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Charge-exchange reactions in a three-body eikonal approach

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Abstract. The three-body eikonal approach to ion–atom collisions based on the Alt–Grassberger–Sandhas equations is developed. The amplitudes for scattering and charge exchange, written in the impact parameter representation and using the eikonal approximation, are represented as a sum of two terms. One of them describes the scattering via the Coulomb potential acting between the colliding heavy particles. The second one could be factored into a product of two terms. One is an explicitly known factor which contains all the information about the interaction between the heavy particles. The remaining part does not contain any reference to this interaction any longer. For these residual amplitudes effective-two body equations are written down. Explicit expressions for the effective potentials occurring therein, for both the scattering and the transfer channels, are derived in the lowest order approximation. This approach is then used to calculate total and partial cross sections for the electron capture processes in collisions of the ions H^+, He^{2+} and Li^{3+} with atomic hydrogen. The latter is taken to be in its ground state, except for the case of incident H^+ when the target hydrogen atom is considered also in some low-lying excited states.

1. Introduction

Avakov *et al* (1990b, hereafter referred to as I) have developed the impact parameter Faddeev approach (IPFA) in the Alt–Grassberger–Sandhas (AGS) form for systems of three charged particles. This approach has then been employed by Avakov *et al* (1990a, hereafter referred to as II) and Avakov *et al* (1992) to calculate electron transfer in reactions of fully stripped ions colliding with atomic hydrogen and multielectron targets. The AGS integral equations for scattering and electron transfer amplitudes pertaining to ion–atom collisions were solved in the K-matrix Born approximation which reduces them to a system of algebraic equations. In the concrete calculations of charge-exchange processes the occurring effective potential was taken into account in its lowest-order approximation which corresponds to the electron-transfer ('pole') amplitude.

On the other hand, it was shown by Belkić *et al* (1979) that in the eikonal approximation the amplitude for electron transfer, when written in the impact parameter representation, can be represented as a product of two factors. The first factor is explicitly expressed through the internuclear Coulomb potential, while the second one does not depend on this interaction at all. In the present paper an analogous expression for the amplitude in the impact parameter representation in eikonal approximation is derived for general binary processes. Integral equations of the AGS form are obtained for that part of the amplitude which does not depend on the internuclear interaction. That is, when calculating the effective potentials occurring

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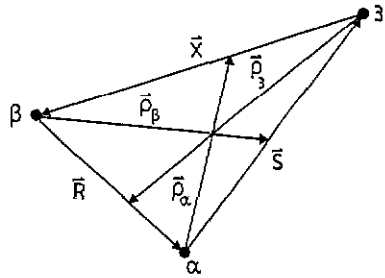

Figure 1. Relative coordinates in three-particle system.

herein, e.g., via the quasi-Born expansion method (Alt *et al* 1967), terms containing the interaction between the heavy particles do not occur any longer.

This approach is used to calculate total and partial cross sections of electron transfer in collisions of the fully stripped ions H^+, He^{2+} and Li^{3+} with hydrogen atoms being both in the ground and in some low-lying excited states. In contrast to the calculations from II and from Avakov *et al* (1992), the present ones approximately take into account the effective potential in the scattering channels as well.

First results were published in a brief report in Alt *et al* (1993).

Atomic units are used throughout the paper.

2. Eikonal amplitudes and three-body equations

We consider a system of three charged particles α, β and 3, where α and β are heavy particles (nuclei) and particle 3 is an electron. The index γ will be used to characterize either the channel containing the heavy particle γ and a bound state of the other nucleus and the electron 3, or the γ subsystem consisting of the heavy particle not equal to γ and the electron 3. That is, we always have either $\gamma = \alpha$ or $\gamma = \beta$. In terms of the AGS three-body transition operators $U_{\beta\alpha}$ the on-shell amplitudes describing the transition from channel α to channel β have the form

$$T_{\beta\alpha}(q'_\beta, q_\alpha) = \langle q'_\beta, \varphi_\beta | U_{\beta\alpha} | \varphi_\alpha, q_\alpha \rangle \tag{1}$$

where q_γ is the relative momentum of the fragments in channel γ. Note that the energy dependence of the various quantities will be suppressed unless required for clarity. The bound state wavefunction in configuration space, $\varphi_\gamma(r_\gamma)$, is the solution of the Schrödinger equation

$$(\hat{E}_\gamma - k_\gamma - V_\gamma)\varphi_\gamma(r_\gamma) = 0 \tag{2}$$

belonging to the binding energy $\hat{E}_\gamma$, V_γ being the Coulomb potential between the electron and the nucleus in subsystem γ. Furthermore, $k_\gamma = -\Delta_{r_\gamma}/2\mu_\gamma$ is the kinetic energy operator of relative motion of the two bound particles, and μ_γ their reduced mass. The transition operators are defined as

$$U_{\beta\alpha} = \bar{\delta}_{\beta\alpha} G_\alpha^{-1} + \bar{V}_\beta + \bar{V}_\beta G \bar{V}_\alpha. \tag{3}$$

