i T^{-1}$ is used, Eq. (5) is solved approximately. Moreover, as we will use quasirelativistic Darwin spinors to describe the initial and final non-distorted-wave functions, Eqs. (1a) and (1b) will also be solved in an approximate way. Otherwise, we must deal with complicated calculations associated with the introduction of *exact* continuum- and bound-state spinors. Exact Coulomb-Dirac wave functions have been used to describe the electron states for ionization reactions [13]. The Coulomb-Dirac continuum wave function has been represented by a partial-wave expansion. Due to numerical difficulties, the partial-wave summation is restricted to angular-momentum quantum numbers $|\kappa| \le 10$. The convergence of the summation is unsatisfactory at high kinetic electron energies. The problem is partly corrected by using relativistic Furry (Sommerfeld-Maue) and Darwin wave functions [12]. In the MCDW model the distortion continuum factors correspond to high-energy electrons (electrons moving with velocities in modulus equal to the collision velocity). Therefore, the use of Darwin wave functions and Furry distortions operators is justified in the present case. Then, the first order of the transition amplitude as a function of the impact parameter $\boldsymbol{\rho}$ can be written as [10]

$$\begin{aligned}\mathcal{A}_{if}(\boldsymbol{\rho}) &= -i\int_{-\infty}^{+\infty} dt \int d\mathbf{r}_T [T\chi'_f(\mathbf{r}'_P,t')]^\dagger W_i \chi_i^+(\mathbf{r}_T,t)\\ &\cong -i\int_{-\infty}^{+\infty} dt \int d\mathbf{r}_T [T\chi'_f(\mathbf{r}'_P,t')]^\dagger [-ic(\alpha T\Omega_i T^{-1} - T\Omega_i T^{-1}\alpha)\cdot\nabla_{\mathbf{r}_T}\Phi_i\\ &\qquad + c^2(\beta T\Omega_i T^{-1} - T\Omega_i T^{-1}\beta + T\Omega_i T^{-1} - \beta T\Omega_i T^{-1}\beta)\Phi_i] .\end{aligned} \tag{14}$$

Expression (14) is equivalent to Eq. (48) of Ref. [10], where Darwin spinors are used to represent the initial and final K-shell bound states. For the reaction without electron spin flip, it is easy to show that as $c\to\infty$, we recover the K-K shell nonrelativistic CDW approximation. Moreover, for ultrarelativistic velocities ($\gamma\to\infty$), we obtain the UCDW model. So, even using approximated initial and final distorted spinors, we recover the corresponding asymptotic energy limits. This is an indication of the consistence of the approximations used.

When the impact energy decreases, the case with change of the electron spin is expected to give negligible contributions compared with the process without spin flip.

In order to give a numerical evaluation of the cross sections, we use the transformation

$$\mathcal{A}_{if}(\boldsymbol{\rho}) = (2\pi)^{-1}\int d\boldsymbol{\eta}\,\mathcal{R}_{if}(\boldsymbol{\eta})\exp(-i\boldsymbol{\eta}\cdot\boldsymbol{\rho}) , \tag{15}$$

where $\mathcal{R}_{if}(\boldsymbol{\eta})$ is the scattering matrix element as a function of the transverse momentum transfer $\boldsymbol{\eta}$. Using some approximations, $\mathcal{R}_{if}(\boldsymbol{\eta})$ can be calculated as indicated in Refs. [10] and [14]. For the cases with and without spin flip, we thus obtain analytical expressions for $\mathcal{R}_{if}(\boldsymbol{\eta})$ which are easy to compute. Also, we must note that as $c\to\infty$, we recover the nonrelativistic CDW matrix element $\mathcal{R}_{if}(\boldsymbol{\eta})$ [10].

Differential and total cross sections can then be computed by using the expressions

$$\frac{d\sigma}{d\Omega} = M_P^2\gamma^2 v^2 |\mathcal{R}_{if}(\boldsymbol{\eta})|^2 \tag{16}$$

and

$$\sigma = \int d\boldsymbol{\eta} |\mathcal{R}_{if}(\boldsymbol{\eta})|^2 , \tag{17}$$

respectively.

