Exact second Born electron capture for $p+\text{He}$

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Formulation and exact numerical calculation of differential and total 1s-1s electron-capture cross sections with the use of the second Born approximation with the free-wave Green's function are presented. At energies above 15 MeV there appears in the differential cross section a peak characteristic of a second Born or two-step process. For total cross sections, our calculations show that below 7 MeV the second-order cross section is larger than the first-order cross section, indicating a breakdown of second-order Born approximation with the free-wave Green's function. Results using the peaking approximation of Drisko converge to our exact second Born results only at energies well above 30 MeV. According to our exact second-Born calculations, observation of the angular distribution above 15 MeV should reveal structure related to at least one two-step mechanism for electron capture.

I. INTRODUCTION

Electron capture has the interesting feature that, at asymptotically high velocities, the second term in the Born series dominates over all other orders. This is borne out[1,2] by the total capture cross section which decreases as v^{-11} in the second order, but decreases as v^{-12} in the first order. Consequently, understanding of electron capture is related directly to an understanding of the second Born approximation.

As is well known,[1] at very high velocities the second Born approximation is a quantum description of a simple two-step process suggested[3] long ago by Thomas. In the first step of the classical Thomas model the projectile scatters the electron by 60° with a speed equal to the speed of the projectile. In the second step the electron is elastically rescattered by the target nucleus so that it travels along with the projectile. The connection of this simple classical model with the quantum-mechanical second Born approximation is described[1,4] in the literature.

Over the past several years, a number of useful second Born calculations using peaking approximations, valid for very high projectile velocities, have been published[5-7] as well as calculations[8-11] based on approximations related to the second Born approximation and numerical second Born calculations[9,12,13] (for $p+\text{H}$) at energies below a few MeV.

Recently, exact numerical second Born calculations at velocities above a few MeV/amu have been briefly reported[14] for 1s-1s transfer in $p+\text{H}$. These calculations yielded two major results: (1) It was found that, below 3 MeV, the second-order Born cross section is greater than the first-order cross section, which, in turn, is greater than the measured cross section at those energies where measurements exist. This indicates that the second-order Born approximation is not adequate in describing cross sections below 3 MeV for $p+\text{H}$ and that higher-order terms have to be included. (2) Above 5 MeV there appears in the differential cross section a peak at an angle of 0.054° in the center-of-mass (c.m.) system. This is the recoil angle of a proton scattering an electron into 60° and thereby is related to the first step of the Thomas two-step model.

This paper is an extension of earlier $p+\text{H}$ work to $p+\text{He}$, and also contains the basic formulation of exact second Born calculations not included in the previous paper.[14] Here, features of exact numerical second Born calculations for $p+\text{He}$ are presented and compared to results based on peaking approximations.[2,5-7] It is also illustrated and emphasized that, at high velocities, differential cross sections are more sensitive to the influence of second Born effects than total cross sections for 1s-1s electron capture, and that observing the differential cross section could provide an interesting experimental test of second Born effects.

II. FORMULATION

The differential cross section in the second Born approximation, proportional to the square of the sum of first- and second-order matrix elements, is given by

$$\frac{d\sigma}{d\Omega}=\frac{\mu_i\mu_f}{4\pi^3}\frac{k_f}{k_i}\,|\,T_{\rm if}^{\rm I}+T_{\rm if}^{\rm II}\,|^2\,, \tag{1}$$

where

$$T_{\rm if}^{\rm I}=\langle\phi_f\,|\,V_f\,|\,\phi_i\rangle \tag{2a}$$

and

$$T_{\rm if}^{\rm II}=\langle\phi_f\,|\,V_fG^+V_i\,|\,\phi_i\rangle\ . \tag{2b}$$

Here, ϕ_i and ϕ_f are the initial and final unperturbed states, V_i and V_f the initial and final potentials, μ_i and μ_f the initial and final reduced masses, k_i and k_f the initial and final momenta, and G^+ a Green's-function operator.

