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Two-state atomic expansion methods for electron capture from multielectron atoms by fast protons

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The two-state, two-center atomic expansion method of Bates for charge transfer is generalized to calculate cross sections of electron capture from inner shells of multielectron atoms by fast protons. In the limit of small capture probabilities, the connections of the present approach with various first-order Born theories are investigated. It is shown that these Born methods for electron capture of multielectron atoms can be obtained from the present approach by further approximations. The method is applied to obtain cross sections of electron capture from C, N, O, Ne, and Ar atoms by fast protons in the energy region where the projectile velocity is nearly equal to the K-shell-electron orbital velocity of these atoms. Results of the calculations are compared with experimental measurements.

I. INTRODUCTION

The transfer of an electron from target to projectile during ion-atom collisions is the subject of recent experimental and theoretical investigations. It is known that this process plays an important role in vacancy production in ion-atom collisions.[1]

For collisions in which the projectile velocity is much smaller than the characteristic orbital velocity of the active electron to be transferred, the molecular theory (MO) of Fano and Lichten[2] has been applied successfully to explain qualitatively the observed low-energy ion-atom collision phenomena.[3] Recent developments by Briggs and Macek,[4] and by Taulbjerg *et al.*[5] have put the MO theory in quantitative form for K-shell vacancy transfer in symmetric and asymmetric ion-atom collisions.

For fast collisions such that the projectile velocity is comparable to or greater than the characteristic orbital velocity of the active electron, the capture of bound electrons from the target atom is less well understood. Whereas the first Born approximation or its variations have been useful in describing excitation and ionization in fast collisions,[6] considerable contention still persists in the application of the first Born theory in rearrangement collisions, particularly for the electron-capture process.[6,7,8] Even in the simplest resonant charge-transfer process, $p+\mathrm{H}(1s) \rightarrow \mathrm{H}(1s)+p$, the various first Born theories predict substantially different capture cross sections. Attempts to generalize these first-order Born theories to multielectron ion-atom collisions create even further questions.

Historically, the $p+\mathrm{H}(1s) \rightarrow \mathrm{H}(1s)+p$ resonant charge exchange has been calculated in the Oppenheimer,[9] Brinkman, and Kramers (OBK)[10] approximation. In the OBK approximation, the nuclear-nuclear interaction was completely neglected in evaluating the first Born transition amplitude. This is justified in that the nuclear-nuclear interaction can only deflect the trajectory of the projectile and does not change substantially the total electron-capture cross sections. Later, similar first-order approximations were adopted by Bates and Dalgarno,[11] and by Jackson and Schiff[12] (JS), but with the internuclear potential also included in the first Born amplitude.[13] As argued by Bates and Dalgarno, the complete nuclear-nuclear interaction is included in the perturbation on the grounds that this would compensate to some extent for the nonorthogonality of the wave functions of the initial and final states, and would consequently lead to more realistic cross sections.[13] Interestingly, the cross sections calculated in this method are much smaller than those calculated by the OBK method and agree much better with experimental data.

Recently, both the OBK and JS methods have been generalized to calculate electron-capture cross sections in multielectron ion-atom collisions.[14-17] Like the prediction in the proton-hydrogen resonant capture, the OBK approximation always predicts cross sections much higher than experimental results. Diverse efforts have been attempted to correct this either by reducing the OBK prediction by a semiempirical factor,[18,19] by semiempirical method,[20] or by introducing different amounts of core-core interactions.[21]

The straightforward generalization of the JS method includes the interaction between the two bare nuclei in the perturbation.[12,16,17] This method apparently fails because the predicted capture cross sections are a few orders of magnitude too high. For example, cross sections for the

capture of K-shell electrons of Ar atoms by protons are predicted to be about 320 times larger than experimental data.[16]

Much of the discrepancy mentioned in the above is due to the fact that no proper allowance had been made for the nonorthogonality of the initial- and final-state wave functions. Bates[22] was the first to note that if the nonorthogonality is properly treated, the difficulty formally associated with the choice of internuclear potential can be resolved.

In this paper, we extend the method of Bates to electron capture in multielectron ion-atom collisions within the independent-electron approximation. This approximation treats only the electron to be transferred as active; the others are treated as passive and provide only screening during the collision process.

In Sec. II, the Bates method is reviewed. The connections of Bates method, in the limit of small capture probability, to the different first Born methods are discussed in Sec. III. In Sec. IV, this method is applied to the capture of K-shell electrons of C, N, O, Ne, and Ar atoms by fast protons. The validity of the present method is discussed in Sec. V.

