Differential cross sections for electron capture in fast proton–multielectron-atom collisions

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Differential cross sections for electron capture in fast-proton–multielectron-atom collisions are obtained by using the eikonal approximation for the internuclear interaction and the two-state, two-center atomic-expansion method for the electron-capture amplitude in the impact-parameter formulation. The importance of the internuclear potential and the various approximations for the electron-capture probability for the differential cross section is examined. It is found that when the projectile deflection is included, the two-state, two-center atomic-expansion method can predict differential cross sections with good agreement with experimental data of Cocke *et al.* and of Bratton *et al.*

I. INTRODUCTION

Differential cross sections for electron capture in ion-atom collisions often exhibit detailed information not evident in the integrated total cross sections and are very valuable to our understanding of Coulombic rearrangement collisions. Such data also can serve as a severe test of various theoretical models for charge transfer. Unfortunately, for fast incident ions, the angular distributions are peaked in the forward direction and there are very few experimental data available.[1,2]

In the last few years, the theoretical studies of electron capture in *fast* ion-atom collisions, particularly the capture of K-shell electrons by fast protons, are almost all based upon the first-order plane-wave Born approximation.[3-6] Because of the nonorthogonality of initial- and final-state wave functions, there are many versions of first-Born theories for charge transfer. However, most of these theories are known to predict *total* capture cross sections a few times to a few orders of magnitude too high.

Among the first-order Born theories, the well-known Oppenheimer, Brinkman, and Kramers (OBK) approximation[7] is known to predict K-shell electron-capture cross sections about a factor of 3 too high for fast protons on heavy target atoms. The straightforward generalization[5,6] of the Jackson-Schiff[8] approach, in which the internuclear interaction between two bare nuclei is also included in the first-Born transition amplitude (to be called the full Born theory), has been shown to predict electron-capture cross sections a few orders of magnitude too high when compared with experimental data. Both theories are incapable of predicting total capture cross sections to within a factor of 2 or better and cannot be accepted as reliable *ab initio* theories for electron capture at high velocities.

A modified first-Born theory proposed by Omidvar *et al.*[4] [Born (C)] and by Halpern[9] indicated that the total capture cross sections in fast ion-atom collisions can be predicted to within a factor of 2 in the high-velocity region. The theory is also a generalization of the Jackson-Schiff approach except that the internuclear potential in the first-Born transition amplitude is assumed to be between the projectile and an almost completely screened target atom. The target nucleus, in this model, is assumed to be completely screened by all the electrons except the active one which is to be captured. Like the full Born theory, the Born (C) theory also reduces to the approximation of Jackson and Schiff if the target atom is hydrogen. The results of Born (C) calculations indicate that the *total* cross sections are *adequately* predicted by the theory. Unfortunately, the foundation of the Born (C) theory, that the target nucleus is almost completely screened by the other electrons, obviously cannot be accepted on physical grounds, particularly when the capture is from the K shell of the target. One would expect that the capture in this case occurs near the K-shell radius of the target atom where the outer electrons do not completely screen the target nucleus.

One interesting result of the Born (C) theory is the prediction of a dip structure in the angular distribution for electron capture. However, this structure was not confirmed in the earlier data of Cocke *et al.*[1] where the K-shell capture angular cross sections of 6-MeV protons on Ar atoms were measured, nor in the more recent data of Bratton *et al.*[2] where the angular distributions for electron capture of 293-keV protons on He atoms were measured. Thus, the Born(C) approximation, though capable of predicting total capture cross sections to better than a factor of 2 in certain energy regions, is unsound and its prediction of angular distribution is in disagreement with existing experimental data.

