Application of the Schwinger Principle to Direct Excitation of Atoms or Ions by Impact of Bare Nuclei at Intermediate Velocities

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A variational scattering amplitude derived in the impact-parameter formalism is used to investigate the electronic excitation of highly charged ions by ion impact at intermediate velocities. This treatment predicts that the cross sections tend to finite limits when the charge of the projectile increases. This feature is illustrated by the good agreement between our theoretical and experimental results for the excitation of Fe^{24+} by He, N, and Ar. The excitation of H by H^+ is studied as a check of our theory.

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Atomic collision cross sections have been studied extensively as functions of impact energies. Recently, the occurrence of biological and solid state physics experiments with beams of highly charged ions issuing from accelerators[1] has reflected a new trend in atomic collision physics. There is a need to investigate cross sections as a function of the projectile charge Z_P at a given impact velocity v. Many of the above-mentioned experiments are performed at intermediate velocities[2] where conventional treatments require very large basis sets although a significant improvement was made recently by means of triple-center expansions.[3] We present here the general conclusions of a new method based on the variational principle of Schwinger.[4] This principle has already been employed successfully in electron-molecule scattering.[5] Our method was especially designed by two of us,[6] for applications to excitation of hydrogenlike ions of nuclear charge Z_T in collision with bare nuclei of charge $Z_P \lesssim Z_T$ at intermediate velocities, i.e., $v \sim Z_T$ (atomic units are used throughout). We feature briefly the treatment; analytical and computational details are given elsewhere.[6] Let $|\psi_\alpha^+\rangle$ and $|\psi_\beta^-\rangle$ be the scattering wave functions defined, in a collision *without rearrangement,* by the Lippmann-Schwinger equations

$$|\psi_\alpha^+\rangle = |\alpha\rangle + G_T^+ V |\psi_\alpha^+\rangle, \tag{1}$$

$$|\psi_\beta^-\rangle = |\beta\rangle + G_T^- V |\psi_\beta^-\rangle, \tag{2}$$

where G_T^+ are the unperturbed target Green's functions, V is the perturbing potential, and $|\alpha\rangle$ and $|\beta\rangle$ are respectively the initial and final states. The well-known Schwinger scattering amplitude is[4]

$$T_{\beta\alpha} = \frac{\langle\beta|V|\psi_\alpha^+\rangle\langle\psi_\beta^-|V|\alpha\rangle}{\langle\psi_\beta^-|V - VG_T^+V|\psi_\alpha^+\rangle}. \tag{3}$$

$T_{\beta\alpha}$ is stationary with respect to small errors in $|\psi_\alpha^+\rangle$ and $|\psi_\beta^-\rangle$. By expanding $|\psi_\alpha^+\rangle$ and $|\psi_\beta^-\rangle$ on two truncated basis sets $\{|i\rangle\}$ and $\{|j\rangle\}$, respectively, one obtains[7]

$$T_{\beta\alpha} = \sum_{i=1}^{N}\sum_{j=1}^{N} \langle\beta|V|i\rangle D_{ij}^{-1}\langle j|V|\alpha\rangle, \tag{4}$$

where D^{-1} is the inverse of the matrix D of elements

$$D_{ji} = \langle j|V - VG_T^+V|i\rangle. \tag{5}$$

The expression (4) is now stationary with respect to the truncations of both basis sets $\{|i\rangle\}$ and $\{|j\rangle\}$; it is exact when they are complete. For present purposes (heavy-particle collisions), a straight-line impact-parameter Schwinger amplitude $\mathscr{A}_{\beta\alpha}(\rho)$ is used, where ρ is the impact parameter. The internuclear distance is $\mathbf{R} = \boldsymbol{\rho} + \mathbf{Z}$, where Z is the coordinate along the straight path of the projectile. $\mathscr{A}_{\beta\alpha}(\rho)$ is derived from the eikonal expressions of both $T_{\beta\alpha}$ and the Lippmann-Schwinger equations[8]

$$|\psi_k^\pm(Z)\rangle = |k(Z)\rangle + \int_{-\infty}^{+\infty} dZ'\, G_T^\pm(Z - Z')V(Z')|\psi_k^\pm(Z')\rangle \quad (k = \alpha, \beta). \tag{6}$$