Here the conventional notations are used: $\bar{\delta}_{\beta\alpha} = 1 - \delta_{\beta\alpha}$ is the anti-Kronecker symbol, $\bar{V}_\gamma = V - V_\gamma$ and $V = \sum_{\gamma=1}^{3} V_\gamma$ are the channel and the total interaction, respectively. Furthermore, $G(z) = (z - H_0 - V)^{-1}$ is the full resolvent of the three-particle system and $G_\alpha(z) = (z - H_0 - V_\alpha)^{-1}$ is the resolvent in channel α, H_0 being the free Hamiltonian.

One can rewrite the amplitude (1) in the form (Alt and Sandhas 1980)

$$T_{\beta\alpha}(q'_\beta, q_\alpha) = \delta_{\beta\alpha} t_\alpha(q'_\alpha, q_\alpha) + \langle \Psi_\beta^{(-)}, \varphi_\beta | \tilde{U}_{\beta\alpha} | \varphi_\alpha, \Psi_\alpha^{(+)} \rangle \tag{4}$$

with 'distorted' transition operators $\tilde{U}_{\beta\alpha}$ which are defined as

$$\tilde{U}_{\beta\alpha} = \bar{\delta}_{\beta\alpha} g_\alpha^{-1} + (\bar{V}_\beta - v_\beta) + (\bar{V}_\beta - v_\beta) G (\bar{V}_\alpha - v_\alpha). \tag{5}$$

Here,

$$g_\alpha(z) = (z - H_0 - V_\alpha - v_\alpha)^{-1}. \tag{6}$$

Denoting by e_γ the charge of particle γ, and by ρ_γ the coordinate of particle γ relative to the centre of mass of the other two particles (see figure 1), the distortion potentials v_α and v_β are chosen in configuration space as

$$v_\alpha(\rho_\alpha) = \frac{e_\alpha e_\beta}{\rho_\alpha} \qquad v_\beta(\rho_\beta) = \frac{e_\alpha e_\beta}{\rho_\beta}. \tag{7}$$

The wavefunctions $\Psi_\alpha^{(+)}(\rho_\alpha)$ and $\Psi_\beta^{(-)}(\rho_\beta)$ are solutions of the Schrödinger equations

$$(E - \hat{E}_\alpha - K_\alpha - v_\alpha)\Psi_\alpha^{(+)}(\rho_\alpha) = 0 \tag{8}$$

$$(E - \hat{E}_\beta - K_\beta - v_\beta)\Psi_\beta^{(-)}(\rho_\beta) = 0 \tag{9}$$

satisfying appropriate boundary conditions. Here, $E = \hat{E}_\gamma + q_\gamma^2/2M_\gamma$ is the total three-body energy, with M_γ being the reduced mass of the fragments in channel γ. Moreover, $K_\gamma = -\Delta_{\rho_\gamma}/2M_\gamma$ denotes the kinetic energy operator of relative motion of particle γ and the bound subsystem of the other two particles. The two-body amplitude $t_\alpha(q'_\alpha, q_\alpha)$ in (4) describes the scattering of particle α off the centre of mass of the bound subsystem $(\beta + 3)$ but with the potential v_α.

Since the electron mass is small compared to the masses of the nuclei α and β one can put $\rho_\alpha \simeq \boldsymbol{R}$, $\rho_\beta \simeq -\boldsymbol{R}$, where $\boldsymbol{R}$ is the radius vector of the heavy particle α relative to the heavy particle β. Consequently, to the same accuracy we also have

$$v_\alpha(\rho_\alpha) \simeq v_\beta(\rho_\beta) \simeq V_3(\boldsymbol{R}) = \frac{e_\alpha e_\beta}{R}. \tag{10}$$

We consider the amplitude (4) in the eikonal approximation. It is well known that in this approximation the solutions $\Psi_\alpha^{(+)}(\rho_\alpha)$ and $\Psi_\beta^{(-)}(\rho_\beta)$ of (8) and (9), respectively, have the simple form of distorted plane waves

$$\Psi_\alpha^{(+)}(\rho_\alpha) = \mathrm{e}^{\mathrm{i}q_\alpha \cdot \rho_\alpha} \mathcal{F}_\alpha^{(+)}(\rho_\alpha) \qquad \Psi_\beta^{(-)}(\rho_\beta) = \mathrm{e}^{-\mathrm{i}q'_\beta \cdot \rho_\beta} \mathcal{F}_\beta^{(-)}(\rho_\beta) \tag{11}$$

where

$$\mathcal{F}_\alpha^{(+)}(\rho_\alpha) = \exp\{\mathrm{i}\eta_3 \ln(q_\alpha \rho_\alpha - q_\alpha \cdot \rho_\alpha)\} \tag{12}$$

$$\mathcal{F}_\beta^{(-)}(\rho_\beta) = \exp\{-\mathrm{i}\eta_3 \ln(q'_\beta \rho_\beta - q'_\beta \cdot \rho_\beta)\}. \tag{13}$$

Here, $\eta_3 = e_\alpha e_\beta / v$ is the Coulomb parameter corresponding to the interaction V_3, with $v = q_\alpha / M_\alpha$ being the relative velocity of colliding particles.

