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# Single-electron Born approximations for charge transfer from multielectron atoms to protons*

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The Born approximation, including the internuclear interaction, is used to compute cross sections for the transfer of one electron from a multielectron atom to an incident proton. When the full internuclear interaction is included, the results lie far above high-energy experimental $K$-shell data for $p$ + Ar. However, when only enough internuclear interaction is used so that the total projectile-target interaction goes to zero asymptotically in accord with plane-wave functions actually used, fair agreement at high energies is obtained. The latter form of the Born approximation is compared to data on $K$-shell capture from helium as well as argon, in addition to the simpler approximation of Oppenheimer and of Brinkman and Kramers (OBK), where no internuclear interaction is included. The OBK results typically lie a factor of 2 to 8 above the data, while our Born results are within a factor of 2 of most of the existing high-velocity $K$-shell data, i.e., with an accuracy comparable to more sophisticated calculations.

The transfer of an electron from target to projectile during ion-atom collisions has attracted both experimental and theoretical attention over a long period of time. It is known, for example, that this process plays a dominant role in vacancy production and energy transfer in some ion-atom interactions.

An interesting variety of charge-transfer calculations[1] exists. However, with a few notable exceptions, these calculations have been primarily limited to simple systems such as protons on atomic hydrogen or helium, and only 1$s$ (target) to 1$s$ (projectile) transitions have usually been considered On the other hand there have been many measurements of electron capture by protons and other ions from multielectron atoms. In these measurements capture occurs from a variety of target states (often not primarily 1$s$ levels) to a variety of projectile states. The need for further calculations is clear.

We restrict ourselves to nonradiative charge-transfer calculations. A number of difficulties are encountered in such calculations. This is the case even at high energies where one might hope to be able to apply the first-order perturbation theory using static atomic wave functions, i.e., the Born approximation. In this respect the convergence of the Born series is not entirely clear. It has been shown that for proton-hydrogen electron-transfer collisions in the range of the relatively high impact energies of a few MeV, the second Born terms are comparable in magnitude to the first Born terms.[2] As the energy increases the contribution to the cross section from the second-order terms becomes larger, since this contribution falls with respect to the impact energy $E$ as $E^{-5.5}$, while the contribution due to the first-order terms falls as $E^{-6}$. At higher energies of the order of 100 MeV another change in the behavior of the cross section for the same process takes place and the cross section falls as $E^{-3}$ (Ref. 3).

This behavior is due to backscattering and comes from the first-order terms. However, the latter behavior holds only for symmetric collisions where the masses of the projectile and target nucleus are equal,[3,4] and does not hold for the majority of the ion-atom collisions considered within our simple model. For energies of the order of 100 MeV relativistic corrections also become important.[5]

The internuclear (or core) interaction plays an important role in the behavior of the cross section. This role has been treated extensively in the literature. It has been shown that at the limit of very high energies, in an exact calculation involving heavy projectiles, contributions of the core interaction are (except for an over-all phase) of the order of $m(M_P+M_T)/4M_PM_T$, where $m$, $M_P$ and $M_T$ are, respectively, the masses of the electron, projectile, and target nucleus.[6] Nevertheless, the core interaction is not negligible in an approximate calculation, and is not negligible in an exact calculation for finite impact energies. Indeed, as we shall later demonstrate, the full Born approximation is quite sensitive to the strength of this internuclear interaction. Such sensitivity to the core term is absent in Born calculations of excitation and ionization, where owing to the orthogonality of the initial and final states the core term vanishes. For the case of charge transfer, improved agreement with measurements can be obtained by enforced orthogonalization of the initial- and final-state wave functions.[7] This orthogonalization has not been done here.

In this paper we discuss the role of the internuclear interaction in the Born approximation. Cross sections have been computed for transfer of an electron from the $K$ shell of a multi electron atom to all significant levels of the formed H atom. We have approximated the target wave function of the $K$-shell electron as a hydrogenic wave function parametrized by an effective nuclear charge $Z_{\text{eff}} = Z_2 - 5/16$, where $Z_2$ is the bare nuclear charge[8] of the target. Realizing the sensitivity of the charge-exchange cross section to the value of the effective charge, introduction of this effective charge is a weakness of our model. The kinematics of the reaction are determined using an ionization potential for the target electron determined from experimental data as described below.