In Table I, total cross sections for the $H^+ + H(1s)$ reaction at nonrelativistic impact energies from 50 keV up to 10 MeV are presented for the cases with and without spin flip. It appears that when the collision velocity decreases,

TABLE I. Non-spin-flip and spin-flip total cross sections for $H^+ + H(1s)$ electron capture (in m^2). The MCDW results are present calculations based on Ref. [10]. The CDW results are obtained from Ref. [3]. The numbers in square brackets give the power of 10 multiplying the preceding number.

	Theory		
		MCDW	
Energy (keV)	CDW	Nonflip	Flip
50	6.95[−21]	6.94[−21]	5.75[−30]
100	6.39[−22]	6.37[−22]	1.46[−30]
250	1.38[−23]	1.37[−23]	1.67[−31]
500	4.83[−25]	4.81[−25]	2.57[−32]
1000	1.29[−26]	1.29[−26]	3.32[−33]
2500	8.42[−29]	8.40[−29]	1.84[−34]
5000	1.68[−30]	1.68[−30]	1.88[−35]
10 000	3.19[−32]	3.21[−32]	1.81[−36]

MCDW presents the correct behavior in the sense that spin flip becomes less and less important in comparison with the non-spin-flip case. Also, non-spin calculations are compared with nonrelativistic CDW results using Ref. [3] (see also Belkič, Gayet, and Salin [15]). The agreement obtained is excellent.

In Table II our results are compared with calculations previously presented [8] but using the relativistic Oppenheimer-Brinkman-Kramers (ROBK), RE, relativistic first-order Born with Coulomb boundary conditions (R1B) [16], and RSE approximations. As done before, the system studied is $H^+ + H(1s)$ but at 100 keV impact energy. A good qualitative agreement with the other theories is obtained, with the exception of RSE which, as discussed before, fails at this low velocity.

In order to obtain a stringent test of the convergence of the MCDW approximation on the nonrelativistic CDW one, we also compare differential cross sections for the system indicated above at the nonrelativistic 300 keV and 10 MeV collision energies for the non-spin-flip reaction. The agreement between MCDW and CDW results is so close that they cannot be distinguished in Figs. 1(a) and 2(a). Moreover, for the 10-MeV case, the relativistic model reproduces a pronounced dip overlapping the Thomas's peak which in the nonrelativistic models is shown to come from interferences between intermediate projectile and target continuum states [17,18]. The dip also appears as a spurious structure at the lower impact-energy case. Calculations with a matrix continuum intermediate-state approximation (MCIS) are also presented for both cases. In this model, introduced by

TABLE II. Non-spin-flip and spin-flip total cross sections for $H^+ + H(1s)$ electron capture (in atomic units) at 100 keV. ROBK, RE, R1B, and RSE results are extracted from Ref. [8]. The MCDW results are present calculations based on Ref. [10]. The numbers in square brackets give the power of 10 multiplying the preceding number.

Theory	σ_{nonflip}	σ_{flip}	$\sigma_{\text{flip}}/\sigma_{\text{nonflip}}$
ROBK	1.22[0]	4.39[−10]	3.60[−10]
RE (prior)	1.99[−1]	2.83[−10]	1.42[−9]
RE (post)	1.99[−1]	2.83[−10]	1.42[−9]
R1B	2.25[−1]	1.76[−10]	7.82[−10]
RSE	5.3[−2]	6.3[−3]	1.2[−1]
MCDW	2.27[−1]	5.20[−10]	2.29[−9]

