# Coulomb boundary conditions in high-energy theories for electron-capture processes

Nobuyuki Toshima and Takeshi Ishihara
*Institute of Applied Physics, University of Tsukuba, Tsukuba, Ibaraki 305, Japan*
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We examine various high-energy approximation methods, with and without boundary corrections for electron-capture processes. From the comparison of the calculated differential cross sections for the proton plus hydrogen-atom system, we show that the boundary correction does not always improve the results. The internuclear interaction must be fully taken into account to explain the experimental results.

## I. INTRODUCTION

More than five decades have passed since Oppenheimer[1] and, subsequently, Brinkmann and Kramers[2] calculated electron-capture cross sections by means of the first-order Born formula, neglecting the internuclear interaction completely. This approximation (OBK) overestimates cross sections by as much as a factor of 5. Two decades later, Bates and Dalgarno[3] and Jackson and Schiff[4] (JS) calculated the first-order Born cross sections for the proton–hydrogen-atom ($p+\mathrm{H}$) collision, including the internuclear interaction in the transition operator. They found that this interaction affects cross sections considerably and reduces them to experimental results. However, a difficulty arose in the physical interpretation, because the contribution of the internuclear interaction was expected to be negligibly small at the energy region studied. Moreover, it was found later that the JS approximation predicts cross sections in violent disagreement with experiments for $K$-shell capture in asymmetric systems such as protons on argon.[5]

On the other hand, analyzing the two-state close-coupling scheme, Bates[6] pointed out that the nonorthogonality of the atomic wave functions of the initial and the final states should be taken into account properly, even for the first-order treatment. Soon after, Bassel and Gerjuoy[7] have shown that the distorted-wave Born approximation (DWBA), in which the distortion potential is an interaction averaged over the electron distribution of the initial or final state, is closely related to Bates's version of the first-order formula. Both of them agree well with experiments.

It is well known that the long-range nature of the Coulomb interaction brings about mathematical difficulties in treating collision processes and requires special account for its proper application. Nevertheless, the scattering formalism developed for short-range potentials has been often applied without modification to systems with Coulomb interactions. Dewangan and Eichler proposed a new first-order theory referred to as the boundary-corrected first-order Born (B1B) approximation,[8] which satisfies the Coulomb boundary conditions in both entrance and exit channels. The B1B approximation coincides with the JS approximation accidentally for the $p+\mathrm{H}$ system. This clarifies why the JS approximation gives good results only for this particular system. The DWBA and the Bates formulas also satisfy the Coulomb boundary conditions,[9] and the difference from the B1B approximation consists in the choice of the distortion potentials that are well defined only at the asymptotic region of infinite separation.

The eikonal approximation[10,11] has been applied widely to electron-capture processes successfully. While it gives good agreement with experiments in both integrated and differential cross sections, it does not satisfy the Coulomb boundary conditions in one of the channels. In this paper we remedy this defect by introducing the boundary-corrected eikonal approximation, which is derived from the usual eikonal amplitude by a modification based on the distorted-wave formalism. We calculate differential cross sections and compare them with other theories satisfying Coulomb boundary conditions. We show that the boundary correction does not always improve the differential cross sections. Atomic units are used throughout unless otherwise stated.

## II. THEORY

Consider the electron-capture process between a bare projectile ion $P$ with a charge $Z_P$ and a target atom consisting of a nucleus $T$ with a charge $Z_T$ and an electron $e$,

$$(T+e)+P \rightarrow T+(P+e)\ , \tag{1}$$

where parentheses denote a bound state. We adopt the impact-parameter method and assume that the projectile moves along a straight-line trajectory with a constant velocity $\mathbf{v}$. The internuclear distance vector measured from the target nucleus $T$ is expressed as $\mathbf{R}=\mathbf{b}+\mathbf{v}t$, where $\mathbf{b}$ is the impact parameter. The total Hamiltonian is given by

$$H_0=-\frac{1}{2}\Delta-\frac{Z_P}{r_P}-\frac{Z_T}{r_T}+\frac{Z_PZ_T}{R}=H+\frac{Z_PZ_T}{R}\ , \tag{2}$$

where $\mathbf{r}_P$ and $\mathbf{r}_T$ are the electron positions referring to $P$ and $T$, respectively. Since $R$ is a function of $t$ only, the internuclear interaction $Z_PZ_T/R$ can be totally absorbed into a phase factor which represents the distortion to each channel wave function, $\phi_i$ and $\phi_f$. The transition amplitude is then written as