Not all first-order Born theories predict a dip in the angular distribution for electron capture. For example, both the OBK[4] and the full Born approximation[5] mentioned above for protons on Ar atoms do not predict such a dip. Since both theories do not predict total cross sections correctly, the meaningfulness of applying these two theories to differential cross sections is limited. By normalizing the total OBK cross sections to experimental results, it was found that the angular distributions predicted by the OBK theory fall off too rapidly at large angles when compared with experimental data of Cocke *et al.* This large-angle behavior is "corrected" in the CBK method of Belkić and Salin[10] by introducing the Coulomb-deflection effect of the projectile due to the Coulombic interactions between the projectile and the target nucleus. Rogers and McGuire,[11] on the other hand, in their SBK model, proposed that the deflection is better described by the interaction of the projectile with a static potential of the target. Both methods yield the same total capture cross section as the OBK theory but the shape of the angular distribution is superior to the OBK prediction when compared with data in Refs. 1 and 2.

Thus, we conclude that the first-order Born theories described in the previous paragraphs are inadequate for describing electron capture for fast ion-atom collisions. A desirable theory should be capable of predicting accurate total and differential capture cross sections.

In a recent article,[12] one of us showed that the *total K-K* capture cross sections for fast ion-atom collisions can be predicted by the two-state atomic-expansion method of Bates if the projectile velocity is camparable to the orbital velocity of the target K-shell electrons. It was shown, in another article[13] (henceforth called I), that in the limit of small capture probability, the two-state atomic-expansion method can be reduced to various first-Born theories if further (as yet unjustified) approximations are made. In this paper, we will discuss the differential cross sections predicted by the method of I.

The theory in I is formulated in the impact-parameter approximation and will be briefly reviewed in Sec. II. In order to discuss the angular distributions within the impact-parameter approximation, we have to apply an eikonal theory for the motion of the projectile. This is done in Sec. III. The results of our calculations are compared with the experimental data in Sec. IV. In Sec. V, we study the impact-parameter dependence of the capture probability $P(\rho)$ for p-H at 120 keV and p-He at 293 keV in the OBK, Born(C), and the two-state atomic-expansion approximations. It is shown that the shape of $P(\rho)$ predicted by the Born(C) (and the Jackson-Schiff) theory is very different from the other two theories. The normalized OBK capture probabilities, surprisingly, are very similar to the shape predicted by the two-state atomic expansion method. This similarity explains why the CBK and SBK theories of Refs. 10 and 11 are capable of predicting the shape of the differential cross sections.

II. TWO-STATE ATOMIC-EXPANSION METHOD FOR ELECTRON CAPTURE

The method is discussed in detail in I. We employ the independent-electron model in which only the electron to be captured is considered. This active electron is solved in a time-dependent potential of the nuclear field of the projectile with charge Z_B and of the target with charge Z_A. By expanding the time-dependent electronic wave function in terms of traveling eigenfunctions of the target and of the projectile and including only initial- and final-state wave functions, a set of coupled first-order differential equations for the scattering amplitudes (the elastic and capture amplitudes) are obtained. In this paper, we will limit ourselves to the situation in which the capture probability is small. The following conclusions from I are useful:

(i) If the distortion of the target electron by the projectile is neglected, the electron-capture amplitude $b(\rho)$ at each impact parameter ρ and each energy E obtained from the two-state, two-center atomic-expansion method is equivalent to the usual first-Born transition amplitude *if* the final wave function $|f\rangle$ is orthonormalized to the initial wave function $|i\rangle$. That is, replacing $|f\rangle$ by $|f^N\rangle$, where

$$|f^N\rangle = \frac{|f\rangle - |i\rangle\langle i|f\rangle}{1-|\langle i|f\rangle|^2}\,, \tag{1}$$

the transition amplitude becomes

$$b(\rho) = \int_{-\infty}^{\infty} \frac{\langle i|V|f\rangle - \langle i|f\rangle\langle i|V|i\rangle}{1-|\langle i|f\rangle|^2}\, e^{-i\omega t}\,dt\,,$$

$$= \int_{-\infty}^{\infty} \frac{\langle i|\, V - \langle i|V|i\rangle |f\rangle}{1-|\langle i|f\rangle|^2}\, e^{-i\omega t}\,dt\,, \tag{2}$$

where ω is the energy defect between initial and final states and appropriate translational factors are understood to be included in the definition of $|i\rangle$ and $|f\rangle$.[13]

(ii) If $|\langle i|f\rangle|^2$ is neglected in (2), $b(\rho)$ becomes equivalent to the wave version of the *distorted-wave approximation* of Bassal and Gerjuoy,[14] even though the "extra term" $\langle i|V|i\rangle$ in (2) in our derivation originates from the consideration of nonorthogonality of initial- and final-state wave functions.