If $E_i$ and $E_f$ stand for the initial and final center-of-mass energies, and $I_i$ and $I_f$ for the ionization potentials of the $K$ shells of the target and the hydrogen atom, through the conservation of energy we must have $E_i - I_i = E_f - I_f$. Since the final state is

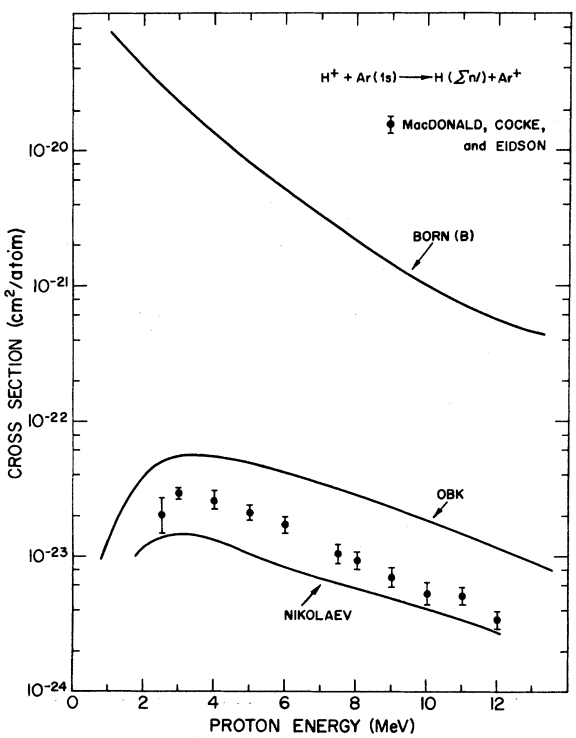


FIG. 1. Electron capture cross sections for $p$ + Ar. The OBK results correspond to choice (A) in the text where the internuclear interaction $V_c$ is set to zero, while Born (B) corresponds to $V_c = +Z_2 e^2/R$. Nikolaev's results include an empirical factor times the OBK results.

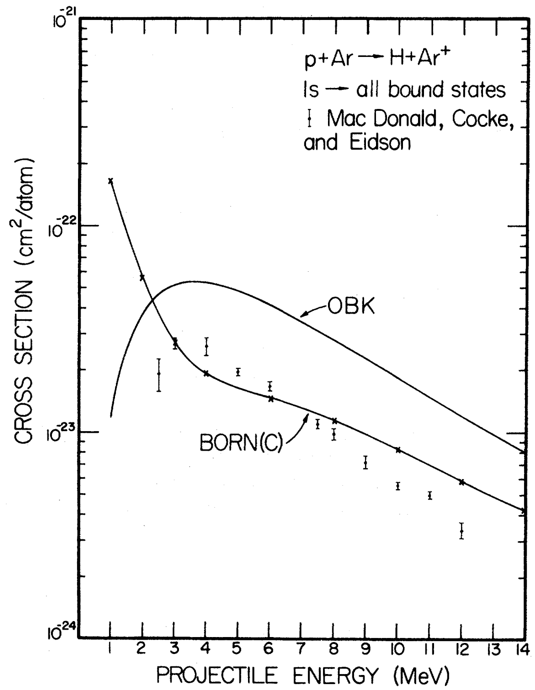


FIG. 2. Electron capture cross sections for $p$ + Ar. The OBK result corresponds to choice (A) with $V_c = 0$, while Born (C) uses $V_c = e^2/R$. The data are that of Macdonald, Cocke, and Eidson (Ref. 11).

an excited state of atomic hydrogen we have $I_f = n^{-2}$Ry. For $I_i$ we have used the experimental value instead of the hydrogenic value of $Z_{\text{eff}}^2$ Ry. The use of the actual, instead of the hydrogenic, ionization potential has the disadvantage of making the prior and post forms of the charge-exchange amplitudes unequal. We use here the prior form of the amplitude.