The full three-particle resolvent takes the form

$$G(E) \simeq G^e(E) = (E - k_\alpha - K_\alpha^e - V + \mathrm{i}0)^{-1} = \left[E - k_\alpha + \frac{q_\alpha^2}{2M_\alpha} + \mathrm{i}\frac{q_\alpha}{M_\alpha}\frac{\partial}{\partial z_\alpha} - V + i0 \right]^{-1} \tag{14}$$

where z_α is the projection of ρ_α onto the direction of q_α. Taking into account the result of the action of the operators $G^e(E)$ and $g_\alpha^{-1}(E)$ onto the functions of the relative coordinate ρ_α standing to the right of them, one obtains the amplitude $T_{\beta\alpha}(q'_\beta, q_\alpha)$ in eikonal approximation in the form

$$T_{\beta\alpha}(q'_\beta, q_\alpha) = \delta_{\beta\alpha}\, t_\alpha(q'_\alpha, q_\alpha) + \int \mathrm{d}^3R\, \mathrm{d}^3\rho_3\, \mathcal{F}_\beta^{(-)*}(\rho_\beta)\, \mathcal{F}_\alpha^{(+)}(\rho_\alpha) \times \mathrm{e}^{\mathrm{i}q'_\beta\cdot\rho_\beta} \varphi_\beta^*(r_\beta)\, U_{\beta\alpha}^{(0)}\, \varphi_\alpha(r_\alpha) \mathrm{e}^{\mathrm{i}q_\alpha\cdot\rho_\alpha}. \tag{15}$$

Here and in what follows the variables ρ_α, r_α, ρ_β and r_β are considered to be expressed as linear combinations of $\boldsymbol{R}$ and ρ_3. The transition operator

$$U_{\beta\alpha}^{(0)} = \bar{\delta}_{\beta\alpha} G_\alpha^{-1} + (\bar{V}_\beta - v_\beta) + (\bar{V}_\beta - v_\beta)\tilde{G}(\bar{V}_\alpha - v_\alpha) = \bar{\delta}_{\beta\alpha} G_\alpha^{-1} + V_\alpha + V_\alpha \tilde{G} V_\beta \tag{16}$$

is seen to be equal to the eikonal approximation of the original operator $U_{\beta\alpha}$, equation (3), with $V_3 \equiv 0$. Hence all information about the effects of the heavy-heavy interaction V_3 is contained solely in the scattering amplitude $t_\alpha(q'_\alpha, q_\alpha)$ and in the phase factor $\mathcal{F}_\beta^{(-)*}(\rho_\beta)\mathcal{F}_\alpha^{(+)}(\rho_\alpha)$. In fact, setting $M_\alpha \simeq M_\beta \simeq M$, $|q_\alpha| \simeq |q'_\beta| \simeq Mv$ and $\rho_\alpha \simeq \rho_\beta \simeq R = (b^2 + Z^2)^{1/2}$, where b is the impact parameter or, equivalently, the component of $\boldsymbol{R}$ in the plane perpendicular to q_α, and Z is the component of $\boldsymbol{R}$ in the direction of q_α, we can estimate that

$$\mathcal{F}_\beta^{(-)*}(\rho_\beta)\mathcal{F}_\alpha^{(+)}(\rho_\alpha) \simeq (Mvb)^{2\mathrm{i}\eta_3}. \tag{17}$$

In the case of direct scattering ($\alpha \to \alpha$) one also has

$$\mathcal{F}_\alpha^{(-)*}(\rho_\alpha)\mathcal{F}_\alpha^{(+)}(\rho_\alpha) \simeq (Mvb)^{2\mathrm{i}\eta_3}. \tag{18}$$