(iii) If the $\langle i|V|i\rangle$ term is also dropped from (2), we obtain the impact-parameter version of the OBK[7] approximation.

(iv) For K-K electron capture, $\langle i|V|i\rangle$ as given in Eq. (15) of I is

$$\langle i|V|i\rangle = \frac{Z_B}{R}\left[1-(1+Z_A R)e^{-2Z_A R}\right], \tag{3}$$

where R is the internuclear separation. For large $Z_A R$, $\langle i|V|i\rangle \approx Z_B/R$. For small $Z_A R$, $\langle i|V|i\rangle \approx 0$. Thus, if we approximate $\langle i|V|i\rangle$ by its small-$Z_A R$ limit, we obtain the equivalent OBK approximation in the impact-parameter approach. If we approximate $\langle i|V|i\rangle$ by its large-$Z_A R$ limit, then we have the equivalent Born(C) approximation.[4] However, this equivalence has a different physical interpretation. The Born(C) "potential" in our approach originates from the incomplete treatment of nonorthogonality of initial- and final-state wave functions, rather than the almost complete screening of the target nucleus by the passive electrons during the capture, as given in Refs. 4 and 9. Approximating $\langle i|V|i\rangle$ by Z_B/R will be adequate for the total capture cross section if the capture for a given incident energy E comes primarily from impact parameters greater than the K-shell radius. However, it is obvious that $\langle i|V|i\rangle$ cannot be approximated by Z_B/R for small $Z_A R$. Thus, we expect the Born(C) prediction for $b(\rho)$ will be different from (2) for small impact parameters or for large angles.

The full Born approximation[5] mentioned in Sec. I corresponds to replacing $\langle i|V|i\rangle$ by $Z_A Z_B/R$. This "approximation" obviously is invalid if the target nuclear charge Z_A is not equal to 1. This explains the failure of the full Born theory in predicting total-capture cross sections.[5,6]

The two-state atomic-expansion method outlined in I has been applied to obtain total electron capture cross sections for ion-atom collisions in Ref. 13. In the small-capture-probability limit, the total cross sections for the capture from the K-shell of C, N, O, Ne, and Ar atoms are given in I and the results are shown to agree well with experimental data. To see whether the theory is also adequate for differential cross sections, we have to compare our calculations with the experimental data of Refs. 1 and 2.

III. DIFFERENTIAL CROSS SECTIONS

The two-state atomic-expansion method discussed in I as summarized in Sec. II is formulated in the impact-parameter approximation in which it is assumed that the projectiles follow classical trajectories throughout the collision. Such a procedure is valid insofar as the total cross section is concerned, as has been established by various authors.[15] However, the impact-parameter treatment is unsatisfactory for the calculation of angular distributions, particularly since, in practice, most impact-parameter calculations assume straight-line trajectories and it therefore is paradoxical even to define a differential cross section.

In principle, it is possible to formulate the heavy-particle rearrangement collisions also in the quantal approach.[16] On the other hand, one would like to have the simplification introduced by the impact-parameter approximation. It is desirable to have a theory of differential cross sections for heavy-particle collisions which gives differential cross sections identical to the quantal treatment to first order in the ratio of the electron mass to the mass of the heavy nuclei, since this is the limit where the impact-parameter approximation is expected to be valid. This is achieved by employing the eikonal approximation. This approximation has been formulated by Schiff,[17(a)] Glauber,[17(b)] and others[18] from the partial-wave analysis in which they replace the summation over partial waves by an integral, and the Legendre polynomials by their asymptotic form. It also has been formulated by McCarroll and Salin[19] and others,[20] in the context of atomic collisions, by deriving the desired equation from the full quantal formalism in which all quantities are replaced by their limits as the masses of the atomic nuclei become infinite. Their result for the differential cross section for transition from K shell to K shell in the center-of-mass system is given by

