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Strong-potential Born-approximation electron-capture cross sections for realistic atomic potentials

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The strong-potential Born approximation to the single-electron capture amplitude in asymmetric ion-atom collisions is discussed in the context of a realistic atomic potential. When final-state binding effects of the captured electron are neglected, a simple connection between the amplitude in the actual atomic-potential case and the one obtained employing a scaled-hydrogenic model is derived which involves the competing effects of an off-shell multiplicative term depending on the residual, target-ion charge and a phase factor containing the difference of the s-wave phase shifts for the two potentials.

The plane-wave Born approximation (PWBA) to the inner-shell ionization amplitude[1] has long been an established cornerstone of atomic-collision theory. Numerous corrections[2] to this basic nonrelativistic scattering amplitude have been enumerated and applied, including binding, polarization, recoil, and relativistic effects.[3] While more elaborate methods for treating ionization now exist,[4] the conceptual simplicity of the PWBA and its overall good agreement with experiment[2] support its use as a lowest-order ionization theory.

Surprisingly, a similar picture of electron capture from inner shells has taken much longer to be developed even though conceptually the capture process can be viewed as an ionization of the electron into the projectile's outgoing direction followed by attachment. Difficulties stemming from the long-range nature of the Coulomb interaction have slowed progress in this area. In recent years, the strong-potential Born (SPB) approximation[5,6] to the electron-capture amplitude has been discussed in a certain limit[6] as the PWBA analogue. Specifically, the SPB amplitude can be shown to represent the folding of an ionization amplitude with the final bound-state momentum distribution in the limit of negligible final-state binding effects of the captured electron.

Implementation of the PWBA has often involved using a scaled-hydrogenic (SH) model in place of the computationally more demanding true atomic potential. Application of the SPB theory has to date used only the SH model. Calculated SPB cross sections for electron capture agree well with experiment,[7,8] but at lower impact energies in less asymmetric situations, e.g., in proton-carbon collisions,[6] theory diverges from experiment sooner than with the PWBA for ionization. Since the SPB theory is so closely tied to the PWBA, this is somewhat puzzling.

In this paper, the low-energy discrepancy is explained by correctly relating[9,10] the SH model to the actual atomic-potential case. As a result, theory and experiment are seen to agree much better in the carbon example while for protons on argon, where larger impact velocities are encountered in a more asymmetric system, results are not altered greatly, in agreement with the conclusions of Macek.[10] A consistent, unified treatment of ionization and capture within the Born approximation is thus obtained. In the following discussion atomic units are used.

Consider the transfer of an active electron to a bare projectile ion from a target ion consisting of nonactive electrons plus nucleus. The incident-channel perturbation $V_{Pe}+V_{PT}$ is a sum of the electron-projectile potential $V_{Pe}=-Z_P/r$ and the interionic potential V_{PT} which reduces asymptotically to Coulomb form with charge Z_aZ_P, where Z_a is the asymptotic target-ion charge. The shielding of the target nucleus of charge Z_T by the nonactive electrons leads to the value Z_a. For neutral targets Z_a is unity; consequently, the initial perturbation is dipolelike.

The SPB approximation to the exact transfer amplitude is obtained by replacing[6] the full Green operator with the Green operator for the target spectrum plus plane-wave projectile motion, and, in contrast to the general case[11] where infinities arise, the resulting amplitude is well defined in the neutral-target case because the initial perturbation is dipolelike. Furthermore, if final-state binding effects involving the captured electron are neglected, the intermediate off-energy-shell electronic scattering state $\psi^-_{\mathbf{s},\varepsilon}$ is reduced to a single continuum state $Q\psi^-_{\mathbf{s}}$ of the target with wave vector $\mathbf{s}$. The off-shell energy is $\varepsilon=p^2/2$.

The factor Q has the same form, namely,

$$Q(Z,s,p)=e^{\pi\nu/2}\Gamma(1-i\nu)[(s-p)/(s+p)]^{i\nu},$$

regardless of whether the assumed potential is pure- or modified-Coulomb in character.[9,10] The charge Z in the modified case is the asymptotic one Z_a and ν denotes Z/p. It is assumed that $s>p$. Use of this "near-shell" wave-function approximation in the amplitude introduces[6,9] errors of order $(s^2-p^2)/(s+p)^2$. The interionic terms are removed from the amplitude using Wick's theorem.[12]