 

$$t_{fi}=-ib^{2i\nu}\int_{-\infty}^{\infty}\langle\phi_f|V_f|\Psi_i\rangle dt\ , \tag{3}$$

with $\nu=Z_TZ_P/v$. The total electronic wave functions $\Psi_i$ satisfies the Schrödinger equation

$$\left[H-i\frac{\partial}{\partial t}\right]\Psi_i(\mathbf{r}_T,t)=0\ , \tag{4}$$

with the initial condition $\Psi_i\rightarrow\phi_i$ as $t\rightarrow-\infty$. The initial and final channel wave functions, $\phi_i(\mathbf{r}_T,t)$ and $\phi_f(\mathbf{r}_P,t)$, are the traveling atomic orbitals that satisfy

$$\left[H_{i,f}-i\frac{\partial}{\partial t}\right]\phi_{i,f}=0 \tag{5}$$

where

$$H_i=H-V_i\quad\text{with }V_i=-Z_P/r_P\ , \tag{6}$$

and

$$H_f=H-V_f\quad\text{with }V_f=-Z_T/r_T\ . \tag{7}$$

Introducing a distortion potential $U_f(R)$ to cancel the Coulomb tail of $V_f$, $t_{fi}$ is rewritten as[12]

$$t_{fi}=-ib^{2i\nu}\int_{-\infty}^{\infty}\langle\chi_f|V_f-U_f|\Psi_i\rangle dt\ . \tag{8}$$

The distorted wave $\chi_f$ satisfies

$$\left[H_f+U_f-i\frac{\partial}{\partial t}\right]\chi_f=0\ , \tag{9}$$

with the condition $\chi_f\rightarrow\phi_f$ as $t\rightarrow\infty$. Note that $\chi_f$ together with the phase factor due to the internuclear interaction, that is a part of $b^{2i\nu}$, satisfies the correct Coulomb boundary conditions in the final channel. The distorted-wave Born approximation

$$t_{fi}^{\mathrm{DW}}=-ib^{2i\nu}\int_{-\infty}^{\infty}\langle\chi_f|V_f-U_f|\chi_i\rangle dt \tag{10}$$

is obtained by replacing $\Psi_i$ in Eq. (8) by the distorted wave $\chi_i$ defined by

$$\left[H_i+U_i-i\frac{\partial}{\partial t}\right]\chi_i=0\ , \tag{11}$$

with the condition $\chi_i\rightarrow\phi_i$ as $t\rightarrow-\infty$. If we choose $U_i$ to cancel the Coulomb tail of $V_i$, $\chi_i$ together with the part of $b^{2i\nu}$ satisfies the correct Coulomb boundary conditions in the initial channel. Among various possibilities, we examine the following two typical choices of $U_i(R)$ and $U_f(R)$:

$$U_i(R)=-\frac{Z_P}{R}\quad\text{with }U_f(R)=-\frac{Z_T}{R}\ , \tag{12a}$$

and

$$U_i(R)=\langle\phi_i|V_i|\phi_i\rangle\quad\text{with }U_f(R)=\langle\phi_f|V_f|\phi_f\rangle\ . \tag{12b}$$

We call the formula Eq. (10) using the potentials (12a) the B1B approximation,[8] and the formula using the potentials (12b) the DWBA.

On the other hand, in the OBK amplitude

$$t_{fi}^{\mathrm{OBK}}=-ib^{2i\nu}\int_{-\infty}^{\infty}\langle\phi_f|V_f|\phi_i\rangle dt\ , \tag{13}$$

the channel wave functions do not satisfy the Coulomb boundary conditions. The eikonal approximation takes account of the Coulomb boundary conditions in only one of the channels. The post-form eikonal amplitude is given by

$$t_{fi}^{\mathrm{eik}}=-ib^{2i\nu}\int_{-\infty}^{\infty}\langle\phi_f|V_f|\psi_i\rangle dt\ , \tag{14}$$

with

$$\psi_i=\phi_i\exp\left[-i\int_{-\infty}^{t}V_i dt'\right]\ , \tag{15}$$

and $V_i=-Z_P/r_P$. In order to make the interaction short ranged, we modify the final state similarly to Eq. (8),

$$t_{fi}^{\mathrm{BE}}=-ib^{2i\nu}\int_{-\infty}^{\infty}\langle\chi_f|V_f-U_f|\psi_i\rangle dt\ . \tag{16}$$

We call this formula the boundary-corrected eikonal approximation, in which the Coulomb boundary conditions are satisfied in both entrance and exit channels.