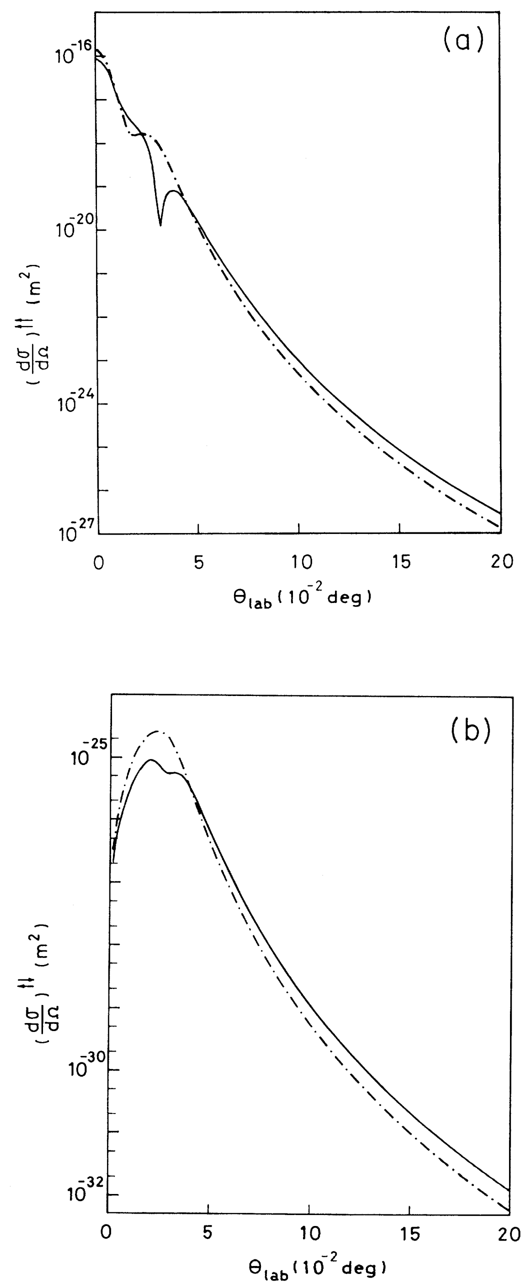

FIG. 1. (a) Theoretical differential cross sections $(d\sigma/d\Omega)^{\uparrow\uparrow}$ for electron capture without spin flip in the $H^+ + H(1s) \rightarrow H(1s) + H^+$ system as a function of the laboratory scattering angle θ for an impact energy of 300 keV. The theoretical models shown are ——, MCDW; —·—·—·, MCIS; — — —, CDW (indistinguishable from MCDW in this figure). (b) Same as (a) but for the case with spin flip, $(d\sigma/d\Omega)^{\uparrow\downarrow}$.

McCann [19], only the entry channel is distorted by using the same initial distorted-wave function as in MCDW. The agreement between MCIS and MCDW differential cross sections is very good, except that MCIS, as expected, only shows one peak that does not present interference effects. Also, nonrelativistic Eikonal calculations [7] are displayed in Fig. 2(a). The RE-differential cross section must converge to them at the energy considered. It is evident from the observation of the figure that the characteristic peak of the two-step mechanism of electron capture will be not represented by RE. Non-spin-flip differential cross sections calculated with the MCDW and MCIS approximations are introduced in Figs. 1(b) and 2(b) at 300 KeV and 10 MeV impact energies, respectively.

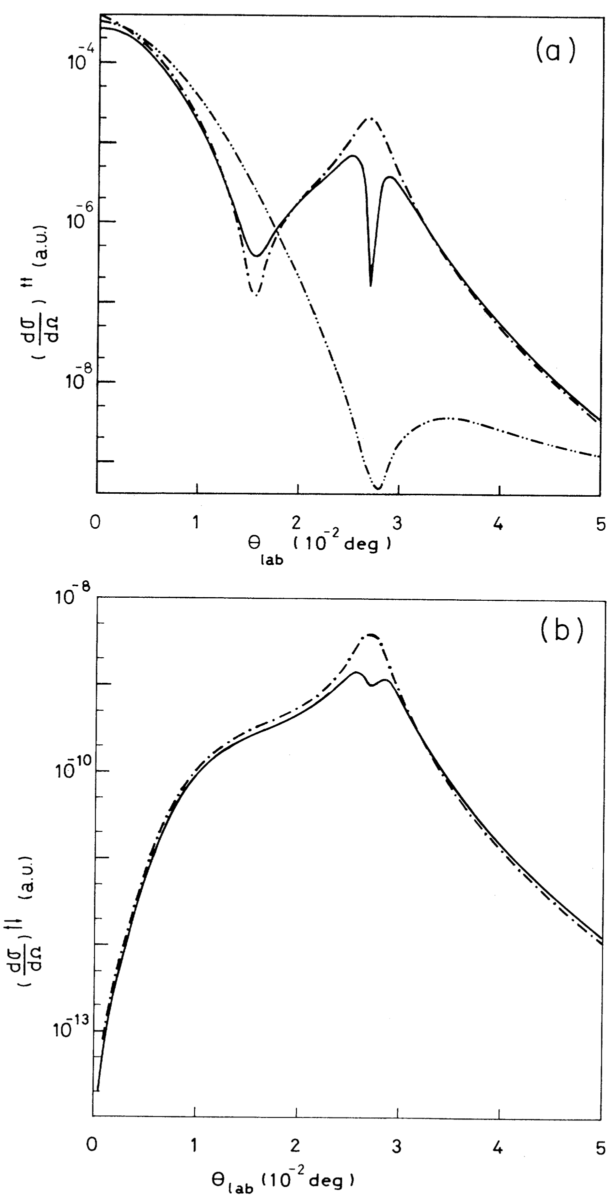

FIG. 2. (a) Same as Fig. 1(a) but for an impact energy of 10 MeV. In addition, —..—..—, SE from Ref. [7]. (b) Same as (a) but for the case with spin flip, $(d\sigma/d\Omega)^{\uparrow\downarrow}$.