The unperturbed propagators $G_T^\pm$ are defined by the equation

$$(H_T - iv\,\partial/\partial Z)G_T^\pm(Z - Z') = \delta(Z - Z'), \tag{7}$$

where H_T is the target Hamiltonian. The initial conditions are $G^\gamma(z) = 0$ if $\gamma z < 0$ ($\gamma = \pm$). The derivation of $\mathscr{A}_{\beta\alpha}(\rho)$ is similar to the quantum derivation of $T_{\beta\alpha}$. Thus $\mathscr{A}_{\beta\alpha}(\rho)$ has the same form (4) as $T_{\beta\alpha}$ but the integrations in the matrix elements run over the electronic coordinates and over Z only. In the following, we are dealing with excitation from the ground state. Hence, both basis sets $\{|i\rangle\}$ and $\{|j\rangle\}$ are restricted to the lowest unperturbed target states, including $|\alpha\rangle$ and $|\beta\rangle$, i.e., they belong to the basis set $\{|\nu\rangle\}$ of eigenstates of $H_T - iv\,\partial/\partial Z$.

With the origin taken on the target nucleus, the states $|\nu\rangle$ are $\phi_\nu(\mathbf{x})\exp[-(\epsilon_\nu/v)Z]$ in the configuration space, where ϕ_ν and ϵ_ν are respectively the eigenfunctions and eigenenergies of the target and $\mathbf{x}$ is the internal electron coordinate. In $\mathscr{A}_{\beta\alpha}(\rho)$, the actual perturbing potential is obtained by omission of the long-range projectile-target Coulomb interaction,[9] i.e., $V=Z_P(R^{-1}-|\mathbf{R}-\mathbf{x}|^{-1})$. The first-Born-type terms of D_{ji} read[6]

$$\langle j|V|i\rangle=\int_{-\infty}^{+\infty}dZ\exp\left(i\frac{\epsilon_j-\epsilon_i}{v}Z\right)W_{ji}(\rho,Z), \tag{8}$$

where W_{ji}, which can be evaluated analytically,[6] is

$$W_{ji}(\rho,Z)=Z_P\int_{-\infty}^{+\infty}d^3x\,\phi_j^*(\mathbf{x})(R^{-1}-|\mathbf{R}-\mathbf{x}|^{-1})\phi_i(\mathbf{x}). \tag{9}$$

By expansion of G_T^+ on the basis set $\{|\nu\rangle\}$, the second-Born-type terms of D_{ji} may be written[6]

$$\langle j|VG_T^+V|i\rangle=-\frac{i}{v}\,\mathrm{S}_\nu\int_{-\infty}^{+\infty}dZ\exp\left(i\frac{\epsilon_j-\epsilon_\nu}{v}Z\right)W_{j\nu}(\rho,Z)\int_{-\infty}^{Z}dZ'\exp\left(i\frac{\epsilon_\nu-\epsilon_i}{v}Z'\right)W_{\nu i}(\rho,Z'). \tag{10}$$

It is worth noting that the functions $W_{\nu\nu'}$ defined in (9) are *exactly* $\propto Z_P$. Since $\langle j|V|i\rangle$ and $\langle j|VG_T^+V|i\rangle$ depend on Z_P only through the functions $W_{\nu\nu'}$, one has clearly from (8) and (10)

$$\langle j|V|i\rangle=Z_PB_{ji}^{\mathrm{I}}, \tag{11}$$

$$\langle j|VG_T^+V|i\rangle=Z_P^2B_{ji}^{\mathrm{II}}, \tag{12}$$

where B_{ji}^{I} and B_{ji}^{II} are respectively the values of $\langle j|V|i\rangle$ and $\langle j|VG_T^+V|i\rangle$ for $Z_P=1$. Thus the matrix elements in $\mathscr{A}_{\beta\alpha}$ must be evaluated only once for $Z_P=1$, which is a great numerical advantage of our treatment. From (5) and the scaling laws (11) and (12) one has

$$D_{ji}=Z_PB_{ji}^{\mathrm{I}}-Z_P^2B_{ji}^{\mathrm{II}}. \tag{13}$$

It is readily seen that, for Z_P *large enough*, $Z_P^2B_{ji}^{\mathrm{II}}$ dominates $Z_PB_{ji}^{\mathrm{I}}$, whatever i and j. In this case, all matrix elements of D become $\propto Z_P^2$. Therefore, all matrix elements of D^{-1} are $\propto Z_P^{-2}$. From (4) and (11), one sees that $\mathscr{A}_{\beta\alpha}(\rho)$ tends to be constant when $Z_P\to\infty$. It turns out that both *differential and total cross sections of excitation* of a given target at a given velocity have *finite limits* when $Z_P\to\infty$. These new important conclusions hold as long as the approximation of straight-line trajectories of the heavy particles is valid.