In this work, the potential V_i (or V_f) is taken to be the Coulomb interaction, $V_{\rm BK}$, between the active electron and the projectile (or target) nucleus, and G^+ is taken to be the free-wave Green's function G_0^+. Other choices for V and G are possible,[15,16] and the choice could be significant at intermediate velocities. However, the leading-order second Born term at very high velocities, i.e., the v^{-11} term, is independent of the choice of V and G. Since $V_{\rm BK}$ is sometimes called the Brinkman-Kramers (BK) potential, we refer to our second- (first-) order calculation as a second- (first-) order BK calculation.

The algebraic reduction[2,14,17] of Eq. (1) yields

$$T_{\rm if}^{\rm I}=\frac{-2^5\pi(abZ_1Z_2)^{5/2}}{b\,(a^2Z_1^2+p^2)^2(b^2Z_2^2+q^2)} \tag{3a}$$

and

$$T_{\rm if}^{\rm II}=\frac{-2^5(abZ_1Z_2)^{7/2}}{b\pi^3}\int\frac{d\vec{\rm P}}{P^2(b^2Z_2^2+|\,\vec{\rm P}-\vec{\rm q}\,|^2)^2}\int\frac{d\vec{\rm Q}}{Q^2(a^2Z_1^2+|\,\vec{\rm Q}+\vec{\rm p}\,|^2)^2(\,|\,\vec{\rm Q}+\vec{\rm V}_1\,|^2+D^2)}\,, \tag{3b}$$

where Z_1 (Z_2) is the projectile (target) charge and with $\epsilon\to0+$,

$$\vec{\rm q}=b\vec{\rm k}_i-\vec{\rm k}_f,\quad a=\frac{M_1}{M_1+1},\quad \vec{\rm p}=a\vec{\rm k}_f-\vec{\rm k}_i,\quad b=\frac{M_2}{M_2+1}\,,$$
$$D^2=\frac{a}{b}(\vec{\rm P}-\vec{\rm q})^2-(a\vec{\rm P}+\vec{\rm p})^2+abZ_2^2-2ai\epsilon,\quad \vec{\rm V}_1=a\vec{\rm P}+\vec{\rm p}\ . \tag{4}$$

This corresponds to Eq. (8.4.18) in McDowell and Coleman.[17] It may be easily shown[18] at this point that Eqs. (3a) and (3b) are each invariant if $(Z_1,\vec{\rm P},-\vec{\rm q})$ are interchanged with $(Z_2,\vec{\rm Q},\vec{\rm p})$. This corresponds to detailed balancing or time-reversal invariance.

The integral over $\vec{\rm Q}$ in Eq. (3b) is not directly available in the current literature. It may be evaluated in closed form using the integral of Lewis.[19] The result for 1s-1s transfer is

$$T_{\rm if}^{\rm II}=\frac{2^4(abZ_1Z_2)^{5/2}Z_2}{a\pi}\times\int\frac{d\vec{\rm P}}{P^2(b^2Z_2^2+|\,\vec{\rm P}-\vec{\rm q}\,|^2)^2}\times\left[\frac{2\alpha\gamma\dfrac{d\beta}{dZ_1}-\beta\dfrac{d(\alpha\gamma)}{dZ_1}}{(\beta^2-\alpha\gamma)\alpha\gamma}+\left[\frac{\dfrac{1}{2}\dfrac{d(\alpha\gamma)}{2Z_1}-\beta\dfrac{d\beta}{dZ_1}}{(\beta^2-\alpha\gamma)^{3/2}}\right]\{\ln[\beta+(\beta^2-\alpha\gamma)^{1/2}]-\ln[\beta-(\beta^2-\alpha\gamma)^{1/2}]\}\right] \tag{5a}$$

with the restriction that

$$-\pi<\arg[\beta\pm(\beta^2-\alpha\gamma)^{1/2}]\le\pi\,,$$

where

$$\alpha\gamma=[aP^2+(aZ_1+D)^2]\times(P^2+aZ_1^2)\left[\frac{a}{b}(\vec{\rm P}-\vec{\rm q})^2+abZ_2^2\right],$$

$$D=(D^2)^{1/2}=\left[\frac{a}{b}(\vec{\rm P}-\vec{\rm q})^2-(a\vec{\rm P}+\vec{\rm p})^2+abZ_2^2-2ai\epsilon\right]^{1/2}, \tag{5b}$$

$$\beta=D(p^2+a^2Z_1^2)+\frac{a^2}{b}Z_1(\vec{\rm P}-\vec{\rm q})^2+a^2bZ_1Z_2^2\ .$$

It is noted that the sign of Re(D) is the same as the sign of ϵ.