In the above text we have derived the approximate formulas for $t_{fi}$ after eliminating the internuclear interaction by introducing the phase factor $b^{2i\nu}$. We can also formulate similar approximation methods retaining the internuclear interaction as a part of $V_i$ and $V_f$. In the latter treatment, the B1B and the DWBA formulas are the same as Eq. (10). The internuclear interaction cancels completely in the interaction $V_f-U_f$, and its distortion in $\chi_i$ and $\chi_f$ is combined to give precisely the factor $b^{2i\nu}$.

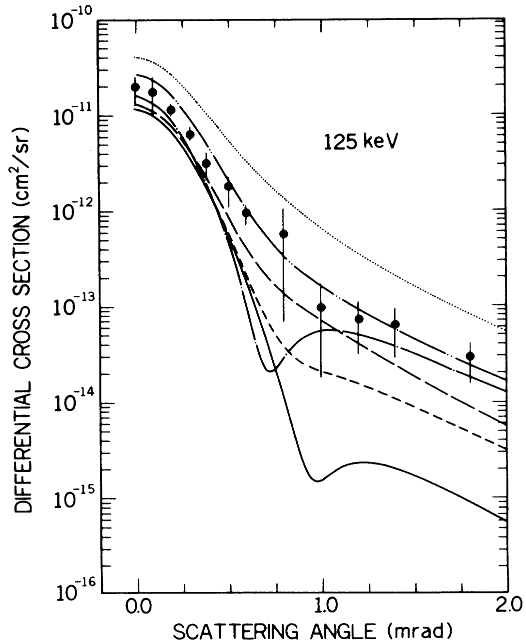


FIG. 1. Differential cross sections for $p+\mathrm{H}(1s)\rightarrow\mathrm{H}+p$ in center-of-mass scattering angle and a proton energy of 125 keV. Theoretical cross sections: dotted, OBK; dot-dashed, B1B; double-dot-dashed, DWBA; long dashed, eikonal; short dashed, DWBA eikonal; solid, B1B eikonal (see text). Experimental data are from Ref. 14.

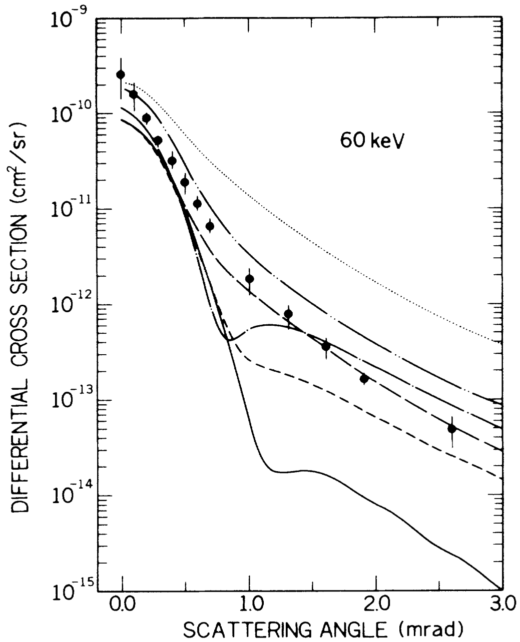


FIG. 2. The same as Fig. 1, but for 60 keV.

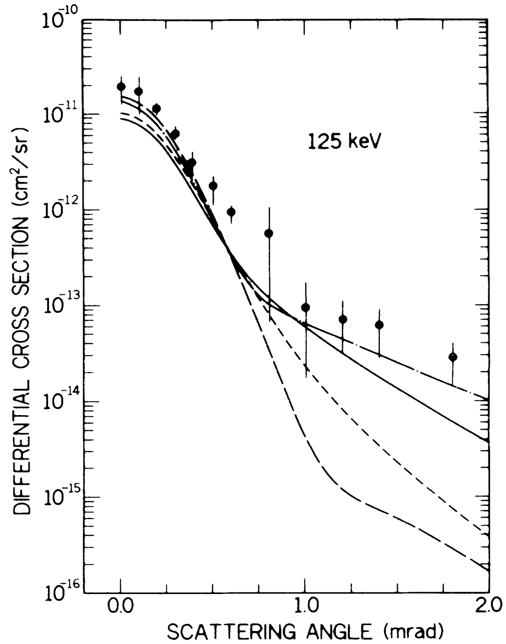


FIG. 3. The same for Fig. 1, but the phase factor $b^{2i\nu}$ is neglected (see text).