In the following applications, the sum over ν in (10) is truncated. Indeed the truncation is irrelevant to the variational procedure. Hence the sum over ν has been limited to the lowest target bound states which are necessary to get a reasonable convergence. The continuum states $|\nu\rangle$ have been ignored although they were shown to contribute slightly to the excitation transition at intermediate velocities.[10,11] However, our first application to the excitation of hydrogen atoms by protons, made as a test, shows this contribution to be small. In Figs. 1 and 2 are represented the differential cross sections for the reaction

$$H^++H(1s)\to H^+H(n=2)$$

at 50- and 100-keV proton energies in the laboratory. In the later case our calculations were performed at 105 keV to compare with the experimental total cross sections. The set of states $|i\rangle$ is composed of the hydrogenlike states $1s$, $2s$, $2p_0$, and $2p_{\pm1}$ only. The states $|\nu\rangle$ included in the calculations are all hydrogenlike states between $1s$ and $5g$, but similar results were obtained by including only all states s, p, and d with principal quantum numbers $n=1,\ldots,5$. A reasonable agreement with the experimental differential cross sections[12] is found. At 50 keV, the disagreement between the second Born approximation and the experimental data, which are normalized to the first Born approximation at 200 keV,[12,15] indicates that perturbation theory is not valid at such low velocities. At both energies our results are close to those of the coupled-state equations[13] with two basis sets containing up to seven s, five p, and three d target orbitals,[16] except for small scattering angles at 50 keV where our results seem too small. Also displayed in Fig. 1 are Shakeshaft's coupled-equation results[11] with 35 scaled hydrogenic wave functions on both centers. Our total cross sections agree well with the experimental data,[15] normalized as indicated before, and with the results of Shakeshaft[11] at both energies (Table I).

Then, our theory has been applied successfully to the excitation of $Fe^{24+}(1s^2)$ impinging on various light atoms at 400 MeV (low side of the intermediate-velocity region). Since the targets are neutral atoms, no direct capture from the ion can occur. Furthermore, because of the quite small relative velocity, target electrons cannot directly excite the ion. Finally the K shell of Fe^{24+} is compact enough to consider that excitation is only due to the charge Z_P of the target nucleus. The orbitals of Fe^{24+} are considered as hydrogenlike orbitals around a charge $Z_T=25$ (full electronic screening). Calculations were performed with all s, p, and d states $|\nu\rangle$ up to $n=5$ for the single excitation of the $2s$, $2p$, $3s$, and $3p$ levels of Fe^{24+}. For the excitation of the $n=2$ and $n=3$ levels the sets $\{|i\rangle\}$ are made of $1s$, $2s$, $2p_0$, $2p_{\pm1}$, and $1s$, $3s$, $3p_0$, $3p_{\pm1}$,