Let us rewrite the integral term on the right-hand side of (15) in the form

$$\frac{1}{2\pi} \int \mathrm{d}^2b\, \mathrm{e}^{\mathrm{i}q_\perp\cdot b} (Mvb)^{2\mathrm{i}\eta_3} \mathcal{T}_{\beta\alpha}^{(0)}(b) \tag{19}$$

where $q_\perp$ is the transverse component of the momentum transfers

$$p = q_\alpha - q'_\beta \mu_\beta / m_3 \qquad q = q_\alpha \mu_\alpha / m_3 - q'_\beta \tag{20}$$

in the rearrangement case, and of

$$q = q_\alpha - q'_\alpha \tag{21}$$

for scattering. Here μ_β and μ_α are the reduced masses of the pairs $(\alpha+3)$ and $(\beta+3)$, respectively, and $m_3 = 1$ is the electron mass in atomic units. The quantity

$$\mathcal{T}^{(0)}_{\beta\alpha}(b) = 2\pi e^{-iq_\perp\cdot b}\iint dZ d^3\rho_3\, e^{iq'_\beta\cdot\rho_\beta}\varphi^*_\beta(r_\beta)U^{(0)}_{\beta\alpha}\varphi_\alpha(r_\alpha)e^{iq_\alpha\cdot\rho_\alpha} \tag{22}$$

depends neither on the interaction V_3, nor on the transverse components $q_\perp$.

The transition amplitude in the impact parameter representation, $\mathcal{T}_{\beta\alpha}(b)$, is related to the one in the momentum representation, $T_{\beta\alpha}(q'_\beta, q_\alpha) \simeq T_{\beta\alpha}(q_\perp)$, by the transformation (see I)

$$\mathcal{T}_{\beta\alpha}(b) = \frac{1}{2\pi}\int d^2q_\perp e^{-iq_\perp\cdot b}T_{\beta\alpha}(q_\perp) \qquad = \tilde{\mathcal{T}}_{\beta\alpha}(b)\, e^{i(m_\alpha - m_\beta)\varphi_b} \tag{23}$$

where m_γ is the azimuthal quantum number of the bound electron in subsystem γ, and φ_b is the azimuthal angle of b. By using (23) with (19) one can rewrite (15) in the impact parameter representation as

$$\mathcal{T}_{\beta\alpha}(b) = \delta_{\beta\alpha}\tau_\alpha(b) + (Mvb)^{2i\eta_3}\mathcal{T}^{(0)}_{\beta\alpha}(b) \tag{24}$$

where $\mathcal{T}^{(0)}_{\beta\alpha}(b)$ is given by (22), and $\tau_\alpha(b)$ which corresponds to the amplitude $t_\alpha(q_\perp)$ by

$$\tau_\alpha(b) = 2i\pi v\{e^{2i\eta_3\ln(Mvb)} - 1\}. \tag{25}$$

Thus, the amplitudes $\mathcal{T}_{\beta\alpha}(b)$ are determined once $\mathcal{T}^{(0)}_{\beta\alpha}(b)$ have been calculated. To solve the latter problem one should use the usual AGS integral equations but with the internuclear Coulomb potential V_3 switched off.

It proves advantageous to decompose the momentum space amplitude $T^{(0)}_{\beta\alpha}(q'_\beta, q_\alpha)$ corresponding to $\mathcal{T}^{(0)}_{\beta\alpha}(b)$ as

$$T^{(0)}_{\beta\alpha}(q'_\beta, q_\alpha) = \delta_{\beta\alpha}t'_\alpha(q'_\alpha, q_\alpha) + \tilde{T}^{(0)}_{\beta\alpha}(q'_\beta, q_\alpha) \tag{26}$$

with

$$\tilde{T}^{(0)}_{\beta\alpha}(q'_\beta, q_\alpha) = \langle\Psi'^{(-)}_\beta, \varphi_\beta|\tilde{U}^{(0)}_{\beta\alpha}|\varphi_\alpha, \Psi'^{(+)}_\alpha\rangle. \tag{27}$$

The transition operator $\tilde{U}^{(0)}_{\beta\alpha}$ occurring here is given by

$$\tilde{U}^{(0)}_{\beta\alpha} = \bar{\delta}_{\beta\alpha}(g'_\alpha)^{-1} + (V_\alpha - v'_\beta) + (V_\alpha - v'_\beta)\tilde{G}(V_\beta - v'_\alpha) \tag{28}$$

where

$$g'_\alpha(z) = (z - H_0 - V_\alpha - v'_\alpha)^{-1} \tag{29}$$

with the distortion potentials chosen as

$$v'_\alpha = -\frac{e_\alpha}{\rho_\alpha} \qquad v'_\beta = -\frac{e_\beta}{\rho_\beta}. \tag{30}$$

The wavefunctions $\Psi'^{(+)}_\alpha(\rho_\alpha)$ and $\Psi'^{(-)}_\beta(\rho_\beta)$ are solutions of the Schrödinger equations

$$(E - \hat{E}_\alpha - K_\alpha - v'_\alpha)\Psi'^{(+)}_\alpha(\rho_\alpha) = 0 \tag{31}$$

$$(E - \hat{E}_\beta - K_\beta - v'_\beta)\Psi'^{(-)}_\beta(\rho_\beta) = 0. \tag{32}$$

Furthermore, the amplitude $t'_\alpha(q'_\alpha, q_\alpha)$ describes scattering of particle α off the centre of mass of the subsystem $(\beta + 3)$ with potential v'_α.