II. ATOMIC EXPANSION METHOD

Developed by Bates in 1958, the atomic expansion method was designed to properly account for the nonorthogonality of the initial- and final-state wave functions in the electron-capture process.

In the Bates method, the motion of the electrons and the nuclei in ion-atom collisions is separated by using the perturbed-stationary-state (pss) method[23]; the motion of the nuclei is treated classically. The attractive nuclear field experienced by the electrons during the collision depends upon the trajectories of the two nuclei. In this paper, we are dealing with high-velocity projectiles; thus straight-line trajectories will be adopted.

To study electron-capture problems in multielectron ion-atom collisions, many approximations can be made if only the capture of inner-shell electrons is to be treated. In principle, the Bates approach can be used to deal with multielectron wave functions. However, it has been shown that electron correlation and exchange effects are not very important for the electron-capture process in the proton-helium system.[24-26] We thus expect the independent-electron model to be adequate, particularly for capture from the inner shells of atoms.

In this approximation, the wave function of the active electron is governed by the time-dependent Schrödinger equation

$$\left(H_e - i\frac{\partial}{\partial t}\right)\Psi(\vec{r},t) = 0, \tag{1}$$

where

$$H_e = -\tfrac{1}{2}\nabla^2 - Z_A/r_A - Z_B/r_B \tag{2}$$

is the effective Hamiltonian of the active electron. In Eq. (2), Z_A and Z_B are the effective charges experienced by the electron; r_A and r_B are the positions of the electron with respect to the target A and to the projectile B, respectively. Atomic units will be used.

Equations (1) and (2) are to be solved with proper boundary conditions at $t = -\infty$. The method adopted by Bates is to expand $\Psi(\vec{r},t)$ in terms of the traveling eigenstates of the target and of the projectile. The following derivation can be found in the paper of Bates[22] or in the book by McDowell and Coleman.[6] We will summarize it below for later discussion.

The time-dependent wave function $\Psi(\vec{r},t)$ can be expanded generally as

$$\Psi(\vec{r},t) = \sum_n a_n(t)\,\phi_n(\vec{r}_A)\exp\left[-i\left(\tfrac{1}{2}\vec{v}\cdot\vec{r} + \tfrac{1}{8}v^2t + \epsilon_n t\right)\right] + \sum_m b_m(t)\phi_m(\vec{r}_B) \times \exp\left[-i\left(-\tfrac{1}{2}\vec{v}\cdot\vec{r} + \tfrac{1}{8}v^2t + \epsilon_m t\right)\right], \tag{3}$$

where $\phi_n(\vec{r}_A)$ $[\phi_m(\vec{r}_B)]$ is the stationary eigenfunction of the target (projectile) with eigenenergy ϵ_n (ϵ_m), $\vec{v}$ is the velocity of the projectile in the laboratory frame and $\vec{r}$ is the position vector of the electron with respect to the midpoint of the internuclear axis.[27] In Eq. (3), the velocity-dependent exponents are introduced to preserve translational invariance.

To describe electron capture, the simplest approximation to Eq. (3) is to retain only the two states which are relevant to the capture process, the initial state of the target and the final state of the projectile. To simplify the notation, we rewrite Eq. (3) (in a self-evident way) as

$$\Psi(\vec{r},t) = a(t)\,\phi_A\exp\left[-i\left(\tfrac{1}{2}\vec{v}\cdot\vec{r} + \tfrac{1}{8}v^2t + \epsilon_A t\right)\right] + b(t)\,\phi_B\exp\left[-i\left(-\tfrac{1}{2}\vec{v}\cdot\vec{r} + \tfrac{1}{8}v^2t + \epsilon_B t\right)\right]. \tag{4}$$

Substitution of Eq. (4) into Eq. (1) yields a set of coupled equations:

$$\begin{aligned} i(1-s^2)\,\dot{a} &= a(h_{AA} - s_{AB}h_{BA}) + b(h_{AB} - s_{AB}h_{BB})\,e^{i\omega t}, \\ i(1-s^2)\,\dot{b} &= b(h_{BB} - s_{BA}h_{AB}) + a(h_{BA} - s_{BA}h_{AA})\,e^{-i\omega t}, \end{aligned} \tag{5}$$