An amplitude is thus obtained which represents the capture analogue of the PWBA for ionization:

$$A_{\rm SPB}=\int d\mathbf{k}\,\tilde{\phi}_f^*(\mathbf{k})Q(Z_a,|\mathbf{v}+\mathbf{k}|,p)^* \times A_{\rm PWBA}(\mathbf{v}+\mathbf{k},\mathbf{k}-\mathbf{K}), \quad (1)$$

where

$$A_{\rm PWBA}(\mathbf{s},\mathbf{q})=\tilde{V}_{Pe}(\mathbf{q})\langle\psi_{\mathbf{s}}^-(\mathbf{r})|e^{i\mathbf{q}\cdot\mathbf{r}}|\phi_i(\mathbf{r})\rangle$$

is the PWBA amplitude for the ionization of an electron in the direction $\mathbf{s}$ with a transfer of momentum $\mathbf{q}$. The momentum spread $\mathbf{k}$ about the projectile velocity $\mathbf{v}$ in the continuum wave function in Eq. (1) is accounted for also in the momentum transfer in the ionization. The momentum transferred to the projectile is denoted by $\mathbf{K}$ with $K^2=K_z^2+K_\perp^2$ and $K_z=-v/2-(\varepsilon_B+\varepsilon_f)/v$; $\mathbf{K}_z$ is taken to be parallel to $\mathbf{v}$. The experimental binding energy ε_B is used in defining $\mathbf{K}_z$. The final bound-state wave function is ϕ_f and the off-shell energy is $p^2/2=v^2/2+\mathbf{v}\cdot\mathbf{k}+\varepsilon_f$ with ε_f the final binding energy. A momentum-space function is denoted by a tilde.

Evaluations of Eq. (1) have so far used a scaled-hydrogenic model where $\psi_{\mathbf{s}}^-(\mathbf{r})$ is calculated for the scaled-Coulomb potential $V_{Te}(r)=-Z_s/r+V_0$. The constant V_0 is chosen, as in ionization case, so that the active electron's initial binding energy corresponds to the experimental value;[13] the scaled charge Z_s is determined by Slater's inner screening rules.[14] Since the scaled-Coulomb potential differs only slightly from the true atomic one in the inner region $r\lesssim 1/Z_s$, the form of the wave function $\psi_{\mathbf{s}}^-(\mathbf{r})$ also varies little there.

Although the *forms* of the two continuum wave functions in the inner region are quite similar, they do possess an overall phase difference, viz., $\exp[i\sigma_0(Z_s,p)]$ compared to $\exp\{i[\sigma_0(Z_a,p)+\delta_0(Z_a,p)]\}$. The s-wave Coulomb phase shift $\sigma_0(Z,p)$ for charge Z and wave vector p is $\arg\Gamma(1-iZ/p)$, and $\delta_0(Z,p)$ denotes the short-range phase shift (relative to Coulomb waves). In the PWBA, this difference of phase has no bearing on the cross section since the latter is proportional to $|A_{\rm PWBA}|^2$. In the SPB approximation, the presence of $A_{\rm PWBA}$ in a momentum integral leads to a different result.

For the SH model the asymptotic charge Z_a in $Q(Z_a,|\mathbf{v}+\mathbf{k}|,p)$ is Z_s (or possibly Z_T). In the actual atomic-potential case for neutral targets Z_a is unity. Since Z_s is much greater than one, the factor Q can be expected to produce quite a different effect in the two models. In order to maintain a general discussion in the following, Z_a is kept in the atomic-potential amplitude.

The local version[15] of the Hartree-Fock approximation due to Slater and here denoted Hartree-Fock-Slater (HFS) is chosen as a realistic atomic potential. Amplitudes for the scaled hydrogenic (SH) and HFS pictures are then given by

$$A_{\rm SPB}^{\rm SH}=\int d\mathbf{k}\,\tilde{\phi}_f^*(k)Q(Z_s,|\mathbf{v}+\mathbf{k}|,p)^*A_{\rm PWBA}^{\rm SH}(\mathbf{v}+\mathbf{k},\mathbf{k}-\mathbf{K}), \quad (2)$$

$$A_{\rm SPB}^{\rm HFS}=\int dk\,\tilde{\phi}_f^*(\mathbf{k})Q(Z_a,|\mathbf{v}+\mathbf{k}|,p)^*e^{-i\Delta(p)}A_{\rm PWBA}^{\rm SH}(\mathbf{v}+\mathbf{k},\mathbf{k}-\mathbf{K}), \quad (3)$$

with

$$\Delta(p)=\sigma_0(Z_s,p)-\sigma_0(Z_a,p)-\delta_0(Z_a,p).$$

The label SH indicates use of a scaled-hydrogenic continuum wave function in a matrix element. Equation (3), the key result of this paper, correctly relates the near-shell SPB amplitude for a realistic atomic potential to the SH amplitude.

