Coupled-channel eikonal approach to electron capture

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We develop an alternative close-coupling scheme based on an eikonal-distorted-wave expansion. The convergence of the basis expansion is improved remarkably at intermediate and high energies in comparison with the ordinary expansion in terms of the unperturbed atomic orbitals. The present electron-capture cross sections of a proton from atomic hydrogen agree well with those of elaborate large-scale close-coupling calculations above 15 keV, even within a two-state approximation. A question is raised as to the effect of the Coulomb boundary conditions to the Oppenheimer-Brinkman-Kramers approximation. [S1050-2947(99)07909-3]

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I. INTRODUCTION

The atomic-orbital close-coupling (AOCC) method [1–3] is one of the most reliable theoretical descriptions of ion-atom collisions, and has been successfully applied to various processes in a wide range of collision energies. One inconvenient characteristic of this method might be the long CPU time required for achieving satisfactory convergence of the expansion. Even for the simplest system

$$p+\mathrm{H}(1s)\rightarrow\mathrm{H}(1s)+p, \tag{1}$$

a large number of basis states have to be employed in order to take proper account of the contribution of continuum states, which affect the electron capture cross sections indirectly even in the energy region of hundreds of keV where the first-order contribution is expected to be dominant but the Thomas double scattering process [4,5] is not yet significant. The electron-capture cross section is generally overestimated above 100 keV when only the initial and final states are used for the expansion [1], while other perturbative distorted-wave approaches such as the eikonal approximation [6,7] work well there. The overestimated capture cross sections gradually decrease as we add more states to the basis functions. Not only excited states but also continuum states are needed in order to achieve convergence. Although this difficulty has been overcome so far owing to the recent rapid progress of high-speed computers [8], it is highly desirable to find better basis functions for a further development of the close-coupling method and for a deeper understanding of the electron-capture processes.

Another requirement of developing a close-coupling formalism arises from the instability problem of excitation and capture cross sections inherent in full two-center AOCC calculations [9,10]. When pseudocontinuum states are used on both centers, excitation and electron-capture cross sections sometimes show unphysical oscillatory structures as a function of the collision energy. In order to remove this instability, the energy spacings between adjacent pseudocontinuum states have to be very small so that a large number of continuum states are required for the expansion. If well-converged capture cross sections are obtained without usage of pseudocontinuum states, we need not worry about this instability problem.

The overestimate of the two-state AOCC capture cross sections is a puzzling problem. It is well-known that the Oppenheimer-Brinkman-Kramers (OBK) approximation [11] generally overestimates capture cross sections, while the so-called Jackson and Schiff approximation [12] shows much better agreement with measurements for process (1). The agreement of the latter approximation is not physically acceptable, since the internuclear interaction should not give such large contribution for ion-atom collisions. Dewangan and Eichler [13] resolved this problem by reformulating the capture theory for the long-range Coulomb potentials. According to their interpretation, the internuclear term $1/R$ of the Jackson-Schiff approximation should be taken as the distortion potential that makes the Coulomb interaction short-ranged. In other words, the overestimate of the OBK capture cross sections are caused by an improper account of the long-range of the Coulomb interactions. However, the distortion potential $1/R$ does not contribute to the transition probability at all in the AOCC formalism, since it is completely absorbed in a phase factor by a kind of gauge transformation [14]. The reduction of the AOCC capture cross sections is achieved only by increasing the number of basis functions. It is quite unclear how the Coulomb boundary condition is related to the convergence problem of the AOCC method.

II. FORMULATION

In this study we unify the close-coupling method and the eikonal approximation to improve the basis-set convergence at intermediate- and high-energy regions. For simplicity we confine our interest to process (1). As a first step we expand the total scattering wave function satisfying the Schrödinger equation in the representation of the impact-parameter method,

$$\left(H-i\frac{\partial}{\partial t}\right)\Psi(\mathbf{r},t)=0, \tag{2}$$

as a linear combination of the target and the projectile atomic orbitals with appropriate electron-translation factors (ETF) attached,

$$\Psi(\mathbf{r},t)=\sum_{n=1}^{N} a_n(t)\phi_n(\mathbf{r},t)\exp(-iE_nt), \tag{3}$$

in the same way as the ordinary close-coupling expansion. In the above expressions $\mathbf{r}$ is a position vector of the transferred electron measured from the coordinate origin, and E_n is the eigenenergy of the nth orbital $\phi_n(\mathbf{r},t)$. We use atomic units in this paper unless otherwise stated. The projectile is assumed to travel at a constant velocity v along a straight-line trajectory throughout the collision. To determine the coefficients $a_n(t)$, we project the Schrödinger equation onto the subspace spanned by the eikonal-distorted states composed of the same number of atomic orbitals ($m=1-N$),