$$\frac{d\sigma}{d\Omega} = \left| i\mu v \int_0^\infty \rho^{1+2i\nu} J_0(\eta\rho) b(\rho)\, d\rho \right| (a_0^2 s_r^{-1}), \tag{4}$$

where μ is the reduced mass, v is the velocity of the projectile, J_0 is the zeroth Bessel function, and $b(\rho)$ is the direct or rearrangement transition amplitude calculated from the impact-parameter approximation. In (4), $\eta = 2\mu v \sin\frac{1}{2}\theta$ and ν is the eikonal phase obtained from treating the nuclear motions semiclassically.

Equation (4) has been applied to calculate the differential cross sections for low-energy ion-atom collisions by Salin and co-workers,[21] where $b(\rho)$ is obtained from the molecular calculation. It has been shown that the differential cross sections for the fundamental proton-hydrogen system[22] are well predicted by Eq. (4). More recent experimental data[23] also confirm the validity of this approach. For ion-atom collisions at higher energies, Eq. (4) has been applied by Belkić and Salin[10] and by Rogers and McGuire[11] to the electron-capture differential cross sections by 6-MeV protons on Ar atoms and by 293-keV protons on He atoms, respectively. Both calculations use the OBK transition amplitude for $b(\rho)$, which is known analytically.

The results of their calculations indicate that improved agreement with experimental data can be achieved by the proper treatment of the projectile motion. In our calculations to be presented in Sec. IV, we will use Eq. (4) but using $b(\rho)$ obtained from the two-state atomic-expansion calculation.

The differential cross sections have also been obtained by treating the projectile's motion *classically*. By assuming Coulomb repulsion between the projectile and the target nucleus, the scattering angle θ and the impact parameter ρ are related by

$$\rho=\frac{13.6}{1000}\frac{Z_A Z_B}{E(\text{keV})}\cot\tfrac{1}{2}\theta=A\cot\tfrac{1}{2}\theta\,, \tag{5}$$

where the last equality defines A. By equating the total inelastic cross sections,

$$\sigma=2\pi\int_0^\infty \rho P(\rho)\,d\rho=\int\frac{d\sigma}{d\Omega}\,d\Omega\,, \tag{6}$$

where $P(\rho)=|b(\rho)|^2$, the differential cross section is related to the transition probability $P(\rho)$ by

$$\frac{d\sigma}{d\Omega}=\frac{A^2}{4}\frac{P(\rho)}{\sin^{4}\frac{1}{2}\theta}\,, \tag{7}$$

where $P(\rho)$ is evaluated at the value of ρ given by Eq. (5).

Equations (5) and (7) are identical to the classical Rutherford-scattering formula except that the scattering cross section is also multiplied by the scattering probability $P(\rho)$. This method of relating differential cross sections to theoretical impact-parameter dependence $P(\rho)$ has been used by many authors,[24] but its validity has been critized by McCarroll and Salin.[19] It is valid only at small impact parameters (or large scattering angles) as has been shown in Ref. 19. However, Eq. (5) is useful in relating ρ and θ as an estimate for the impact parameter ρ for a given scattering angle θ.

IV. COMPARISON WITH EXPERIMENTAL DATA

We have applied Eq. (4) to obtain differential cross sections using the capture amplitude $b(\rho)$ calculated from the two-state atomic-expansion method discussed in I.

In Fig. 1, we show the results of our calculations for the differential electron-capture cross sections by 6-MeV protons from the K shell of Ar atoms. Also shown are the experimental data of Cocke *et al.*,[1] the Born(C) result of Ref. 4 and the CBK result of Belkić and Salin.[10] Note that the Born(C) theory predicts a dip in the angular distributions near $\theta\approx 0.03°$ which is not evident in the experimental data. Our results shown in Fig. 1 are calculated from Eq. (4) assuming a Coulombic interaction between the projectile and the target with effective charge $Z_A=17.6875$. Our result shows