where $\omega = \epsilon_A - \epsilon_B$ and

$$
\begin{aligned}
s_{AB} &= \int \phi_A^* \phi_B e^{(i\vec{v}\cdot\vec{r})}\, d\tau, \\
s_{BA} &= \int \phi_B^* \phi_A e^{(-i\vec{v}\cdot\vec{r})}\, d\tau, \\
h_{AB} &= \int \phi_A^* (-Z_A/r_A)\phi_B e^{(i\vec{v}\cdot\vec{r})}\, d\tau, \\
h_{BA} &= \int \phi_B^* (-Z_B/r_B)\phi_A e^{(-i\vec{v}\cdot\vec{r})} d\tau, \\
h_{AA} &= \int \phi_A^* (-Z_B/r_B)\phi_A\, d\tau, \\
h_{BB} &= \int \phi_B^* (-Z_A/r_A)\phi_B\, d\tau,
\end{aligned}
\tag{6}
$$

and where the integration is over the electronic coordinates. The identities $s_{BA} = s_{AB}^*$ and $s^2 = s_{AB}\, s_{BA}$ are obvious.

Introducing the transformation

$$
\begin{aligned}
a(t) &= d_A(t) \exp\left(-i \int_{-\infty}^{t} \alpha(t')\, dt'\right), \\
b(t) &= d_B(t) \exp\left(-i \int_{-\infty}^{t} \beta(t')\, dt'\right).
\end{aligned}
\tag{7}
$$

Eqs. (5) are simplified to

$$
\begin{aligned}
i\dot{d}_A &= \frac{h_{AB} - s_{AB} h_{BB}}{1 - s^2}\, e^{i\omega t + i\delta} d_B, \\
i\dot{d}_B &= \frac{h_{BA} - s_{BA} h_{AA}}{1 - s^2}\, e^{-i\omega t - i\delta} d_A,
\end{aligned}
\tag{8}
$$

where

$$
\delta = \int_{-\infty}^{t} [\alpha(t') - \beta(t')]\, dt' \tag{9}
$$

and

$$
\begin{aligned}
\alpha(t) &= (h_{AA} - s_{AB} h_{BA})/(1 - s^2), \\
\beta(t) &= (h_{BB} - s_{BA} h_{AB})/(1 - s^2).
\end{aligned}
\tag{10}
$$

Equations (8) are to be solved with the boundary conditions $d_A(-\infty) = 1$, $d_B(-\infty) = 0$ for each impact parameter ρ and each energy. The total capture cross section per atom is obtained from

$$
Q = 2\pi N_A \int_0^{\infty} \rho\, d\rho\, p(\rho), \tag{11}
$$

where $p(\rho) = |b(+\infty)|^2$ is the capture probability and N_A is the number of equivalent electrons in the target shell from which the active electron is captured.

III. CONNECTIONS WITH OTHER BORN APPROXIMATIONS

For collisions in which the capture probabilities are small, the capture amplitude can be solved from Eqs. (8) by first-order approximation. If we set $d_A(t) \equiv 1$, then $d_B(+\infty)$ is given by

$$
d_B(+\infty) = -i \int_{-\infty}^{\infty} \frac{h_{BA} - s_{BA} h_{AA}}{1 - s^2}\, e^{-i\omega t - i\delta}\, dt. \tag{12}
$$

In Eq. (12), the transition amplitude $d_B(+\infty)$ can be easily shown to be independent of any arbitrary internuclear potentials added to the definitions of the matrix elements h_{BA} and h_{AA}. This is due to the fact that the nonorthogonality of initial and final states has been properly accounted for in Eqs. (5) through the introduction of overlap integrals s_{AB} and s_{BA}.

The δ term in Eq. (12) represents the distortion of the electron wave function in the nuclear field of the projectile and the target in the two-state atomic expansion approximation. If this distortion is neglected, then Eq. (12) becomes

$$
d_B(+\infty) = -i \int_{-\infty}^{\infty} \frac{h_{BA} - s_{BA} h_{AA}}{1 - s^2}\, e^{-i\omega t}\, dt. \tag{13}
$$