The results presented in this paper and in our previous paper[14] were obtained through the use of Eqs. (5a) and (3a) in Eq. (1). The second-order BK amplitude, Eq. (5a), was evaluated by integrating numerically. The integrand was carefully studied and integration intervals were chosen appropriate to the mathematical behavior of the integrand. Adopting the notation $\vec{P}=(P,\theta_p,\phi_p)$, the P integration was done first using 25 intervals. Eight-point Gauss-Legendre integration was used over each interval. The integrand was somewhat smoother after the first integration. The θ_p integration was done with 11 intervals with eight-point Gauss-Legendre integration used for each interval. The integrand was then even smoother. The ϕ_p integration was down with three intervals using eight-point Gauss-Legendre integration for each interval. One numerical check was to use sixteen- (rather than eight-) point Gauss-Legendre integration throughout, shifting the mesh as well as doubling the number of mesh points in each dimension. The numerical results were invariant at all angles through four digits.

III. RESULTS

Calculations for 1s-1s capture have been performed for protons incident on atomic helium at projectile energies between 0.1 and 500 MeV. In this section we consider in detail both total and differential cross sections. It is assumed that the helium wave functions are approximately hydrogenic with the effective charge $Z_2^*=1.6875$ and the binding energy $\frac{1}{2}Z_2^{*2}$ (in a.u.).

Total cross sections are presented in Fig. 1. Above the proton laboratory energy of 8 MeV, the second-order BK cross section is smaller than the first-order BK cross section. At energies between 8 and 0.1 MeV, our calculations for second-order BK cross sections give results larger than the first-order BK cross sections. Since the first-order BK cross sections lie above observed results, we conclude that terms of higher order in the BK expansion are required to bring theory into agreement with observation. Only at very high velocities, i.e., above 200 MeV, does the v^{-11} second-order contribution dominate over the v^{-12} contribution. This is evident from the asymptotic velocity formula[2] of Drisko (to which our results reduce well above 200 MeV), namely,

$$\sigma_{\mathrm{BK}\,2}=\sigma_{\mathrm{BK}\,1}\left[0.2946+\frac{5\pi v}{2^{11}(Z_1+Z_2)}\right],$$

where, at asymptotic velocities, $\sigma_{\mathrm{BK}\,1}$ varies as v^{-12}. The asymptotic Drisko formula is also plotted in Fig. 1. In the energy region shown, below 30 MeV, the differences between the asymptotic Drisko formula and the exact numerical calculations are comparable to differences between first- and second-order BK calculations. At higher energies (above 200 MeV) relativistic effects[20] become important, leading, for example, to a v^{-2} dependence for the first-order BK cross section. At lower energies (below 5 MeV), the first-order BK cross sections are closer to the exact results than the asymptotic Drisko formula (which is an approximation to the second-order BK cross section). Hence, the agreement[21] between cross sections derived from the asymptotic Drisko formula and experimental data at intermediate velocities cannot be explained solely on the basis of the second-order BK approximation.

Also plotted in Fig. 1 are un-normalized lines proportional to v^{-11} and v^{-12}. In the energy region shown, most cross sections plotted are closer to a v^{-12} than a v^{-11} dependence. Since relativistic effects are important above 200 MeV, we conclude that studying the velocity dependence of total cross sections for 1s-1s electron capture in $p+\mathrm{He}$ is not a useful method to study second Born effects. We find no reason for this conclusion to change for systems with different projectile or target charges. Studies of total cross sections of systems with exchange between high Rydberg states[22] could, however, be different since the velocity scale shifts to lower velocities.