In the impact parameter representation the decomposition (26) looks as

$$\mathcal{T}^{(0)}_{\beta\alpha}(b) = \delta_{\beta\alpha}\tau'_\alpha(b) + \mathcal{T}^{(0)'}_{\beta\alpha}(b) \tag{33}$$

where

$$\tau'_\alpha(b) = 2i\pi v\{e^{2i\eta_\alpha \ln(Mvb)} - 1\} \tag{34}$$

$$\eta_\alpha = -\frac{e_\alpha}{v}. \tag{35}$$

By using (33) for $\mathcal{T}^{(0)}_{\beta\alpha}(b)$ on the right-hand side of (24) we obtain the final result for the transition amplitude in the eikonal approximation

$$\mathcal{T}_{\beta\alpha}(b) = \delta_{\beta\alpha}\, 2\pi i v\{(Mvb)^{2i(\eta_3+\eta_\alpha)} - 1\} + (Mvb)^{2i\eta_3}\mathcal{T}^{(0)'}_{\beta\alpha}(b) \tag{36}$$

with

$$\eta_3 + \eta_\alpha = \frac{e_\alpha(e_\beta - 1)}{v}. \tag{37}$$

As in (23) we can define $\tilde{\mathcal{T}}^{(0)}_{\beta\alpha}(b)$ via

$$\mathcal{T}^{(0)'}_{\beta\alpha}(b) = \tilde{\mathcal{T}}^{(0)}_{\beta\alpha}(b)e^{i(m_\alpha - m_\beta)\varphi_b}. \tag{38}$$

Note that an analogous factor can be split off from the effective potentials (see below). Hence, if off-shell effects are neglected the amplitudes $\tilde{\mathcal{T}}^{(0)}_{\beta\alpha}(b)$ are found as solutions of the set of coupled algebraic equations

$$\tilde{\mathcal{T}}^{(0)}_{\beta n,\alpha m}(b) = \tilde{\mathcal{V}}^{(+)}_{\beta n,\alpha m}(b) - \frac{i}{4\pi v}\sum_{\gamma,r}\tilde{\mathcal{V}}^{(-)}_{\beta n,\gamma r}(b)\tilde{\mathcal{T}}^{(0)}_{\gamma r,\alpha m}(b) \tag{39}$$

where n, m and r are the full sets of quantum numbers of the bound electron, and $\tilde{\mathcal{V}}^{(\pm)}_{\beta n,\alpha m}(b)$ are the effective potentials to be discussed in detail in the next section. As indicated above the latter coincide with the standard expressions except that they do not contain the interaction between the heavy particles α and β. Thus, calculation of the amplitude $\tilde{\mathcal{T}}^{(0)}_{\beta\alpha}(b)$ and, then by means of (36) of $\mathcal{T}_{\beta\alpha}(b)$, allows us to find scattering and electron transfer cross sections in eikonal approximation.

3. The effective potentials

In the AGS equations for three charged particles (Alt and Sandhas 1980) the effective potentials are defined by

$$\mathcal{V}^{(\pm)}_{\beta n,\alpha m}(q'_\beta, q_\alpha) = \langle \Psi'^{(-)}_\beta | Z_{\beta n,\alpha m}(z) - \delta_{\beta\alpha}\delta_{nm}v'_\alpha | \Psi'^{(\pm)}_\alpha \rangle \tag{40}$$

with

$$Z_{\beta n,\alpha m}(z) = \langle \chi_{\beta n} | G_0 U'_{\beta\alpha}(z) G_0 | \chi_{\alpha m} \rangle. \tag{41}$$

The distortion potential v'_α is given by (30). The bound state form factor of subsystem γ is related to the corresponding wavefunction via $|\chi_{\gamma r}\rangle = V_\gamma|\varphi_{\gamma r}\rangle$. In eikonal approximation, the solutions $\Psi'^{(+)}_\alpha$ and $\Psi'^{(-)}_\beta$ of the Schrödinger equations (31) and (32), respectively, are distorted plane waves

$$\Psi'^{(\pm)}_\alpha(\rho_\alpha) = e^{iq_\alpha\cdot\rho_\alpha}\mathcal{F}'^{(\pm)}_\alpha(\rho_\alpha), \quad \Psi'^{(-)}_\beta(\rho_\beta) = e^{-iq'_\beta\cdot\rho_\beta}\mathcal{F}'^{(-)}_\beta(\rho_\beta) \tag{42}$$

with

$$\mathcal{F}'^{(\pm)}_\alpha(\rho_\alpha) = \exp\{\pm i\eta_\alpha \ln(q_\alpha\rho_\alpha \mp q_\alpha\cdot\rho_\alpha)\} \tag{43}$$

$$\mathcal{F}'^{(-)}_\beta(\rho_\beta) = \exp\{-i\eta_\beta \ln(q'_\beta\rho_\beta - q'_\beta\cdot\rho_\beta)\} \tag{44}$$

$$\eta_\alpha = -\frac{e_\alpha}{v} \qquad \eta_\beta = -\frac{e_\beta}{v}. \tag{45}$$