For high-velocity collisions, $s^2 \ll 1$, Eq. (13) can then be written explicitly as

$$
\begin{aligned}
d_B(+\infty) = -i \int_{-\infty}^{\infty} dt\, d\tau\, \phi_B \left[-\frac{Z_B}{r_B} - h_{AA}\right] \\
\times \phi_A \exp\{-i(\vec{v}\cdot\vec{r} + \omega t)\},
\end{aligned}
\tag{14}
$$

in a form similar to the first Born transition amplitude with $(Z_B/r_B) - h_{AA}$ as the interaction "potential." For capture from the K shell of target A to the K shell of projectile B, h_{AA} is

$$
h_{AA} = (Z_B/R)[-1 + (1 + Z_A R) e^{-2Z_A R}]. \tag{15}
$$

For the charge-exchange $p + \mathrm{H}(1s) \rightarrow H(1s) + p$, $Z_A = Z_B = 1$, Eq. (14) becomes identical to the distorted-wave approximation for electron capture derived by Bassel and Gerjuoy.[28] Thus, Eq. (14) is the generalization of their method to arbitrary Z_A and Z_B. Incidentally, Eq. (14), or more rigorously, Eq. (13), can also be derived from the usual first Born theory if the final-state wave function is required to be orthogonal to the initial-state wave function. Thus, we show that in the limit of small capture probabilities, the two-state atomic expansion method of Bates, the distorted-wave approximation of Bassel and Gerjouy and the first Born theory are all equivalent if the orthogonalized final state is used in the first Born theory.

To explore the meaning of Eq. (14) in more detail, we plot, in Fig. 1, $-R\, h_{AA}/Z_B$ as a function of $Z_A R$, where R is the internuclear separation. The function h_{AA} approaches zero as $Z_A R \rightarrow 0$ and approaches $-Z_B/R$ as $Z_A R \rightarrow \infty$. If

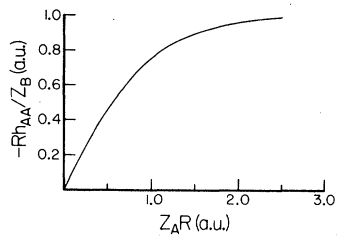

FIG. 1. Plot of $-Rh_{AA}/Z_B$ as a function of Z_AR.

h_{AA} is chosen to be zero in Eq. (14), we recover the usual OBK approximation. From Eq. (13), this is *equivalent* to neglecting the nonorthogonality of initial and final states as was done in the OBK approximation (by setting $s_{BA} \equiv 0$). On the other hand, if the large-R limit of h_{AA} is used in Eq. (14), the expression in the squared bracket becomes $[-Z_B/r_B + Z_B/R]$. In the $p + \mathrm{H}(1s) \rightarrow \mathrm{H}(1s) + p$ capture problem, it becomes $[-1/r_B + 1/R]$ and the second term resembles the internuclear interaction between the protons. This is equivalent to the method of JS in which the internuclear potential is included in the first Born transition amplitude. Therefore, we can interpret that the introduction of the internuclear interaction into the first Born transition amplitude has the effect of partially accounting for the nonorthogonality of the initial and final states in the $p + \mathrm{H}(1s) \rightarrow \mathrm{H}(1s) + p$ reaction at intermediate and large R. However, this similarity *cannot* be generalized to ion-atom collisions of arbitrary Z_A and Z_B. The large R limit of h_{AA} is Z_B/R instead of the internuclear interaction Z_AZ_B/R. This partially explains why the straightforward generalization of the JS method to ion-atom collisions by including a full internuclear interaction results in unrealistic capture cross sections. Incidentally, the large-R limit of h_{AA} has also been introduced recently[15] in the Born amplitude, under the assumption of almost complete screening of the target nucleus charge by the passive electrons. This assumption is *not* valid for the capture of K-shell electrons. It is better to interpret Z_B/R as an approximation of the nonorthogonality contribution to the Born amplitude for electron capture and has no relation with the internuclear potential.

It is not difficult to understand why the JS or the Born method of Ref. 15 usually gives better absolute total capture cross section than the OBK approximation. In Fig. 1, h_{AA} is well approximated by its large-R limit $-Z_B/R$ for R near or greater than the K-shell radius. Thus, if the total electron capture comes primarily from large impact parameter ρ, such $\rho Z_A \geq 1$, then the JS or the Born method of Ref. 15 will give reasonable total capture cross sections [as compared with that obtained from Eq. (13)]. However, it must be realized that both methods will fail at small ρ or, correspondingly, at large scattering angles. Also, if the total capture cross section comes primarily from small impact parameters, then the total cross sections calculated from these two methods will be wrong .

It might then be speculated that the OBK method is a better approximation for collisions at small impact parameters. This is not quite true. For small impact parameters, the distortion of the active electron wave function by the projectile is very large and cannot be reasonably approximated by any first-order theory, even such as Eqs. (8) and (13).