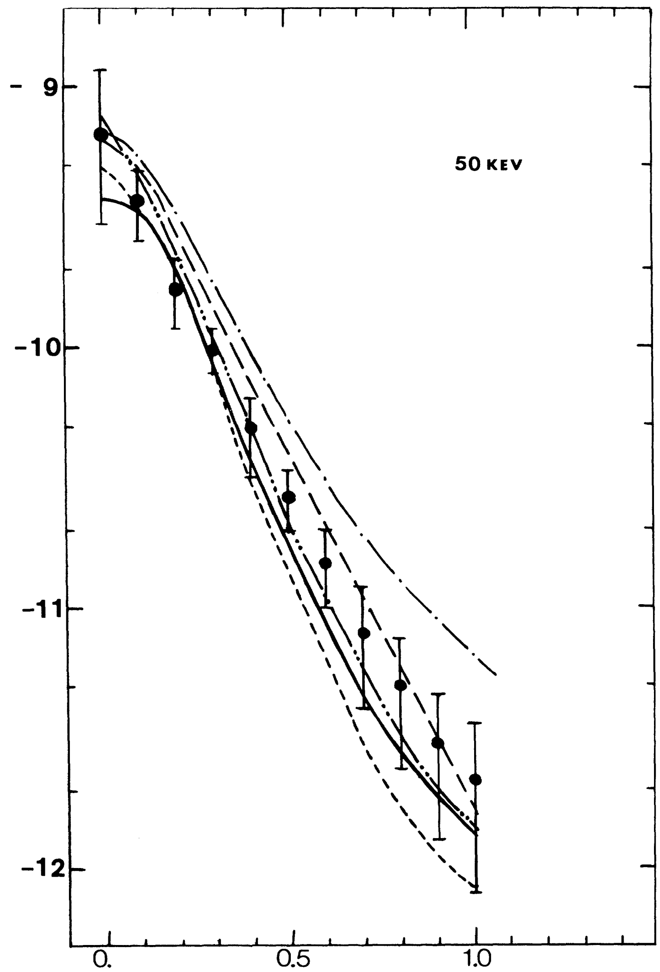

FIG. 1. Excitation of the level $n=2$ of hydrogen atoms by protons. The impact energy is 50 keV in the laboratory. Differential cross sections in cm^2/sr are plotted as functions of the scattering angle in units of 10^{-3} rad in the frame of the center of mass (powers of ten are indicated on the logarithmic vertical scale). Experimental data (Ref. 12); Circles, theoretical data; solid line, present results; double-dot–dashed line, Ref. 13; long dashed line, first Born approximation; dot-dashed line, second Born approximation; short dashed line, Shakeshft's results (Ref. 11) taken in Ref. 14.

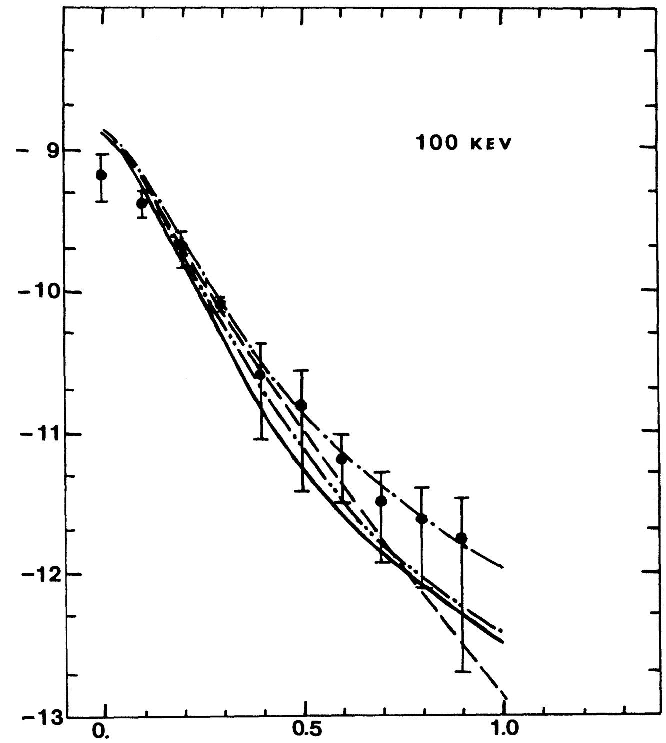

FIG. 2. Same as Fig. 1 at 100-keV impact energy. Actually, our results were calculated at 105 keV.

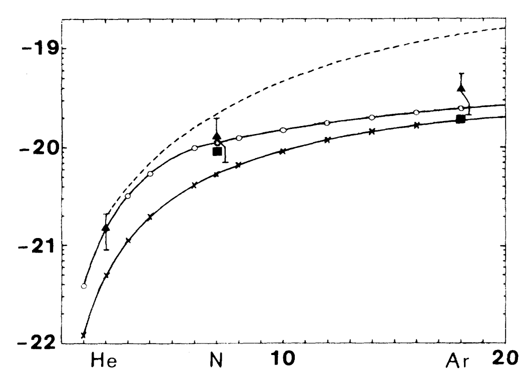

FIG. 3. Excitation of 400-MeV $Fe^{24+}(1s^2)$ impinging on various targets of nuclear charge Z_P indicated on the abscissa axis. The excited levels are $1s$, nl where $n=2$ and $l=0, 1$. The total cross sections per electron in square centimeters, plotted as functions of Z_P, refer to the ordinate axis where a logarithmic scale is used (powers of ten are indicated). $l=0$: line with crosses, present theory; $l=1$: line with circles, present theory; dashed line, first Born approximation; triangles and squares, present experimental data, respectively, without and with subtraction of double-process contribution (Ref. 18) (simultaneous projectile ionization and electron capture from the target) occurring with heavier targets (N,Ar). The precision is the same with both data.

respectively. As a consequence of the variational principle, very stable results ($\sim 10\%$) are found by taking only the initial and final states as set $\{|i\rangle\}$. Our results are displayed in Figs. 3 and 4 together with the experimental data[18] for the excitation of the orbitals $2p$ and $3p$ obtained by two of us (J.P.R. and K.W.), at the Cyclotron à Energie Variable in Orsay, France. Details about the measurements will be given in a forthcoming paper. Good agreement is found, whereas the first Born approximation appears reliable only for $Z_P \ll Z_T$. When $Z_P \simeq Z_T$, our calculations show that second Born terms prevail in the D matrix. It indicates

TABLE I. Total cross sections (in units of 10^{-17} cm^2) for excitation of atomic hydrogen to the $n=2$ level by proton impact at 50 and 105 keV in the laboratory. EXP: experimental data (Ref. 15). Theoretical results: B I and B II are respectively the first and second Born approximations; BDN, Ref. 17; S, Ref. 11 (the result at 105 keV is from Fig. 1 in that paper); SCHW, the present calculations.