Such a structure of the effective potentials $Z_{\beta n,\alpha m}(z)$ results from the following *decomposition of the two-particle T-matrix into a non-separable and a separable term* (Alt *et al* 1967)

$$T_\gamma(z) = T'_\gamma(z) + T^s_\gamma(z) \tag{46}$$

where the latter is of the form

$$T^s_\gamma(z) = \sum_r |\chi_{\gamma r}\rangle\hat{t}_{\gamma r}\langle\chi_{\gamma r}| \tag{47}$$

with

$$\hat{t}_{\gamma r} = (z - \hat{E}_{\gamma r})^{-1}. \tag{48}$$

We recall that in this approach the separable part $T^s_\gamma(z)$ is to be constructed such as to contain all bound state poles in subsystem γ (at energies $\hat{E}_{\gamma r}$) of the original amplitude $T_\gamma(z)$ via $\hat{t}_{\gamma r}$. Consequently, $T'_\gamma(z)$ does not contain any pole contribution. Note that we choose the same notation for the operators in the three-particle and in the two-particle space. However, when considering the corresponding plane wave matrix elements the well known energy shift $z \to z - q^2_\gamma/2M_\gamma$ has to be taken into account.

The presence of the free Green functions G_0 in (41) leads to unpleasant difficulties in the calculation of the effective potentials. They can partly be avoided by using an alternative decomposition of the two-particle T-matrix

$$T_\gamma(z) = \tilde{T}'_\gamma(z) + \tilde{T}^s_\gamma(z) \tag{49}$$

with

$$\tilde{T}^s_\gamma(z) = \sum_r |\chi_{\gamma r}\rangle\hat{t}_{\gamma r}\langle\varphi_{\gamma r}|G_0^{-1}(z). \tag{50}$$

Such a splitting leads to the same structure of the AGS equations. However, the effective potentials $Z_{\beta n,\alpha m}$ are now given as

$$Z_{\beta n,\alpha m}(z) = \langle\varphi_{\beta n}|U'_{\beta\alpha}(z)G_0|\chi_{\alpha m}\rangle. \tag{51}$$

The matrix elements of $U'_{\beta\alpha}$ can be evaluated, e.g., by using the quasi-Born expansion

$$U'_{\beta\alpha} = \bar{\delta}_{\beta\alpha} G_0^{-1} + \sum_\gamma \bar{\delta}_{\beta\gamma}\, \bar{\delta}_{\gamma\alpha}\, \tilde{T}'_\gamma + \ldots. \tag{52}$$

Let us find the lowest order approximations to the effective potential. Insertion of the first term of the expansion (52) into the right-hand side of (51) yields the zeroeth order (in terms of powers of $\tilde{T}'_\gamma$) approximation for the effective potential in the transfer channel

$$\mathcal{V}^{(0)(\pm)}_{\beta n,\alpha m}(q'_\beta, q_\alpha) = \bar{\delta}_{\beta\alpha} \langle \Psi'^{(-)}_\beta, \varphi_{\beta n} | \chi_{\alpha m}, \Psi'^{(\pm)}_\alpha \rangle. \tag{53}$$

The second term in the expansion (52), with V_3 switched off when inserted into (51) and (40) (cf the discussion following (39)), gives rise to the lowest order contribution to the effective potential in the scattering channel

$$\mathcal{V}^{(1)(\pm)}_{\alpha n,\alpha m}(q'_\alpha, q_\alpha) = \langle \Psi'^{(-)}_\alpha, \varphi_{\alpha n} | \tilde{T}'_\beta(z) G_0(z) | \chi_{\alpha m}, \Psi'^{(\pm)}_\alpha \rangle - \delta_{nm} \langle \Psi'^{(-)}_\alpha | v'_\alpha | \Psi'^{(\pm)}_\alpha \rangle. \tag{54}$$

In what follows, when calculating the electron transfer cross sections by (39) we will take into account only the terms $\mathcal{V}^{(0)(\pm)}_{\beta n,\alpha m}(q'_\beta, q_\alpha)$ and $\mathcal{V}^{(1)(\pm)}_{\alpha n,\alpha m}(q'_\alpha, q_\alpha)$ for the effective potentials. In addition, when evaluating $\mathcal{V}^{(1)(\pm)}_{\alpha n,\alpha m}$ we will approximate the amplitude $\tilde{T}'_\beta$ by the potential V_β.