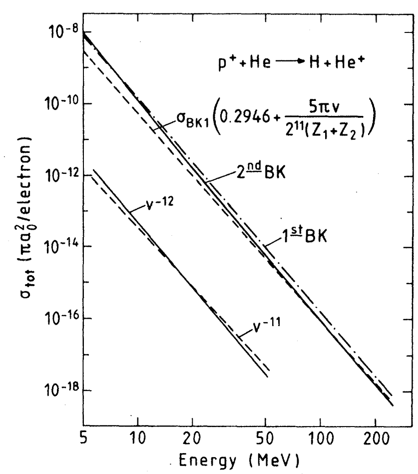

FIG. 1. Total 1s-1s electron-capture cross section vs proton laboratory energy for $p+\mathrm{He}$. Drisko asymptotic form, second-order BK, and first-order BK are in units of πa_0^2/electron. Cross section per atom is twice as large. v^{-12} and v^{-11} curves are unnormalized.

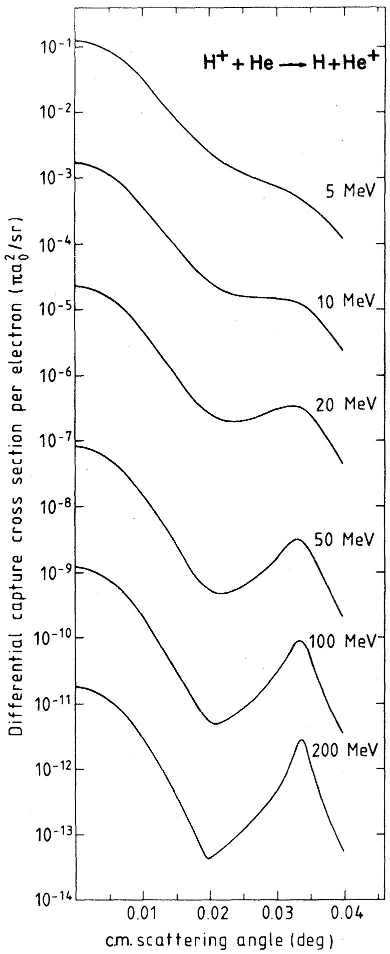

FIG. 2. Differential 1*s*-1*s* electron-capture cross sections vs scattering angle in degrees in the center of mass for $p+$He at various laboratory energies in units of πa_0^2 per electron per sr.

Differential cross sections at energies ranging from 5 to 200 MeV are shown in Fig. 2. Above 10 MeV a peak in the differential cross section appears. This peak is due to structure in the Green's function G in Eq. (2b) occurring at a center-of-mass scattering angle of 0.0338 deg. This is the recoil angle of a proton scattering an electron into 60° (in the laboratory frame), and corresponding to the first step in the two-step model of Thomas. Since this peak is superimposed on a differential cross section which is rapidly decreasing with increasing angle, the peak shifts a little toward smaller angles at lower velocities, where the second Born "two-step" peak is smaller. The peak disappears below 10 MeV for $p+$ He as compared to about 5 MeV for $p+$ H.

Effects of Coulomb deflection by the nuclei are not included in the results shown. Coulomb deflection is important at large scattering angles. Calculations with and without Coulomb deflection were done in the first-order BK approximation. The Coulomb deflection was less than a 30% effect at c.m. angles less than 0.037° at 50 MeV, 0.030° at 20 MeV, and 0.025° at 5 MeV. Thus, for projectile energies above 20 MeV, we do not expect Coulomb deflection to dominate the second Born peak.

Relativistic effects have also been omitted in the present results. Moisiewitsch and Stockman[20] have shown that for $p+$ H, relativistic effects increase the first-order BK cross sections by 40% at $\theta=0°$ at 100 MeV, and decrease monotonically as θ increases, contributing 20% to the total cross section. At 10 MeV, there is a 3% effect on the total cross section. This is consistent with the relativistic impulse approximation of Jakubassa-Amundsen and Amundsen.[23] Since relativistic effects depend primarily on the velocity of the projectile, these results are expected to apply as an estimate to $p+$ He.