Cross sections derived from various evaluations[16] of Eq. (2) have appeared previously; the first results obtained using Eq. (3) are presented here. The evaluation of Eq. (3) employs the dominate peaking of the $\mathbf{k}$ integrand about $k=\pm iZ_P$, which follows from the presence of $\tilde{\phi}_f^*(\mathbf{k})$. The $\mathbf{k}$ integration is carried out in cylindrical coordinates with $\mathbf{k}_z$ taken to be parallel to $\mathbf{v}$. Neglecting the k_ρ dependence of the integrand except in $\tilde{\phi}_f^*(\mathbf{k})$ and $Q(Z_a,|\mathbf{v}+\mathbf{k}|,p)^*$ and performing the k_ρ integration, the peaking in $\tilde{\phi}_f^*$ is seen to translate into poles at $k_z=\pm iZ_P$.

The k_z integration is performed by closing the integration contour in the upper half-plane where only a branch point at iZ_P exists. If k_z is set equal to iZ_P in the integrand except for $\tilde{\phi}_f^*$ and Q^*, the amplitude becomes

$$A_{\rm SPB}^{\rm HFS}=e^{-i\Delta(p_0^*)}A_{\rm PWBA}^{\rm SH}(p_0\hat{\mathbf{v}},iZ_P\hat{\mathbf{v}}-\mathbf{K})I, \quad (4)$$

where

$$I=\int d\mathbf{k}\,\tilde{\phi}_f^*(\mathbf{k})Q(Z_a,|\mathbf{v}+\mathbf{k}|,p)^*$$

and $p_0=v+iZ_P$ with $\varepsilon_f=-Z_P^2/2$ for a $1s$ final state. The approximation in Eq. (4) is much less severe than for a pure SH evaluation because the exponent ν in the energy-phase factor of Q is given by Z_a/p and not Z_s/p. Reference 6 presents a fuller discussion of this "transverse-peaking" approximation.[6]

With this approximation, the phase difference becomes a function of the complex wave vector p_0. Rather than attempt the difficult task of obtaining exact complex phase shifts for a modified-Coulomb potential and since a comparative study of Eqs. (2) and (3) is of interest, the smallness of Z_P/v is used to perform a Taylor expansion of the

phase shifts about v,

$$\Delta(Z,p_0^*)\approx\Delta(Z,v)-iZ_P\Delta'(Z,v)\,,$$

The prime denotes differentiation with respect to the wave vector. The real, short-range phase shifts are obtained by numerical integration of Schrödinger's equation for the HFS potential.[15] To order $(Z_P/v)^2$ it follows from Eq. (4) that

$$A_{\rm SPB}^{\rm HFS}=e^{-Z_P\Delta'(v)}A_{\rm PWBA}^{\rm SH}(p_0\hat{\mathbf{v}},iZ_P\hat{\mathbf{v}}-\mathbf{K})I. \tag{5}$$

Phase factors which cancel when the amplitude is squared have been dropped.

Only the second-order *variation* of the phase shifts as a function of the wave vector plays a role. Figure 1 shows the derivative of the difference of the s-wave phase shifts for the K-shell, scaled-Coulomb, and Hartree-Fock-Slater potentials in carbon and argon. The difference increases as the continuum threshold of the scaled-Coulomb potential is approached; the larger difference seen in the carbon case, which leads to a greater reduction of the cross section, results from the impact energy lying relatively closer to threshold.

For an initial $1s$ state, an explicit evaluation of the ionization amplitude is given by Eq. (5) in the paper by Alston.[6] Assuming $Z_a\le Z_P$, defining $\nu_a=Z_a/(v+iZ_P)$, and writing $[(k^2+Z_P^2)/(2p_0)^2]^{-i\nu_a}$ for $[(|\mathbf{v}+\mathbf{k}|-p)/(|\mathbf{v}+\mathbf{k}|+p)]^{-i\nu}$ to order $(Z_P/v)^2$, one finds for I the expression

$$I=(2^{3/2}Z_P^{5/2}/\pi)e^{\pi\nu_a/2}\Gamma(1-i\nu_a)(2p_0)^{2i\nu_a}\int d\mathbf{k}(k^2+Z_P^2)^{-2-i\nu_a}=\pi^{1/2}(2Z_P)^{3/2}(2p_0/Z_P)^{2i\nu_a}e^{\pi\nu_a/2}\Gamma(\tfrac{1}{2}+i\nu_a)/(1+i\nu_a)\,,$$

which gives

$$|I|^2=\pi^2(2Z_P)^3[2/(1+e^{-2\pi Z_a/v})] \tag{6}$$

to the same order.