IV. K-SHELL ELECTRON CAPTURE OF C, N, O, Ne, AND Ar ATOMS BY FAST PROTONS

The two-state atomic expansion method has previously been applied only to simple atomic systems. (See the review by Bransden.[8]) By comparing with experimental data or with more elaborate calculations, it is concluded that the simple two-state calculations predict reasonable capture cross sections when the projectile velocity is not very far away from the characteristic orbital velocity of the active electrons.

Theoretical calculations of electron-capture cross sections from multielectron atoms have been limited to the OBK or other Born methods.[15-20] The results of these calculations are often unreliable. We have applied the two-state atomic expansion method, under the independent-particle approximation as outlined in Sec. II, to calculate the electron-capture cross sections of the K shell of carbon, nitrogen, oxygen, neon, and argon atoms by fast protons.

The numerical method is straightforward. A screened hydrogenic 1s wave function with effective charge $Z_A = Z - \frac{5}{16}$, where Z is the nuclear charge of the target, is used for the target atom and a bare nuclear charge Z_B is used for the projectile. The matrix elements of Eq. (6) are evaluated by transforming the two-centered integrand to prolate spheroidal coordinates (λ, μ, ϕ).[29] Integrations over ϕ and μ can be carried analytically. The integration over λ is done using 24-point Gauss-Laguerre quadrature, although the 32-point formula has been used also to check the accuracy of the integration. The capture amplitude $b(+\infty)$, or equivalently $d(+\infty)$, is obtained by solving the coupled Eqs. (8), either by direct numerical integration or by an iterative method. The latter method is more suitable for calculating small amplitudes. In particular, the first it-

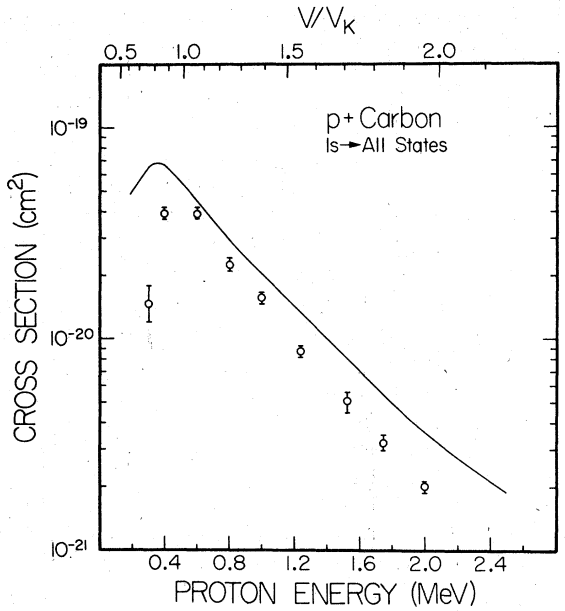

FIG. 2. Electron-capture cross sections from the K shells of carbon atoms by fast protons. The values are the total capture cross sections per target atom, including capture to the exited state of hydrogen atoms. The solid curve is the result of the present calculation. Experimental data are from Rødbro *et al.*, Ref. 33. Also shown are the values of V/V_K, the ratio of the projectile velocity V to the characteristic K-shell orbital velocity of the target atom, defined by $V_K = \sqrt{2I_K}$, where I_K is the K-shell ionization energy.

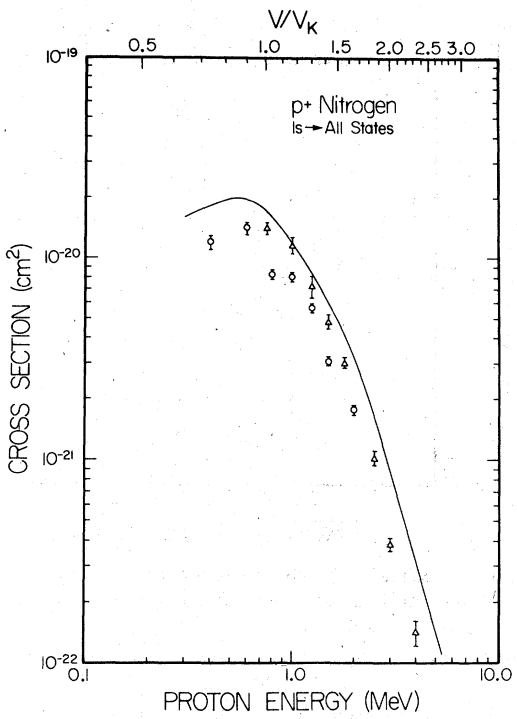

FIG. 3. Same as in Fig. 2, except for nitrogen atoms. Experimental data: Φ, from Rødbro *et al.*, Ref. 33; ⏄, from Cocke *et al.*, Ref. 32.