Differential cross sections were also evaluated in the high-velocity peaking approximation.[2,5,6,17] The results of this peaking approximation (not shown) are in qualitative agreement with the numerical results shown in Fig. 2. That is, the structure, magnitude, and energy dependence of the second Born peak at high velocities, as shown in Fig. 2, is reasonably well reproduced by the Drisko peaking approximation. However, the magnitude of the forward angle scattering cross sections, which are dominant below 10 MeV, are not so well reproduced. To test the range of the validity of the peaking approximation (designed for use at high velocities) calculations were performed at energies below 10 MeV. At 1 MeV, the peaking approximation cross sections are about 5 times smaller than the exact results, while at 0.1 MeV, the peaking approximation is roughly 4 times larger than exact second-order BK results, which, in turn, lie a factor of about 3 above first-order BK cross sections. By comparison, for $p+$ H at 25 keV the peaking approximation second-order BK cross sections are more than an order of magnitude greater than exact results. We conclude that, in these cases at least, the peaking approximation introduced[2] by Drisko is valid only at very high velocities.

In Table I, a sample of numerical values for second-order BK cross sections is given. Total cross sections at each energy were evaluated using a total of 24 differential cross sections with the angular intervals chosen to optimize the integration accuracy. In the regions where our second Born cross sections are meaningful, i.e., above 10 MeV, the electron-transfer cross sections are very small, i.e., smaller than $10^{-9}\pi a_0^2$. At intermediate velocities,

TABLE I. Differential and total cross sections in the second-order Brinkman-Kramers approximation for $p+\mathrm{He}$.

c.m. angle (degrees $\times 10^2$)	c.m. differential cross sections[a] (πa_0^2/sr-electron) Laboratory energy (MeV) 100	50	20	10	1
0.0347	1.21(−9)[b]	8.28(−8)	2.32(−5)	1.70(−3)	1.78(+3)
0.335	9.83(−10)	6.78(−8)	1.92(−5)	1.42(−3)	1.55(+3)
0.706	4.97(−10)	3.50(−8)	1.02(−5)	7.81(−4)	9.90(+2)
1.08	1.65(−10)	1.21(−8)	3.84(−6)	3.14(−4)	4.95(+2)
1.58	2.25(−11)	1.99(−9)	8.00(−7)	7.60(−5)	1.62(+2)
2.05	4.86(−12)	5.20(−10)	2.46(−7)	2.51(−5)	5.49(+1)
2.40	6.95(−12)	5.52(−10)	1.93(−7)	1.65(−5)	2.49(+1)
3.05	3.20(−11)	1.75(−9)	3.12(−7)	1.51(−5)	6.62(0)
3.27	7.39(−11)	2.86(−9)	3.49(−7)	1.37(−5)	4.33(0)
3.35	8.75(−11)	2.97(−9)	3.31(−7)	1.25(−5)	3.67(0)
3.40	8.28(−11)	2.80(−9)	3.10(−7)	1.16(−5)	3.33(0)
3.59	2.94(−11)	1.36(−9)	1.92(−7)	7.86(−6)	2.28(0)
3.93	4.57(−12)	2.76(−10)	5.73(−8)	3.00(−6)	1.16(0)
Total cross sections (πa_0^2/electron)	9.76(−17)	6.25(−15)	1.72(−12)	1.30(−10)	1.74(−4)

[a]Hydrogenic wave functions with $Z_2^*=1.6875$ and $\frac{1}{2}Z_2^{*2}$ (a.u.) for the binding energy were used.
[b]The numbers in parentheses are the exponents of ten.

e.g., 0.1 MeV, where electron transfer can be a dominant collision mechanism, the cross sections are about πa_0^2. With this in mind, we point out that detailed knowledge of our second Born cross sections above 10 MeV for $p+\mathrm{He}$ does not give complete information about electron capture at intermediate velocities, where the Born series (using V_{BK} and G_0) appears not to converge rapidly (cf. earlier discussion of Fig. 1).