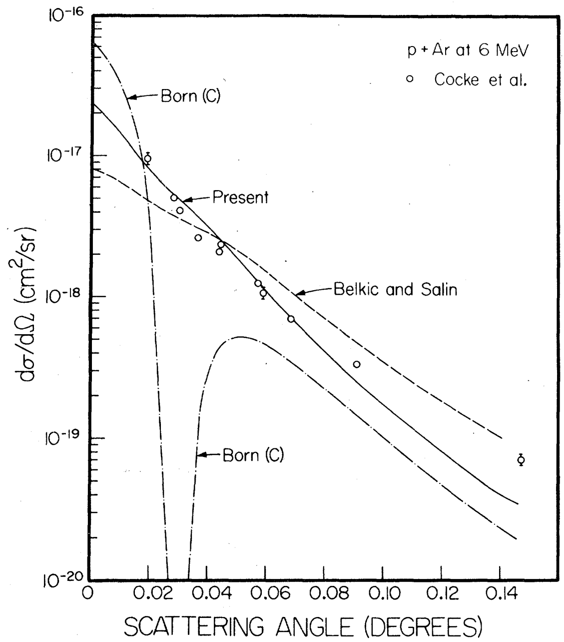

FIG. 1. Differential cross sections for electron capture from the K shell of Ar atoms by 6-MeV protons. The experimental data are from Cocke *et al.*, Ref. 1. The solid curve is the result of the present calculation. The dashed lines are the CBK result of Belkić and Salin, Ref. 10. The Born (C) curve is from Ref. 4.

good agreement with data in the shape and in magnitude. The total cross section calculated at this energy is 15 Mb, to be compared with the experimental value 16.8 ± 0.9 Mb. Also shown in the figure is the result of Belkic and Salin which is in agreement with experimental data at large angles but shows a substantial discrepancy at small angles. In their calculation, they also use Eq. (4) except that the OBK transition amplitude $b(\rho)$ is used.[25]

In Fig. 2, the differential cross sections for electron capture of 293-keV protons on He atoms are presented. The experimental data are from the measurement of Bratton, Cocke, and Macdonald.[2] The theoretical curves are all calculated from the present two-state atomic-expansion method for $b(\rho)$ but using different eikonal phases. The Born(C) result, which is not shown in Fig. 2, again predicts a dip in the angular distribution and is inconsistent with experimental data. Also not shown is the SBK result of Rogers and McGuire.[25] These authors computed the differential cross sections from the OBK amplitude for $b(\rho)$ and used an eikonal phase for the projectile, by assuming the interaction with the target is approximated by a static potential which results from the partial screening of the target nucleus by the other elec-

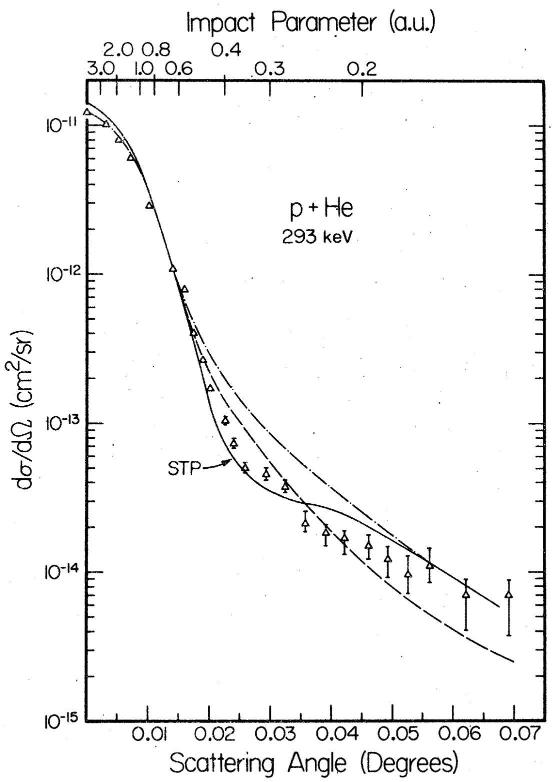

FIG. 2. Differential cross sections for electron capture from helium atoms by 293-keV protons. The experimental data are from Bratton *et al.*, Ref. 2. The three theoretical curves are obtained from the present calculation using different effective charges, see text. The STP curve stands for a static potential for the projectile-target internuclear interaction.