erative solution for $d_B(+\infty)$ is then given by Eq. (12). Depending upon the systems, usually two or three iterations are enough for desirable accuracy. In solving Eqs. (8), we use experimental K-shell ionization energy for ϵ_A and $-Z_B^2/2$ for ϵ_B. By choosing ϵ_A and Z_A separately, the unitarity condition is not imposed in the calculation. This choice of ϵ_A is desirable because the capture probability, as given by its first-order solution Eq. (12), is dominated by the oscillatory function $e^{-i\omega t}$ in the integrand, as well as the damped oscillation in the matrix elements of $-Z_B/r_B - h_{AA}$. This explains why the OBK approximation (obtained by letting $h_{AA} = 0$) usually predicts correct energy dependence for the total capture cross sections, even though the absolute values are often wrong.

The calculated total capture cross sections from the K shells of C, N, O, Ne, and Ar atoms by protons are displayed in Figs. 2–6. They are the total capture cross sections per target atom, including capture to the excited states of the projectile. The theoretical values shown in the figures are obtained from the calculated 1s-1s val-

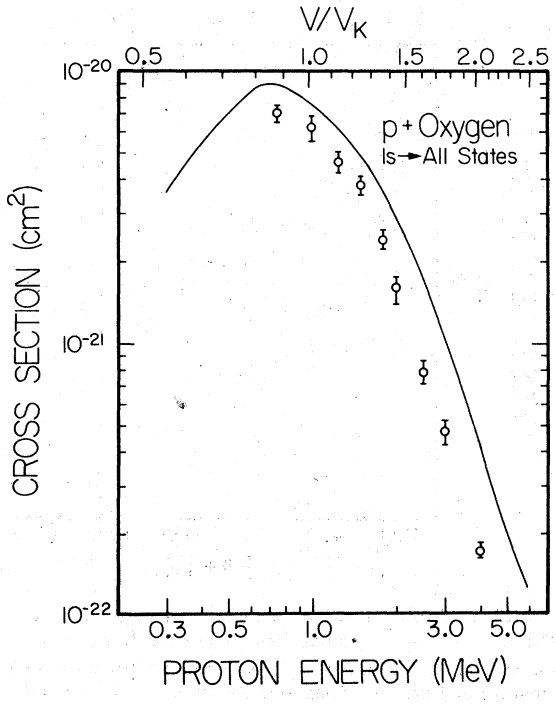

FIG. 4. Same as in Fig. 2 except for oxygen atoms. Experimental data from Cocke *et al.*, Ref. 32.

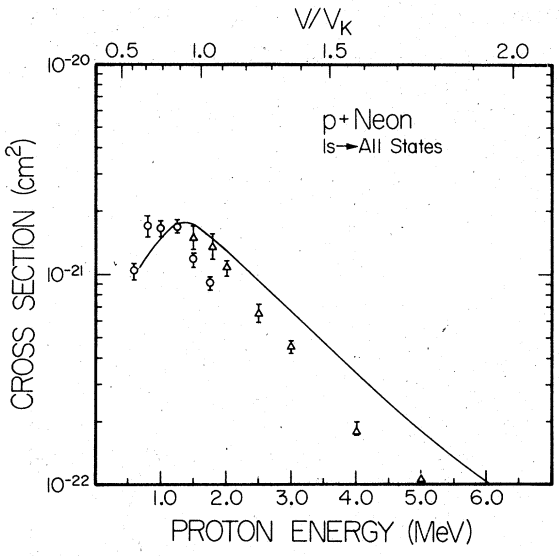

FIG. 5. Same as in Fig. 2 except for neon atoms. Experimental data: Φ, from Rødbro *et al.*, Ref. 33; ⊼, Cocke *et al.*, Ref. 32.

ues by multiplying 1.2, corresponding to the high velocity $1/n^3$ scaling.[30] Experimental data shown on these figures are from Macdonald *et al.*,[31] Cocke *et al.*,[32] and from Rødbro *et al.*[33] For