$$\left\langle \phi_m(\mathbf{r})L_m \left| H - i\frac{\partial}{\partial t} \right| \Psi(\mathbf{r},t) \right\rangle = 0, \tag{4}$$

where $L_m = L_P$ (L_T) when the mth state belongs to the target (projectile). The eikonal phase factors L_P and L_T are defined as

$$L_P = \exp\left(-i\int_{-\infty}^{t} V_P dt' \right), \tag{5}$$

$$L_T = \exp\left(i\int_{t}^{\infty} V_T dt' \right), \tag{6}$$

where V_P (V_T) is the Coulomb interaction between the electron and the projectile (target) proton. These factors are chosen to satisfy the boundary conditions $L_P \to 1$ and $L_T \to 1$ for $t \to -\infty$ and $t \to +\infty$, respectively, and can be rewritten explicitly removing constant phase factors, after integration [7], as

$$L_P = (r_P + z_P)^{-iZ_P/v}, \tag{7}$$

$$L_T = (r_T + z_T)^{iZ_T/v}. \tag{8}$$

In the present system [Eq. (1)] both charges Z_T and Z_P are unity. $\mathbf{r}_P$ and $\mathbf{r}_T$ are the position vectors of the electron measured from the projectile and the target nuclei, respectively, and z_P and z_T are their z components along the incident beam direction. The boundary conditions of L_P and L_T guarantee the orthogonality of the target states before the collision and that of the projectile states after the collision. The orthogonality is required to satisfy the initial condition and to define the transition probabilities at $t \to +\infty$ unambiguously. Under these conditions the transition probability to the projectile state m is given by the squared absolute value of the amplitude $a_m(t=\infty)$.

Equation (4) reduces to coupled differential equation in a matrix form,

$$\tilde{S}\frac{d\mathbf{a}}{dt} = -i\tilde{H}\mathbf{a}, \tag{9}$$

where $\mathbf{a}$ is the state vector whose ith component is the coefficient $a_i(t)$, and the elements of the overlap and the interaction matrices $\tilde{S}$ and $\tilde{H}$ are defined as

$$\tilde{S}_{mn} = \langle \phi_m(\mathbf{r})L_m | \phi_n(\mathbf{r}) \rangle, \tag{10}$$

$$\tilde{H}_{mn} = \langle \phi_m(\mathbf{r})L_m | V_n | \phi_n(\mathbf{r}) \rangle, \tag{11}$$

TABLE I. Convergence of the capture cross sections in cm^2 for $p + \mathrm{H}(1s) \to \mathrm{H}(1s) + p$. The numbers in brackets are the powers of 10 to be multiplied. The three basis sets (a), (b), and (c) contain $n=1$ states, $n=1$ and 2 states, and $n=1$–4 states on both centers, respectively.

E (keV)	(a)	(b)	(c)
12.0	8.97[−16]	8.52[−16]	8.11[−16]
25.0	2.33[−16]	2.62[−16]	2.73 [−16]
50.0	4.63[−17]	5.13[−17]	5.31[−17]
100.0	5.77[−18]	5.99[−18]	5.99[−18]
200.0	4.29[−19]	4.28[−19]	4.28[−18]

where $V_n = V_P$ or V_T when the nth state belongs to the target or to the projectile, respectively. One should note that the first-order solution of the coupled equations reduces to the traditional eikonal approximation in the prior form [6,7] at high energies rather than the symmetric eikonal approximation [15]. The solution of Eq. (4) becomes exact in the limit of the infinity ($N \to \infty$) for the completeness even though the present expansion is not based on the variational principle.

III. RESULTS AND DISCUSSIONS

The computation of the matrix elements (10) and (11) is performed by direct three-dimensional numerical integration in the spheroidal coordinates (ξ, η, φ) for the two-center part and in the spherical coordinates (r, θ, φ) for the single-center part [16]. The Gauss-Laguerre quadruture is used for the ξ and r parts, and the Gauss-Legendre quadruture is used for the η, θ, and φ parts. The number of points used for the Gauss quadrutures is from 24 to 40 depending on the collision energy. The eikonal phase factors make the integrand oscillate rapidly at low energies while the ETF does so at high energies, so that a larger number of points is required there.