Cross sections integrated over transverse momentum transfers, defined as

$$\sigma_{\rm SPB}=(2\pi v^2)^{-1}\int_0^\infty dK_\perp K_\perp|A_{\rm SPB}|^2\,,$$

are shown in Figs. 2 and 3. Results of HFS and SH calculations[17] make use of Eq. (5), with Eq. (6), and Eq. (2), respectively. The argon curves agree quite well with the abundant experimental data of Horsdal-Pedersen *et al.*[8] and differ only slightly from one another. This close agreement supports Macek's general conclusion that the scaled-hydrogenic model does not give greatly different results from a realistic potential model. The phase-derivative term in $A_{\rm SPB}^{\rm HFS}$ generally compensates the larger reduction from Q found in $A_{\rm SPB}^{\rm SH}$. Thus, the two models provide approximately equal results.

In the less asymmetric collision of protons on carbon, results show that good agreement between the two models is again found at higher energies. For lower energies, however, the phase-derivative term gives a relatively larger reduction in the HFS cross section compared to the SH one. Much better agreement with the experimental data of Rødbro, Horsdal-Pedersen, Cocke, and Mac-

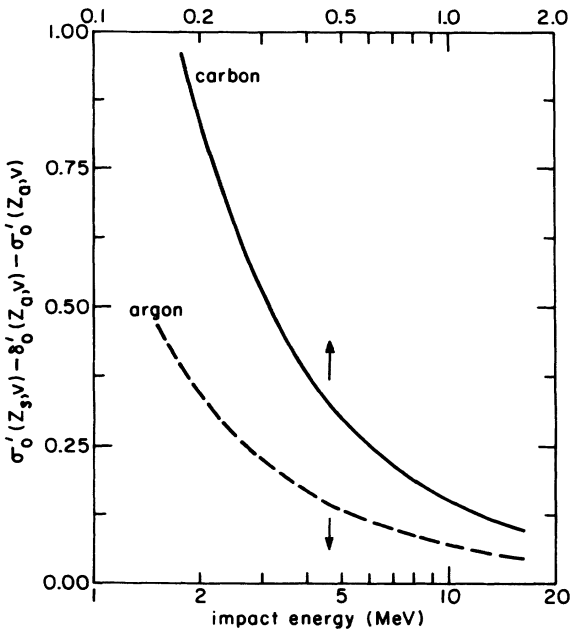

FIG. 1. The derivative with respect to the wave vector of the difference of the s-wave scaled-Coulomb and Hartree-Fock-Slater phase shifts are shown vs a proton-impact energy defined to be 25 keV times the square of the continuum wave vector v in atomic units.

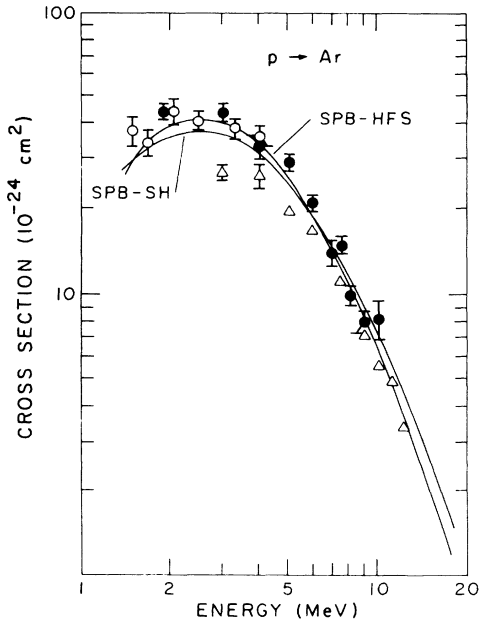

FIG. 2. Strong potential Born cross sections for the capture of a K-shell electron from an argon atom by an incident proton are shown for the scaled-hydrogenic (SH) and more realistic Hartree-Fock-Slater (HFS) models. Experimental data are taken from Horsdal-Pedersen *et al.* (Ref. 8).