One more approximation is connected with the attempt to get rid of the free Green function on the right-hand side of (54). Analogously to what was done in section 2, when using the eikonal approximation one can show that

$$G_0(E) \mathcal{F}'^{(\pm)}_\alpha(\rho_\alpha) e^{iq_\alpha \cdot \rho_\alpha} = \mathcal{F}'^{(\pm)}_\alpha(\rho_\alpha) \tilde{G}_\alpha(E) e^{iq_\alpha \cdot \rho_\alpha} \tag{55}$$

where

$$\tilde{G}_\alpha(E) = (E - k_\alpha - K^e_\alpha - \tilde{v}'_\alpha + i0)^{-1} \tag{56}$$

and $\tilde{v}'_\alpha(\rho_\alpha) = -v'_\alpha(\rho_\alpha)$. Let us write the resolvent $\tilde{G}_\alpha(E)$ as

$$\tilde{G}_\alpha = G_0 + G_0 \tilde{t}'_\alpha G_0 \tag{57}$$

with the transition operator $\tilde{t}'_\alpha$ being defined by

$$\tilde{t}'_\alpha = \tilde{v}'_\alpha + \tilde{v}'_\alpha G_0 \tilde{t}'_\alpha. \tag{58}$$

It is obvious that $\tilde{t}'_\alpha$ does not contain any contribution from bound states since the potential $\tilde{v}'_\alpha$ is positive. Thus, the additional approximation consists in neglecting all terms proportional to $\tilde{t}'_\alpha$ as being of higher order. In other words, for $\tilde{G}_\alpha$ we use its lowest order approximation, $\tilde{G}_\alpha \approx G_0$. Since in (39) the effective potentials are needed on the energy shell only, taking into account (55) one finally has $G_0(\hat{E}_{\alpha m} + q_\alpha^2/2M_\alpha + i0)|\chi_{\alpha m}, q_\alpha\rangle = |\varphi_{\alpha m}, q_\alpha\rangle$ on the right-hand side of (54). Collecting things together we arrive at the following approximate expression for the effective potential in the scattering channel

$$\mathcal{V}^{(1)(\pm)}_{\alpha n,\alpha m}(q'_\alpha, q_\alpha) = \langle \Psi'^{(-)}_\alpha, \varphi_{\alpha n} | V_\beta | \varphi_{\alpha m}, \Psi'^{(\pm)}_\alpha \rangle - \delta_{nm} \langle \Psi'^{(-)}_\alpha | v'_\alpha | \Psi'^{(\pm)}_\alpha \rangle \tag{59}$$

which will be used for the numerical investigations.

3.1. The effective potential: rearrangement channel

According to (53) the effective potential occurring as driving term in the electron transfer channel is explicitly given by

$$\mathcal{V}^{(0)(+)}_{\beta n,\alpha m}(q'_\beta, q_\alpha) = \bar{\delta}_{\beta\alpha} \iint \mathrm{d}^3R\, \mathrm{d}^3r_\beta\, \mathrm{e}^{\mathrm{i}q'_\beta\cdot\rho_\beta} \varphi^*_{\beta n}(r_\beta)\chi_{\alpha m}(r_\alpha) e^{i q_\alpha\cdot\rho_\alpha} D(R). \quad (60)$$

Here, $\chi_{\alpha m}(r_\alpha)$ is the configuration space form factor of the mth bound state in subsystem α. The function $D(R)$ is defined as

$$D(R) = (Mv)^{\mathrm{i}(\eta_\alpha+\eta_\beta)} b^{2\mathrm{i}\eta_\alpha} (R+Z)^{-\mathrm{i}\xi} \quad (61)$$

with

$$\xi = \eta_\alpha - \eta_\beta. \quad (62)$$

When evaluating the integral appearing on the right-hand side of (60) we closely follow the procedure used by Belkić and Taylor (1987). Our aim is to obtain the explicit expression for $\mathcal{V}^{(0)(+)}_{\beta n,\alpha m}$ in the impact parameter representation. The momentum transfers in the rearrangement channel, as defined by equation (20), are

$$p = q_\perp + \hat{v}\left(\frac{v}{2} - \frac{\Delta E}{v}\right) \qquad q = q_\perp - \hat{v}\left(\frac{v}{2} + \frac{\Delta E}{v}\right) \quad (63)$$

where $\hat{v} = v/v$, and $q_\perp$ is the transverse component of p and q. Expression (60) can be rewritten as

$$\mathcal{V}^{(0)(+)}_{\beta n,\alpha m}(q'_\beta, q_\alpha) = \bar{\delta}_{\beta\alpha}(Mv)^{\mathrm{i}(\eta_\alpha+\eta_\beta)} \int \mathrm{d}^3R \mathrm{e}^{\mathrm{i}q_\perp\cdot b} b^{2\mathrm{i}\eta_\alpha} \mathrm{e}^{\mathrm{i}Z(v/2-\Delta E/v)} (R+Z)^{-\mathrm{i}\xi} J(\boldsymbol{R}) \quad (64)$$

with

$$J(\boldsymbol{R}) = \int \frac{\mathrm{d}^3k}{(2\pi)^3} \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}} \tilde{\varphi}^*_{\beta n}(\boldsymbol{k}) \tilde{\chi}_{\alpha m}(\boldsymbol{k}+\boldsymbol{v}). \quad (65)$$