This is also true for the boundary-corrected eikonal approximation (16).

Dewangan[13] introduced the Glauber-eikonal approximation for the $p+\mathrm{H}$ system. He included the internuclear interaction explicitly in the eikonal approximation to eliminate an ill-defined phase factor in the transition amplitude, and discussed the high-energy behavior of the electron-capture cross sections. However, he did not develop a distorted-wave formalism for a general ion-ion collision. Our treatment coincides with his one for the $p+\mathrm{H}$ system.

The scattering amplitude at a scattering angle $\theta$ is calculated by a two-dimensional Fourier transform of a transition amplitude,

$$f(\theta)=\frac{\mu v}{2\pi}\int e^{i\mathbf{q}\cdot\mathbf{b}}t_{fi}(b)d^2b \ , \tag{17}$$

where $\mu$ is the reduced mass and $\mathbf{q}\cdot\mathbf{b}=2\mu v b\sin(\theta/2)$.

## III. RESULTS AND DISCUSSION

We have calculated differential cross sections for $p+\mathrm{H}(1s)\rightarrow\mathrm{H}+p$ using the approximate formulas defined in the preceding sections. The results are compared with experiments in Figs. 1 and 2. All the theoretical results are the sum over final states up to the principal quantum numbers $n=3$. The experimental cross sections[14] are the sum over all final bound states. The OBK cross sections are too large, as expected, but the scattering-angle dependence is reasonably good. We note that Eq. (13) is different from the usual definition of the OBK amplitude in which the phase factor $b^{2i\nu}$ is omitted. Without this phase factor the angular distribution of the OBK cross sections is quite different from the experimental data. It has no effect on the integrated cross sections but it plays a crucial role in the differential cross sections. Both the DWBA and the eikonal cross sections are in good agreement with experiments. The former is a little larger and the latter is a little smaller than the experimental data but their shapes are similar. The B1B cross sections have an undersirable dip around 0.9 mrad. Belkić *et al.*[15] reported that this dip becomes less prominent as we add more and more contributions of final highly excited states. However, they could not remove the dip completely by the summation.

As stated in Sec. II, the distortion potential is not unique in the boundary-corrected eikonal approximation (16). We adopt two types of distortion potentials, Eqs. (12a) and (12b). We call the former the B1B eikonal and the latter the DWBA eikonal approximation. These two boundary-corrected eikonal approximations show poorer agreement with experiments than the original eikonal approximation. The disagreement is serious for the B1B eikonal approximation at large scattering angles. The Coulomb boundary conditions are well defined only at asymptotic region. Nevertheless, it gives a marked effect to the large angle scatterings that are mainly determined by the inner part of the potential.

We attribute these disagreements to the lack of the phase factor $b^{2i\nu}$. Equation (10) apparently contains this factor but it is canceled completely by the phase factors contained in $\chi_i$ and $\chi_f$ in the B1B amplitude for the $p+\mathrm{H}$ system. This may be easily understood if we think of the fact that the B1B approximation coincides with the JS approximation for this system. Similarly, half of this factor is canceled by $\chi_f$ in the B1B eikonal amplitude. In order to confirm this conjecture we calculated cross sections disregarding the phase factor $b^{2i\nu}$. Figure 3 shows the results. All the cross sections are considerably modified, especially at large scattering angles. The dip of B1B cross sections has disappeared and the shape has become much better. The eikonal approximation shows the worst behavior. These results support our conjecture that this phase factor is the most important in the angular distribution. Since this factor is missing in the original B1B amplitude, as stated above, the neglect of this factor in Eq. (10) retrieves it as $b^{-2i\nu}$. The matrix elements of the B1B amplitude are real quantities, so that this factor gives the same effect as $b^{2i\nu}$. On the other hand, this phase factor is completely missing in the modified eikonal amplitude.

It is sometimes claimed that the dip in B1B cross sections is caused by the two-term interactions $V_f - U_f$. The fact that the dips in both the B1B and the B1B eikonal cross sections have disappeared by omitting the phase factor $b^{2i\nu}$ implies that the subtraction of the distortion potential from the interaction is not the only cause of the dip. This point is also confirmed by the fact that the DWBA differential cross sections are free from the dip though the transition operator is also composed of two terms.

The phase factor $b^{2i\nu}$ is the consquence of complete inclusion of the internuclear interaction. If it is modified by a Coulomb boundary condition, some portion of it is lost. Our results show that this factor should be fully included to explain experimental angular distributions.

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