We have checked the convergence for three different sets of basis functions. The smallest set (a) contains only initial and final states, the intermediate-size set (b) contains all the bound states with principal quantum numbers $n=1$ and 2, and the largest set contains all the bound states with $n \leqslant 4$. The capture cross sections of process (1) are compared in Table I. We see an excellent convergence of the present method for the number of basis functions, in contrast to the slow convergence of ordinary coupled-channel methods based on the undistorted-wave-basis expansion.

Figure 1 shows the cross sections of the electron-capture process (1). As seen in Table I, the cross sections of sets (a) and (c) are very close, so that they are indistinguishable in the figure above 100 keV. Since no direct measurement is available for state-specified process (1) we compare the present result with elaborate large-scale AOCC calculations [10], which can be judged to have converged in comparison with even larger calculations [8] and other independent calculations [17]. All the measurements are for the total capture cross sections that contain transitions into all the excited states. The contribution of the excited states is sometimes estimated by dividing the total cross section by a factor of 1.202, which is justified only for the Born approximation. We avoid the unfavorable uncertainty arising from this nor-

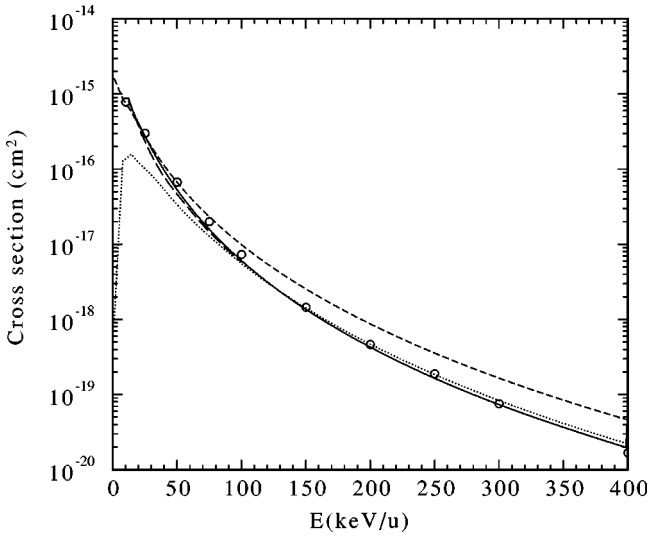

FIG. 1. Electron-capture cross sections for $p+\mathrm{H}(1s)\rightarrow\mathrm{H}(1s)+p$. Solid line and long-dashed line, present coupled-channel eikonal with the largest basis set (c) and the smallest basis set (a), respectively; short-dashed line, two-state AOCC; dotted line, the eikonal approximation. Circles are from the large-scale AOCC calculations, in which 161 states including pseudocontinuum are used on both the target and the projectile [10]. Above 100 keV, the two coupled-channel eikonal cross sections are too close to be distinguished in plotting.

malization procedure by using well-defined theoretical work. As stated above, the ordinary two-state AOCC calculations give overestimated cross sections by a factor of 2–3 above 100 keV, while the eikonal approximation fails to produce the monotonic increase of the cross sections below 50 keV, which is a characteristic behavior of a resonant electron capture of symmetric systems. The present coupled-channel eikonal calculations, on the contrary, gives excellent agreement with the large-scale AOCC calculations even within the two-state approximation in a wide energy region above 15 keV.

The transition probabilities of process (1) are compared at 25 and 100 keV in Fig. 2. At 100 keV the coupled-channel-eikonal probability is very close to that of the perturbative eikonal approximation, while it is closer to that of the two-state AOCC method at 25 keV. The smooth crossover from the perturbative eikonal approximation to the two-state AOCC method for decreasing collision energy is just what we had in mind in formulating the present coupled-channel eikonal approach.

The projection procedure (4) does not automatically maintain the unitarity of the total transition probabilities. In Table II we show the variation of the unitarity (the sum of the probabilities of all the transitions) as a function of the collision energy at the impact parameter $b=1.5$ where the capture probability become maximum. The unitarity violation becomes serious for decreasing collision energy. The broken unitarity arises mainly from the components on the target, namely, the excitation channels. The eikonal distortion [Eq. (6)] on the target states does not disappear at $t=+\infty$, in contrast with the distortion [Eq. (7)] on the projectile states, and hence the projection onto the target states [Eq. (11)] does not lead directly to true excitation. The remaining distortion makes the apparent probabilities of target excitation larger than the real values. To examine the above interpretation, we project the distorted target states $\{\phi_m(\mathbf{r}_T)L_m\}$ back to the undistorted states $\{\phi_m(\mathbf{r}_T)\}$ after the collision:

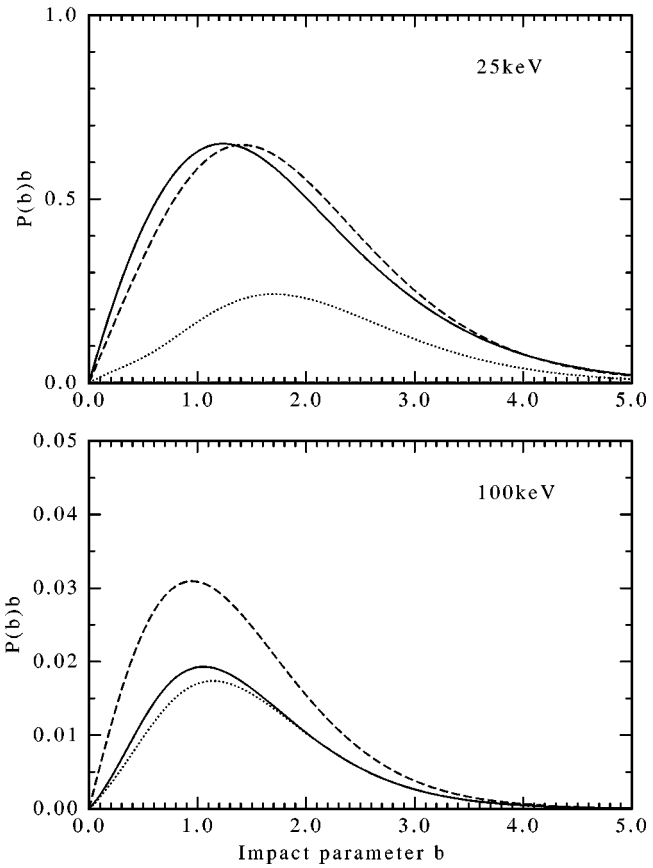

FIG. 2. Electron-capture probabilities for $p+\mathrm{H}(1s)\rightarrow\mathrm{H}(1s)+p$ as a function of the impact parameter b in atomic units. The upper figure is for 25 keV, and the lower for 100 keV. Solid lines, present coupled-channel eikonal probabilities of the largest basis set (c); dashed lines, two-state AOCC; dotted lines, the eikonal approximation.

$$b_m=\sum_k \langle\phi_m|\phi_k L_k\rangle a_k . \tag{12}$$

Note that the above projection does not change the capture probabilities at all since the overlap matrix [Eq. (10)] is diagonal among the projectile states, and the overlaps between the projectile and the target states vanish after the collision. We present the sum of the corrected transition probabilities

TABLE II. Unitarity check of the coupled-channel eikonal calculations for the largest basis set (c) at the impact parameter $b=1.5$. The coefficients a_n give apparent probabilities before correction, and b_n of Eq. (12) gives the probabilities after correction (see the main text).

E (keV)	$\Sigma_n\lvert a_n(t=+\infty)\rvert^2$	$\Sigma_n\lvert b_n(t=+\infty)\rvert^2$
25.0	2.049	1.141
50.0	1.636	1.046
100.0	1.289	1.015
200.0	1.128	1.006

in Table II. The broken unitarity is impressively recovered. The unitarity violation of the apparent probabilities arises from the leak and the inflow of the probabilities due to the difference of the spaces covered by $\{\phi_m(\mathbf{r}_T)L_m\}$ and $\{\phi_m(\mathbf{r}_T)\}$. The unitarity becomes worse below 25 keV even after the correction procedure, and the present method becomes less reliable. Below 15 keV the present capture cross sections exceed the converged cross sections of the large-scale AOCC calculations. However, because the two-state AOCC method works satisfactorily well below 50 keV, we do not have to develop a new formalism there.

The Coulomb boundary condition does not have any effect on coupled-channel eikonal capture cross sections for the same reason as discussed above for the ordinary AOCC method. The reduction of the capture cross sections is caused solely by eikonal phase factors in the transition matrix elements. These factors represent the distortion of electronic wave functions induced by Coulomb forces exerted by the other nuclei. Whereas the effect of the factors diminishes quickly to direct excitation processes as the collision energy increases, it continues to affect rearrangement capture processes up to high collision energies. Since the interaction region in which the electron capture occurs shrinks as the collision energy increases, the decrease of the collision time is balanced by the augmented strength of the Coulomb interaction [14], and the distortion has a sizable effect on the capture cross sections even at high energies. In the ordinary AOCC treatment, this distortion effect of the electronic states can be taken into account only by superimposing a large number of excited states and continuum states. Although the claim of Dewangan and Eichler [13] about the proper account of the Coulomb boundary conditions for the electron capture is physically sound, further intensive analysis and reinterpretation of the perturbative capture theories are required.

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