tron. Since the total OBK cross section is 2.55 times larger than the experimental value, they have to normalize their calculated differential cross sections. After this normalization, their results are in reasonably good agreement with experiment, thus indicating that their method can predict the shape of the differential cross sections well. The three theoretical calculations shown in the figure differ only in the effective charge and the internuclear potentials used. They are all calculated by the two-state atomic-expansion method for $b(\rho)$. The dashed and the dot-dashed curves differ in the effective charge Z_A used in the calculation for $b(\rho)$ and for the Coulombic eikonal phase. For the dashed curve, we use $Z_A = 1.4$. For the dot-dashed curve, we use $Z_A = 1.6875$. The solid curve is calculated using the same $b(\rho)$ as the dot-dashed curve, but the eikonal phase is computed using a static potential similar to that of Ref. 11.

The results in Fig. 2 show that the differential cross sections at small angles are not sensitive to the internuclear potential adopted for the projectile motion. At larger angles, there are significant discrepancies due to the choice of effective charges for the target. Since the large-angle scattering is due to close collisions, it is desirable that the projectile sees a bare nucleus at very small ρ. The choice of a static potential is advantageous over the Coulombic potential in that the close collisions at small ρ and glancing collisions at large ρ are more accurately described. In the present calculation, the solid curve shows a slight shoulder at $\theta \approx 0.03°$. Since the present method tends to overestimate $b(\rho)$ for small ρ,[26] the slight disagreement in Fig. 2 at large angles is not unexpected. It will be desirable to find a more accurate method for computing $b(\rho)$ for small impact parameters to see how the behavior of $d\sigma/d\Omega$ at large angles is changed by the choice of internuclear potential adopted.

V. DISCUSSION

The results presented in Sec. IV clearly indicate that the two-state atomic-expansion method, when used together with Eq. (4), can provide an adequate description for the differential cross sections for charge transfer. The results of the CBK approximation of Ref. 10 and of the SBK approximation of Ref. 11 also indicate that the OBK approximation, when used together with Eq. (4) by a proper choice of eikonal phase, can provide an adequate description for the *shape* of the angular distribution, similar to the well-known fact that the OBK approximation provides a correct charge and energy dependence for the total electron-capture cross sections. On the other hand, the Born(C) method, though capable of predicting reasonable total capture cross sections, is inadequate for the angular distributions. The insufficiency of the Born(C) approximation has already been discussed in Sec. II under the impact-parameter formulation. To see the origin of the difference in the angular distribution, we show the capture probability predicted by the OBK, the Born(C), and the present approximations. This is desirable in view of the recent discussion[27] of the angular distributions for $p + \mathrm{H}(1s) \rightarrow \mathrm{H}(1s) + p$, where a dip is predicted by many versions of the first-order Born theory.

In Fig. 3, we show the impact-parameter dependence of $P(\rho)$ for $p + \mathrm{H}(1s) \rightarrow \mathrm{H}(1s) + p$ at 120-keV proton energies using the three approximations and the impact-parameter version of the approximation of Bassel and Gerjuoy. The OBK probability has been divided by 3.27 so that it gives the same total cross section as the two-state approximation. Note the close similarity in the two curves which explains why the CBK and SBK approximations can predict the shape of the differential cross