Calculations were done to verify the property of detailed balancing by checking to see if the cross sections for $p+\mathrm{He}^+$ were equal, at the same velocity, as those for $\mathrm{H}+\mathrm{He}^{2+}$, i.e., the inverse reaction. These two sets of differential cross sections were found to be identical within numerical accuracy. This provided a useful numerical check on our calculations.

IV. DISCUSSION

One motivation for calculating cross sections for $p+\mathrm{He}$ is that an experiment for $p+\mathrm{He}$ may be performed more easily than for $p+\mathrm{H}$ since helium is more readily available than atomic hydrogen. Since, at high velocity, the cross sections are proportional to Z_2^5, it was also hoped that counting rates for differential measurements would be higher for $p+\mathrm{He}$. However, since the second Born peak does not clearly appear until the proton energy is above 15 MeV in He (compared to about 7 MeV in H), what is gained in counting rates in the Z_2^5 dependence is lost in the E^{-6} dependence.

Another consideration of experimental interest is the size of the radiative electron-capture (REC) cross sections relative to (nonradiative, or direct) electron capture, i.e., the process primarily considered in this paper. Evaluation of nonrelativistic REC total cross sections has been presented by Kleber and Jakubassa[24] and by Briggs and Dettmann.[25] At very high collision velocities, REC is practically the same as radiative recombination.[26] A simple expression for REC total cross sections at very high velocities ($v \gg Z_1$) may be easily found from Eq. (2) of Kleber and Jakubassa, namely,

$$\sigma_{\mathrm{REC}}=1.63Z_1^5E^{-5/2}\times10^{-9}(\pi a_0^2)\ ,$$

where E is the projectile energy in MeV/amu, and Z_1 is the projectile charge. Above about 20 MeV, the REC total cross section is larger than the direct-capture cross section for $p+\mathrm{He}$.

It is also of interest to know the angular distribution for the REC cross sections. This angular distribution depends on the momentum transferred to the projectile by the emitted photon, the electron, and the target nucleus. To our knowledge, no detailed calculation of such an REC differential cross section exists. A simple classical estimate[1] of the maximum deflection angle of the projectile recoiling from the electron and the photon indicates that REC scattering is confined to forward scattering angles smaller than the angle of the second Born peak for $p+\mathrm{He}$ in the energy region shown in our figures. However, recoil from the target nucleus (Coulomb deflection) and quantum effects could spread the distributions to larger angles, in our opinion. Nevertheless, we find nothing to suggest any structure (e.g., a peak) in the REC differential scattering cross sections. In any case, results from a detailed calculation would be useful.

A second peak, not included in our calculations, at a center-of-mass angle of 0.044° may also be observable in helium. As Shakeshaft and Spruch originally observed,[27] this peak corresponds to a rescattering of the captured electron by the second target electron in the second step of the Thomas model. Briggs and Taulbjerg[28] have given an expression for the total cross section at very high velocities, namely,

$$\sigma_{ee}=2^4\pi^2 Z_1^5 Z_2^3 v^{-11}(Z_1+\sqrt{2}Z_2)^{-1} .$$

This may be compared to the total cross section under the Thomas peak considered in this paper due to rescattering of the captured electron by the target nucleus, namely,

$$\sigma_{eN}=2^7\pi^2 Z_1^5 Z_2^5 v^{-11}(Z_1+Z_2)^{-1} .$$

The electron-electron cross section is smaller than the electron-nucleus cross section by a factor of slightly more than $8Z_2^2$. For a helium target the electron-electron cross section is, thus, about 40 times smaller than the electron-nucleus cross section, and the electron-electron peak appears at a larger scattering angle, where effects due to internuclear deflection may also interfere. Hence, in helium at high velocities, some interesting, albeit small, structure may be evident in the differential cross section between the major Thomas peak at 0.034° c.m. and 0.044° c.m., where rescattering due to the second target electron is possibly observable.

V. SUMMARY

In conclusion we point out that differential cross sections for $1s$-$1s$ electron capture are more sensitive to second Born effects between 5 and 200 MeV than total cross sections. These cross sections are, however, small. Nevertheless, studies of electron-capture cross sections at very high velocities may lead to insight into a relatively unexplored area of the three-body problem where second Born effects play a clear and important role.

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