Plane waves are used to describe the relative motion of the target and projectile both initially and finally. The internuclear (core) interaction $V_c$ is used in three versions: (A) $V_c = 0$, corresponding to the approximation of Oppenheimer,[9] and Brinkman and Kramers,[10] (OBK); (B) $V_c = Z_2/R$, using the full internuclear interaction, where $R$ is the internuclear separation; and (C) $V_c = 1/R$, corresponding to a total perturbation potential $V = 1/R - 1/(\vec{r} - \vec{R})$, where $\vec{r}$ is the coordinate of the participating electron. The potential in case (C) goes to zero as $R \to \infty$, in accord with the plane waves used in this approximation.

In Figs. 1 and 2 we compare our three versions of the Born approximation to the data[11] of Macdonald, Cocke, and Eidson for electron capture by protons from the $K$ shell of argon. In these calculations we sum over capture into all final states for $n \leq 3$. The dominant contributions are from the $l = 0$ terms which fall off approximately[4] as $n^{-3}$.

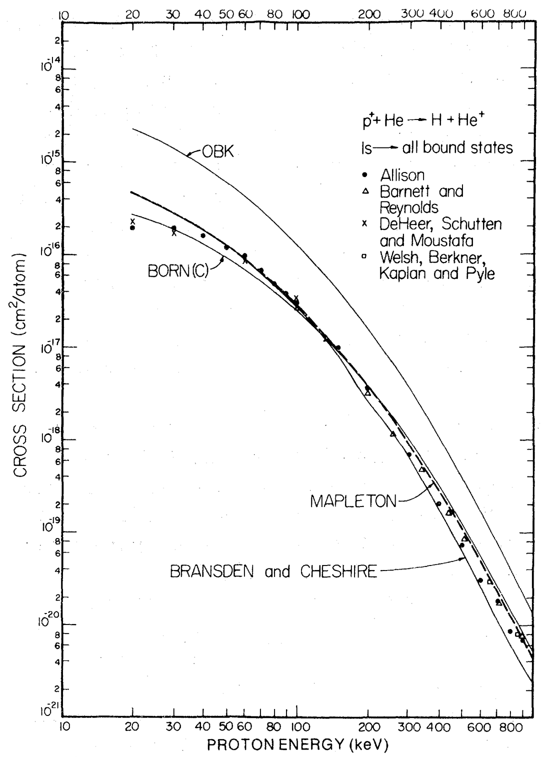


FIG. 3. Electron capture cross sections for $p$ +He versus proton energy in keV. The OBK results correspond to choice (A) with $V_c=0$, while Born (C) uses $V_c=e^2/R$. The data are that of Allison (Ref. 14), Barnett and Reynolds (Ref. 15), DeHeer *et al.* (Ref. 16), and Welsh *et al.* (Ref. 17). More sophisticated calculations due to Mapleton (Ref. 18) and Bransden and Cheshire (Ref. 19; 1$s$-1$s$ only) are also shown.

In Fig. 1 we see that the Born (B) approximation ($V_c=Z_2/R$) lies about two orders of magnitude above the data, and fails to fit the shape of the data as a function of the projectile energy. The simpler OBK results are only a factor of 2 to 4 too large and reflect the shape of the data reasonably well. These results are similar to those for capture into the 1$s$ level recently reported by Halpern and Law.[12]

The semiempirical cross sections of Nikolaev,[13] also shown in Fig. 1, are the product of $\sigma_{\rm OBK}$ and an empirical factor which depends on the relative projectile-target velocity, and the charge of the target nucleus. The factor is chosen so that the best fit is obtained with the measured capture cross sections, summed over all shells of $H_2$, He, $N_2$, Ne, Ar, and Kr. The agreement with measurement does not seem to be totally satisfactory, and it may be that Nikolaev's empirical factor for total cross sections contains corrections for nonhydrogenic outer-shell electrons which do not apply to inner-shell electrons.

In Fig. 2 we compare the OBK and Born (C) calculations ($V_c=1/R$) to the same experimental data. While OBK fits the shape of the data better, especially at low velocities, the Born (C) calculation fits the magnitude better at high velocity.

A more thorough test of this high-velocity result is shown in Fig. 3, where our Born (C) results ($V_c=1/R$) are compared to high-velocity data of Allison,[14] of Barnett and Reynolds,[15] of De Heer, Schutten, and Moustafa,[16] and of Welsh, Berkner, Kaplan, and Pyle,[17] for electron capture by protons from helium. In this calculation we have computed only 1$s$-to-1$s$ charge-transfer cross sections and then multiplied the result by 1.202, corresponding to the high-velocity $n^{-3}$ scaling. Our Born (C) results fit the data to within a factor of 2 at all energies considered here. In contrast, the OBK results, which entirely neglect the internuclear term, lie a factor of 2 to 8 above the data.