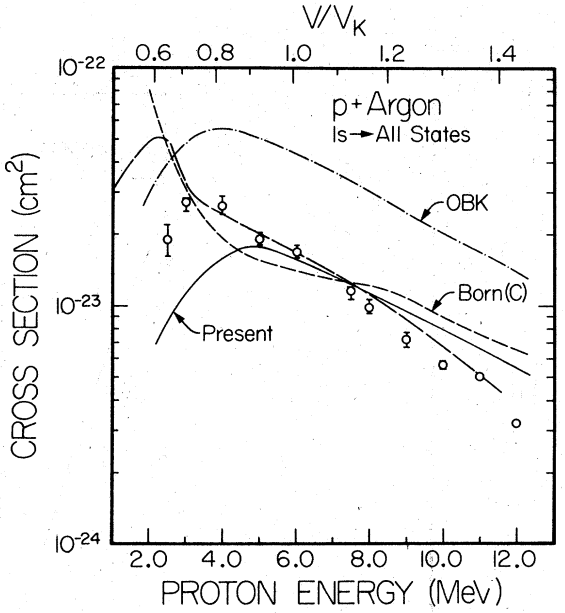

FIG. 6. Same as in Fig. 2 except for argon atoms. Other theoretical results: short-dashed lines, the Born (C) method of Ref. 15; dash-dotted lines, the OBK results of Ref. 15. Long-dashed lines, continuous distorted-wave (CDW) results of Ref. 34. Experimental data are from Macdonald *et al.*, Ref. 31.

C, N, and O, atoms, the experimental data are obtained from measuring capture in CH_4, N_2, and O_2 gases. The experimental K-shell capture cross sections are not expected to change much by any molecular binding effect.

It can be seen from Figs. 2–6 that the calculated values are generally in good accord with experimental data. In Fig. 6, the results of the OBK approximation, the Born method of Omidvar *et al.*,[15] and the continuum distortion-wave method of Belic and McCarroll[34] are also shown for comparison. The OBK predictions shown in Fig. 6 are about three times too large when compared with experimental data. The Born method of Omidvar *et al.*[15] predicts cross sections in reasonable agreement with data at higher energies but the predicted energy dependence differs from the experimental data. The continuum distorted-wave method of Belic and McCarroll[34] also predicts cross sections in excellent agreement with experimental data at the high-energy side,[35] but the energy dependence at the low-energy side is also incorrect.

V. DISCUSSION

From the results of Figs. 2–6, it is clear that the simple two-state expansion method is capable of predicting capture cross sections in *reasonable* agreement with experimental data. However, further improvement of the model is possible. In the following we discuss the limitation of the present method and possible further improvement.

A. Atomic model

In Eqs. (1) and (2), we use the active-electron approximation by disregarding the effects of passive electrons. It is possible to formulate a many-electron theory of electron capture based upon the Bates formulation. In fact, such a theory has been written explicitly by Msezane[36] recently for the two-electron systems. However, the complexity of such a theory for general N-electron problem will make such a formulation impractical in view of the numerical difficulties.

Improvement in the atomic model within the independent-electron approximation can be proceeded by using a more realistic potential $V(r_A)$ for the target atom. For example, the Green-Sellin-Zachor (GSZ) potential of Green *et al.*[37] can be introduced into the Hamiltonian (2).[38] These potentials predict the K-shell ionization energy accurately. We can thus use the eigenstates and eigenenergies generated from this potential in the expansion (4), thus preserving the unitarity relation in the coupled Eqs. (6) and (8). It is hoped that the choice of the more realistic potential will

improve the computed cross sections in the region where the cross section peaks. However, it is *not* expected that the improvement in the atomic model *alone* will make the theoretical calculations agree with experimental data over the entire energy range considered. The convergence of the truncated atomic expansion has to be investigated too.

B. Scattering model

To study the limitation of the two-state atomic expansion method, we examine the well-studied simple reaction $p+\mathrm{H}(1s)\rightarrow\mathrm{H}(1s)+p$. At the low-velocity limit, the potential curves of the quasimolecule H_2^+ are exactly known. These potential curves describe the distortion of the atomic electron wave function by the projectile in the adiabatic limit. By comparing the potential curves calculated by the two-state atomic expansion with the exact H_2^+ potential curves,[39] we can conclude that the two-state representation is adequate for $R\geq 1.0$, but not smaller R. Therefore, we can expect the two-state atomic expansion method adequate for describing the collision $p+\mathrm{H}(1s)\rightarrow\mathrm{H}(1s)+p$ at impact parameters $\rho\geq 1.0$, but not at smaller impact parameters. If the total capture cross section comes primarily from the impact parameters $\rho\geq 1.0$, then the total capture cross section obtained from the two-state atomic expansion will be adequate. This occurs at the intermediate energy region where the projectile velocity nearly matches the orbital velocity of the target electron. As the velocity of the projectile increases, the capture has to occur at smaller impact parameters for the projectile to pick up electrons close to the target nucleus, then the two-state atomic expansion becomes inadequate.[40]