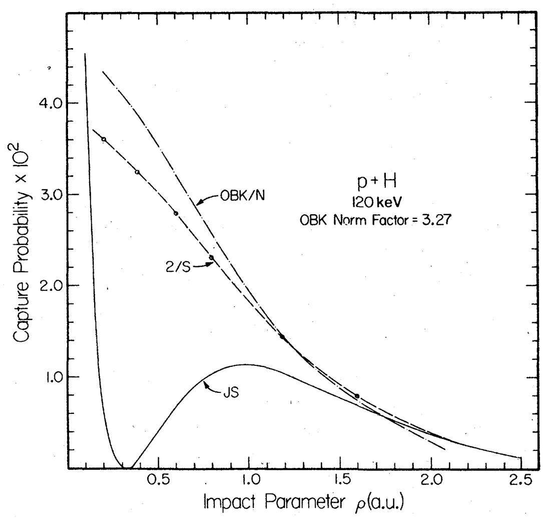

FIG. 3. Impact-parameter dependence of the electron-capture probability in the OBK, the Jackson-Schiff (JS), and the two-state atomic expansion (2/*S*) approximations for proton on hydrogen atoms at 120 keV. The OBK probabilities have been normalized to give total cross sections identical to those of the two-state approximation by dividing by 3.27.

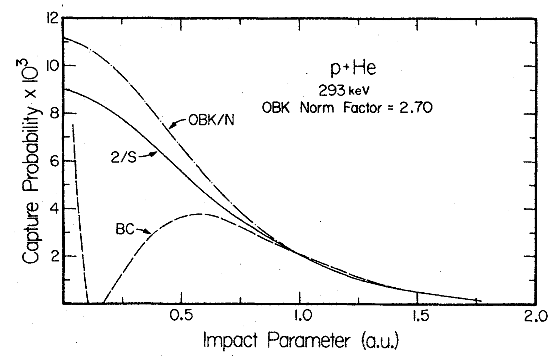

FIG. 4. Same as Fig. 3 except for protons on helium atoms at 293 keV. The curve *BC* represents the Born (*C*) approximation.

sections. On the other hand, the JS approximation [which is identical to Born(C) and the full Born approximation in this system] gives an entirely different shape for $P(\rho)$, particularly at small ρ. This is reflected in the prediction for the angular distributions. The Bassel and Gerjuoy[14] approximation shown as circles in Fig. 3 gives $P(\rho)$ almost identical to the result of the two-state approximation. This is not surprising since the overlap integral $|\langle i|f\rangle|^2$ in Eq. (2) is small and the probability $P(\rho)$ can be calculated by the use of perturbation theory. In Fig. 4, we show a similar $P(\rho)$ plot for 293-keV protons on He atoms. Again, the normalized OBK approximation is in close agreement with the two-state calculation but the Born(C) calculation (designated as *BC* curve) gives an entirely different curve.

It is interesting to comment the rate of convergence of the various methods of Born-series expansion for charge transfer at high velocities. Accepting that there is no dip in the differential cross sections for charge transfer at high velocities (the results of Refs. 1 and 2 certainly support this statement, even though there is no experimental data available for proton-hydrogen atom systems), and the reliability of experimental total capture cross sections, the results of this paper and of Ref. 13 show that the first Born theories like OBK and Jackson-Schiff [or full Born and Born(C) for multielectron systems] approximations *alone* are inadequate for predicting the differential and total cross sections. The second-Born terms for these methods definitely have to be evaluated. Whether the higher-Born terms are needed will not be clear until the second-Born term is computed. However, if the final state is orthogonalized to the initial state,[28] our results indicate that the resulting first-order theory [Eq. (2)] is capable of predicting total and differential electron-capture cross sections in agreement with available experimental data, in the energy region where the theory is expected to be valid. With increasing velocities the importance of higher-order terms for the present method will also increase, as the present method is known to overestimate the total cross sections at high energies.[13,24]

In summary, we have shown that the differential cross sections for charge transfer for fast collisions can be explained by the two-state atomic-expansion method formulated in the impact-parameter approximation, if the projectile motion is properly treated in the eikonal approximation.[4] We also show the inadequacy of the Jackson-Schiff approximation (for protons on hydrogen atoms) and the Born(C) method for the description of differential cross sections for charge transfer despite the fact that these approximations are known to predict total cross sections to better than a factor of 2. The OBK and the full Born approximations, on the other hand, are not well suited to be desirable first-order theories for charge transfer because of the large discrepancy for the total capture cross section. We conclude that Eq. (2) is a more satisfactory first-order Born theory for charge transfer, if the transfer probability is small.

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[26]See the discussion of Sec. V of I.
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