TABLE III. Non-spin-flip and spin-flip total cross sections for 1*s*-1*s* electron capture (in atomic units) for $U^{92+}+U^{91+}$ collisions at 500 MeV/amu. Same captions as for Table II. The results of 36-state coupled-channel calculations are extracted from Ref. [8].

Theory	σ_{nonflip}	σ_{flip}	$\sigma_{\text{flip}}/\sigma_{\text{nonflip}}$
ROBK	1.74[−3]	1.27[−5]	7.30[−3]
RE (prior)	1.40[−4]	8.16[−6]	5.83[−2]
RE (post)	1.40[−4]	8.16[−6]	5.83[−2]
R1B	1.16[−4]	3.98[−6]	3.43[−2]
Close coupling	1.42[−4]	8.14[−6]	5.73[−2]
RSE	2.26[−5]	2.73[−6]	1.21[−1]
MCDW	1.60[−4]	7.36[−6]	4.62[−2]

tively. It is clear that the spin-flip case gives differential cross sections several orders of magnitude lower than the case without spin flip. Also, the spin-flip figures show a double scattering peak. Interference effects appear again in MCDW even if a smooth valley now replaces the pronounced dip of the case without spin flip. It must also be noted that electron spin cannot change in the electron-capture reaction if the projectile is not deflected from its original direction. This is a qualitative distinctive characteristic of the spin-flip case.

The comparison of Tables I and II and Figs. 1 and 2 are a convincing test of the low-velocity convergence of the MCDW and a severe indication of the adequacy of the approximations made during the obtention of $\mathcal{R}_{if}(\boldsymbol{\eta})$. The MCDW approximation thus constitutes an excellent tool to estimate also spin-flip contributions in the case of electron capture even at nonrelativistic velocities.

The RSE approximation has also been shown to fail in comparison with other theoretical predictions, even at a relativistic velocity corresponding to a collision energy of 500 MeV/amu, for the impact of U^{92+} on U^{91+}. In Table III we compare our MCDW results with ROBK, RE, R1B, and close-coupling calculations [8], all of them obtained with bound-state Darwin wave functions. The agreement of MCDW with these theories is very good, even if for this case the validity of the use of Darwin wave functions could be questioned because $Z_{P,T}/c \ll 1$. In our calculations, Darwin spinors are affected by normalization factors as given by Deco and Grün [20]. It has been shown that when scalar eikonal phases are used to distort bound spinors, the associated perturbative potentials present spurious spin-flip contributions as $c \to \infty$, and this criticism was suggested to be valid also for the UCDW and MCDW approximations [8]. We have shown in this work that such spurious contributions do not appear in MCDW in the nonrelativistic energy regime. Also, it must be noted even though these perturbative potentials will also appear related to the distorted channel in models where only one channel is distorted by an eikonal phase, it has been shown that this spurious behavior is mathematically eliminated in such cases [8].

III. CONCLUSIONS

The MCDW behavior at nonrelativistic energies has been studied for electron capture in ion-atom collisions where the electron spin changes or remain unaltered. For the reactions without spin flip, it has been shown analytically and numerically that MCDW approximation goes on the nonrelativistic CDW approximation as $c \to \infty$. For the case with spin flip it has also been numerically proved that the MCDW gives negligible contributions to the cross sections compared with the non-spin-flip case as the impact energy decreases. Therefore, the MCDW does not exhibit unphysical effects in the nonrelativistic domain in contrast with other symmetric theories such as RSE and UCDW. The MCDW which also goes on the UCDW as $\gamma \to \infty$ thus constitutes a powerful tool to describe charge exchange for all collisions velocities for which the impact-parameter approximation may be used.

Differential and total cross sections have been presented and qualitatively analyzed for the cases with and without spin flip. The present work sheds light on a recent paper [8] where the points analyzed here were discussed.

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