	B I	B II	BDN	S	SCHW	EXP
			$E_{\mathrm{lab}}=50$ keV			
$1s \rightarrow 2s$	1.65	5.65	2.69	1.79	1.30	
$1s \rightarrow 2p$	13.32	13.43	9.23	6.88	7.90	
Total	14.97	19.08	11.92	8.67	9.20	10.53 ± 0.64
			$E_{\mathrm{lab}}=105$ keV			
$1s \rightarrow 2s$	0.86	2.07	1.12		0.76	
$1s \rightarrow 2p$	9.28	9.15	8.20		7.79	
Total	10.14	11.23	9.32	8.4	8.54	8.88 ± 0.29

that, at intermediate velocities, perturbation treatments might work only when $Z_P << Z_T$. The agreement between our experimental and theoretical results for $Z_P = 18$ gives evidence for the above-mentioned *saturation* of the excitation cross sections when Z_P is increased. Furthermore, it shows that the Schwinger principle can be a powerful tool to investigate atomic collisions at intermediate velocities when perturbation treatments fail.

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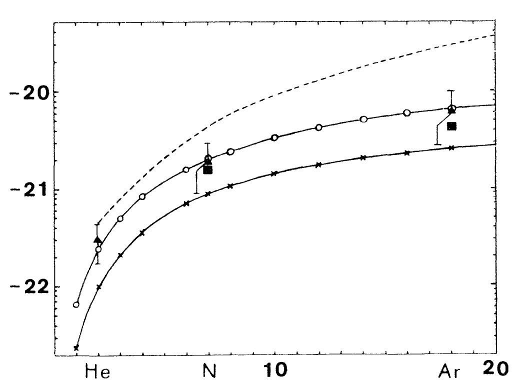

FIG. 4. Same as Fig. 3 but $n=3$.

[1]Proceedings of Models of the Energy Deposition of Ionizing Radiations and the Biological Response, Gesellschaft für Schwerionenforschung, Darmstadt, June 1982 (unpublished); Meeting on the Properties of Heavy Ions in Physics, Biology and Medicine, Institut Curie, Paris, May 1984 (to be published).

[2]R. Gayet, Nucl. Sci. Appl. **1**, 555 (1983).

[3]T. G. Winter and C. D. Lin, Phys. Rev. A **29**, 567, 3071 (1984).

[4]R. G. Newton, *Scattering Theory of Waves and Particles* (McGraw-Hill, New York, 1966), p. 317.

[5]M. E. Smith, R. R. Lucchese, and V. McKoy, Phys. Rev. A **29**, 1857 (1984), and references therein.

[6]B. Brendlé, thèse de troisième cycle, Université de Bordeaux I, 1984 (unpublished) (available at author's address; text in french); B. Brendlé and R. Gayet, to be published.

[7]R. R. Lucchese and V. McKoy, Phys. Rev. A **25**, 1963 (1982).

[8]R. K. Janev and A. Salin, Ann. Phys. (N.Y.) **73**, 136 (1972).

[9]Dž. Belkić, R. Gayet, and A. Salin, Phys. Rep. **56**, 279 (1979).

[10]R. Shakeshaft, J. Phys. B **8**, 114 (1975), and Phys. Rev. A **14**, 1626 (1976).

[11]R. Shakeshaft, Phys. Rev. A **18**, 1930 (1978).

[12]J. T. Park, J. E. Aldag, J. L. Peacher, and J. M. George, Phys. Rev. Lett. **40**, 1646 (1978).

[13]B. H. Bransden and C. J. Noble, Phys. Lett. **70A**, 404 (1978).

[14]J. T. Park, in *Advances in Atomic and Molecular Physics,* edited by D. R. Bates and B. Bederson (Academic, New York, 1983), p. 85.

[15]J. T. Park, J. E. Aldag, J. M. George, and J. L. Peacher, Phys. Rev. A **14**, 608 (1976).

[16]J. Callaway, M. R. C. McDowell, and L. A. Morgan, J. Phys. B **8**, 2181 (1975).

[17]B. H. Bransden, D. P. Dewangan, and C. J. Noble, J. Phys. B **12**, 3563 (1979).

[18]J. P. Rozet, K. Wohrer, A. Chétioui, A. Jolly, C. Stephan, and B. Brendlé, and R. Gayet, to be published.