Also shown in Fig. 3 are more sophisticated calculations of Mapleton,[18] who does a more thorough treatment in first-order perturbation, and of Bransden and Cheshire,[19] who apply a more rigorous impulse approximation. The accuracy of our simple Born (C) results ($V_c=1/R$) is comparable to these more complete calculations in this case.

In Fig. 4 we present differential scattering cross

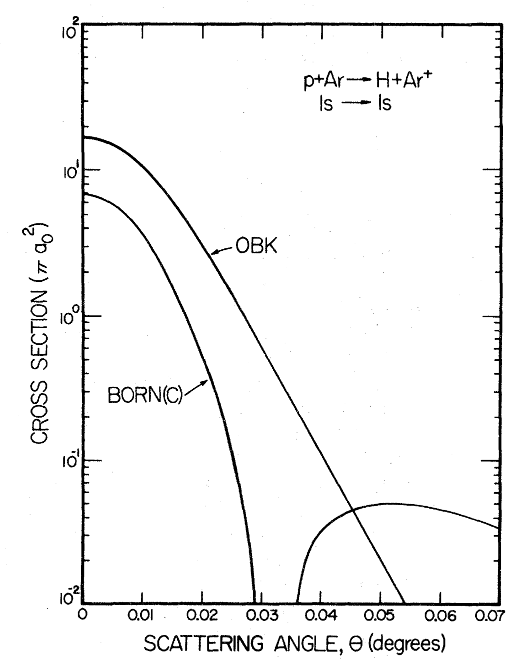


FIG. 4. Theoretical angular distributions $d\sigma/d(\cos\theta)$ for electron capture by 6-MeV protons in argon. The scattering angle $\theta$ is the angle between the initial and final momenta in the center of mass. In this case, laboratory angles are comparable.

sections for 1$s$-to-1$s$ transfers to protons from argon. There is a minimum in our Born (C) results at forward angles corresponding to projectile impact parameters comparable to the radius of the $K$ shell. This minimum, not found in the OBK calculation, is often present in first-order perturbation calculations[7,20,21] which include internuclear contributions. The position of the minimum varies from calculation to calculation, and it is not clear which calculation, if any, gives the correct minimum. On the other hand, measurement of these distributions might provide a useful benchmark for various theories.

The phenomenological agreement of our Born (C) results with data for total cross sections for charge transfer from 1$s$ target levels to protons is clearer than the justification of the particular choice of core interaction used to obtain our present results. Indeed further tests of this approximation with experimental data would be helpful in assessing its validity. On the other hand, it is well known that for $p+\mathrm{H}$, the results of Jackson and Schiff[22] are in significantly better agreement with observations than the OBK results. In this case, both Born approximation (B) and (C) reduce to the Jackson and Schiff results since $Z_2=1$.

In this connection a scaling law due to Mapleton[1] should be mentioned. According to this scaling law the OBK cross section for any given proton–multielectron-atom charge transfer is calculated. The result is then multiplied by the ratio of the full Born to the OBK cross sections for the proton–hydrogen-atom charge transfer with the same impact energy as the multielectron-atom case. This scaling law leads to results which agree to better than a factor of 2 with the experimental data for He. The results for O and Ar are also impressive. The main weakness of this scaling law is the scaling of a nonresonance cross section (proton–multielectron-atoms) by a resonance cross section (proton–hydrogen-atom). The cross sections for these two cases have different functional forms in the OBK and the full Born approximations, and as was mentioned earlier, they have distinctly different asymptotic power laws with respect to the impact energy.

Setting $V_c=1/R$ in our Born (C) results helps to compensate for ignoring Coulomb distortions when the projectile is close to the nucleus. While such Coulomb distortions are probably small at high velocities for the OBK term, impact-parameter calculations of Schiff[20] indicate that internuclear contributions may be large at small distances where Coulomb effects may be important. It may be that it is important to pair opposite charges at high velocities to ensure that the total interaction goes to zero asymptotically. However, in atomic charge transfer it is difficult to conclusively justify either of these explanations.

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