Within the method of Bates, the charge exchange $p+\mathrm{H}(1s)\rightarrow\mathrm{H}(1s)+p$ has been studied by the multistate atomic expansion method[41] by using the Sturmian basis set[42] and by the pseudostate method.[43] In the multistate expansion method of Ref. 41, excited hydrogenic orbitals are used in the expansion of Eq. (3). It was found that the electron-transfer cross sections are not changed substantially by the inclusion of the excited states. However, this does not imply that the two-state calculation has converged in all the cases studied. It actually happens that the excited states included in the expansion are not important for this particular reaction. This can be easily understood from the discussion in the previous paragraph. It was shown there that the inadequacy of the two-state atomic expansion occurs at small $R\leq 1.0$ where the electronic motion cannot be represented by the excited-state wave functions of the target or the projectile because of the diffuse nature of these functions, but can only be represented by the continuum functions. The Sturmian basis set and the pseudostates are all chosen in the hope that the continuum states are thus partially accounted for. In Table I, we compare the two-state calculation of McCarroll[44] and the pseudostate calculation of Cheshire *et al.*[43] for the reaction $p+\mathrm{H}(1s)\rightarrow\mathrm{H}(1s)+p$. We can see the two-state calculations are quite adequate for $E_p\leq 100$ keV, but as E_p increases, the two-state calculations overestimate the capture cross sections by a factor of 2 as the contributions of capture from small impact parameters to the total cross section increase.

From Table I and the discussion above, it becomes clear that the two-state approximation is best in the energy region where $v_p\approx v_{el}$. The method becomes inadequate as the projectile energy increases, eventually reducing to the OBK approximation at extremely high energies. It is interesting to mention that this implies all the first Born approximations for electron transfers are inadequate, even at high energies. This is not inconsistent with the conclusion of Drisko[45] that the second Born term is more important than the first Born term in the extreme limit of high energies.

By examining the results of our calculations in Figs. 2–6, our values at the high-energy side are about a factor of 2 higher than experimental data. Thus one might speculate that the continuum states are also very important in our calculations. At this moment we tend to believe this is not the case. The discrepancy probably can be reduced

TABLE I. Comparison of the two-state calculations [a] and the pseudostate calculations [b] for the total capture cross sections for $p+\mathrm{H}(1s)\rightarrow\mathrm{H}(1s)+p$ reactions. The cross sections are given in cm^2. $A(-B)=A\times 10^{-B}$.

Energy (keV)	Two-state [a]	Pseudostate [b]
4	1.15(−15) [c]	1.13(−15)
10	7.79(−16) [c]	7.77(−16)
15	5.60(−16)	5.81(−16)
20	4.18(−16) [c]	4.14(−16)
25	2.76(−16)	2.93(−16)
40	1.51(−16) [c]	1.13(−16)
60	4.98(−17) [c]	4.20(−17)
100	1.012(−17)	8.89(−18)
300	1.711(−19)	8.51(−20)
1000	5.12(−22)	2.63(−22)

[a] Two-state calculations from McCarroll, Ref. 41.

[b] Pseudostate calculations from Cheshire *et al.*, Ref. 42.

[c] Interpolated from Ref. 41.

by including a few more atomic states of the target atom into expansion (3). It is noted that some excited orbitals of the target atoms have radii smaller or comparable to the radius of the 1*s* orbital of the hydrogen atom. The restriction of the two-state atomic expansion with basis functions differing substantially in the size of orbitals might have forced those amplitudes which would have otherwise ended up in the direct excitation channels into the electron-capture channel. The validity of this speculation has to be substantiated by actual calculations.

In summary, we applied the two-state atomic expansion method to compute the electron-capture cross sections of C, N, O, Ne, and Ar atoms. Comparisons of this method with other first-order Born methods are made to elucidate the region of validity of these methods. The limitation and possible further improvement of the present model is also discussed.

Note added in proof. The revised experimental electron capture cross sections for protons on carbon atoms at low energies, in units of 10^{-18} cm^2, are 0.81 ± 0.05 at 400 keV, 0.88 ± 0.08 at 300 keV, and 0.8 ± 0.08 at 250 keV of proton energies (J. R. Macdonald, private communication). These revised values are in good agreement with our calculations in Fig. 2.

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