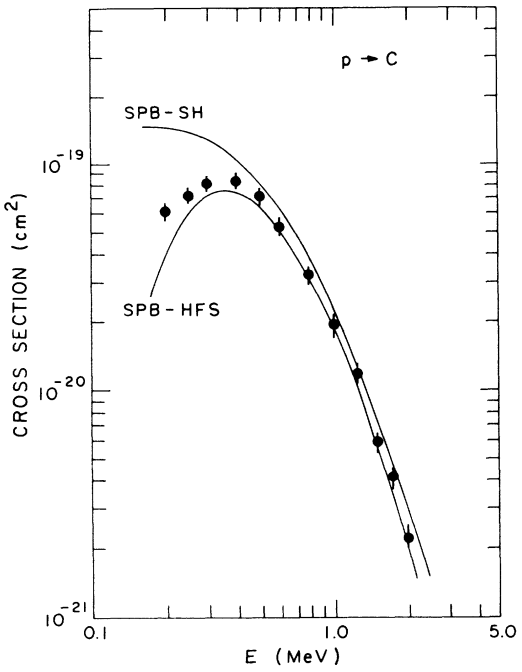

FIG. 3. Strong potential Born cross sections for the capture of a K-shell electron from a carbon atom by an incident proton are shown. Experimental data are taken from Rødbro *et al.* (Ref. 7). See Fig. 2 for curve designations.

donald[7] is found. The sharp rise in the carbon curve in Fig. 1 corresponds directly with the cross-section reduction seen in Fig. 2. The 0.2–0.6 MeV energy range in carbon is rather closer to the threshold of the scaled-Coulomb potential than the 2.0–6.0 MeV range is in argon and, consequently, the phase difference is larger for carbon. The overall phase difference of the HFS and SH wave functions combined with the final-state momentum integration leads to different cross sections. Clearly, previous SPB calculations for less asymmetric collisions should be reconsidered in the light of the present analysis.[16]

The good agreement now found between the realistic atomic-potential model and experiment for both carbon and argon mirrors more closely that found between the PWBA ionization results and experiment, but previously unattained in the SPB capture results. A careful reanalysis of the relationship of the scaled-hydrogenic model to the atomic-potential model has produced the improvement. Although the present evaluation of the SPB amplitude is approximate, the modification of the amplitude seen in Eq. (3) is independent of this. A more accurate calculation could be obtained by employing an HFS version of A_{PWBA} which, however, appears under the $\mathbf{k}$ integral. As the connection between the PWBA and the SPB, which has been strongly emphasized here, is a direct one [Eq. (5)], corrections[2,3] to the PWBA can be readily incorporated into the present SPB approximation.

[1]E. Merzbacher and H. W. Lewis, in *Handbuch der Physik,* edited by S. Flugge (Springer, Berlin, 1958), Vol. 34, p. 166.

[2]G. Basbas, W. Brandt, and R. Laubert, Phys. Rev. A **7**, 983 (1973); **17**, 1655 (1978).

[3]M. H. Chen, B. Crasemann, and H. Mark, Phys. Rev. A **26**, 1243 (1982).

[4]N. Grün, in *Invited Papers of the Fifteenth International Conference on the Physics of Electronic and Atomic Collisons, Brighton, 1987,* edited by H. B. Gilbody *et al.* (North-Holland, Amsterdan, 1988), p. 345.

[5]J. Macek and K. Taulbjerg, Phys. Rev. Lett. **46**, 170 (1981).

[6]J. Macek and S. Alston, Phys. Rev. A **26**, 250 (1982); S. Alston, *ibid.* **27**, 2342 (1983).

[7]M. Rødbro, E. Horsdal-Pedersen, C. L. Cocke, and J. R. MacDonald, Phys. Rev. A **19**, 1936 (1979).

[8]E. Horsdal-Pedersen, C. L. Cocke, J. L. Rasmussen, and S. L. Varghese, J. Phys. B **16**, 1799 (1983).

[9]S. Alston, Phys. Rev. A **38**, 636 (1988).

[10]J. Macek (private communication) and (unpublished).

[11]D. P. Dewangan and J. Eichler, J. Phys. B **19**, 2939 (1986).

[12]J. D. Jackson and H. Schiff, Phys. Rev. **89**, 359 (1953); see footnote on p. 359.

[13]M. O. Krause, Oak Ridge National Laboratory Report No. ORNL-TM-2943, 1970 (unpublished).

[14]J. C. Slater, Phys. Rev. **81**, 385 (1951).

[15]F. Herman and S. Skillman, *Atomic Structure Calculations* (Prentice-Hall, Englewood Cliffs, 1963).

[16]L. J. Dubé, in *Invited Papers of the Fourteenth International Conference on the Physics of Electronic and Atomic Collisons, Palo Alto, 1985,* edited by D. C. Lorents, W. E. Meyerhof, and J. R. Peterson (North-Holland, Amsterdam, 1986), p. 345.

[17]Scaled-hydrogenic results are the transverse-peaking ones of Alston (Ref. 6).