In the momentum space representation the bound state form factor $\tilde{\chi}_{\alpha m}(\boldsymbol{k})$ is related to the corresponding wavefunction $\tilde{\varphi}_{\beta n}(\boldsymbol{k})$ via

$$\tilde{\chi}_{\gamma r}(\boldsymbol{p}) = -\tfrac{1}{2}(p^2 - 2\hat{E}_{\gamma r})\tilde{\varphi}_{\gamma r}(\boldsymbol{p}). \quad (66)$$

The latter is given explicitly by

$$\tilde{\varphi}_{\gamma r}(\boldsymbol{p}) = R_{n_\gamma \ell_\gamma}(p) Y_{\ell_\gamma m_\gamma}(\hat{p}) \quad (67)$$

with

$$R_{n_\gamma\ell_\gamma}(p) = N_{n_\gamma\ell_\gamma} \frac{p^{\ell_\gamma}}{(p^2 - 2\hat{E}_{\gamma r})^{\ell_\gamma+2}} C^{\ell_\gamma+1}_{n_\gamma-\ell_\gamma-1}\left(\frac{p^2+2\hat{E}_{\gamma r}}{p^2-2\hat{E}_{\gamma r}}\right) \quad (68)$$

$$N_{n_\gamma\ell_\gamma} = (2\pi)^{3/2}\left[\frac{2^{4\ell_\gamma+5} n_\gamma (n_\gamma-\ell_\gamma-1)!}{\pi(n_\gamma+\ell_\gamma)!}\right]^{1/2} \ell_\gamma!(-2\hat{E}_{\gamma r})^{(2\ell_\gamma+5)/4}. \quad (69)$$

Here, $r = (n_\gamma, \ell_\gamma, m_\gamma)$ denotes the set of quantum numbers of the bound electron, and $\hat{E}_{\gamma r} = -e_\gamma^2/2n_\gamma^2$ is the corresponding binding energy. Furthermore, $C^{\ell_\gamma+1}_{n_\gamma-\ell_\gamma-1}(\cdot)$ are the Gegenbauer polynomials which can be expressed as

$$C^{\ell_\gamma+1}_{n_\gamma-\ell_\gamma-1}\left(\frac{p^2+2\hat{E}_{\gamma r}}{p^2-2\hat{E}_{\gamma r}}\right) = \frac{\Gamma(n_\gamma+\ell_\gamma+1)}{\Gamma(n_\gamma-\ell_\gamma)\Gamma(2\ell_\gamma+2)} \sum_{k=0}^{n_\gamma-\ell_\gamma-1} \frac{a_k}{(p^2-2\hat{E}_{\gamma r})^k}. \tag{70}$$

The coefficients a_k occurring herein satisfy the recurrence relations

$$a_k = a_{k-1} \cdot 2\hat{E}_{\gamma r} \frac{(n_\gamma+\ell_\gamma+k)(n_\gamma-\ell_\gamma-k)}{k(\ell_\gamma+k+1/2)} \qquad a_0 = 1. \tag{71}$$

After straightforward manipulations of the integral (65) we arrive at an expression for $\mathcal{V}^{(0)(+)}_{\beta n,\alpha m}(q'_\beta, q_\alpha)$ from which it is possible to obtain the effective potential in the impact parameter representation as follows (see I):

$$\mathcal{V}^{(0)(+)}_{\beta n,\alpha m}(q'_\beta, q_\alpha) = \frac{1}{2\pi}\int \mathrm{d}^2b\, \mathrm{e}^{\mathrm{i}q_\perp\cdot b}\, \tilde{\mathcal{V}}^{(0)(+)}_{\beta n,\alpha m}(b)\, \mathrm{e}^{\mathrm{i}(m_\alpha-m_\beta)\varphi_b}. \tag{72}$$

Omitting an inessential complex constant we then find

$$\begin{aligned}
\tilde{\mathcal{V}}^{(0)(+)}_{\beta n,\alpha m}(b) = {} & -\bar{\delta}_{\beta\alpha}\frac{b^{2\mathrm{i}\eta_\alpha}}{4(2\pi)^{3/2}} N_{n_\alpha\ell_\alpha} N_{n_\beta\ell_\beta} \frac{\Gamma(n_\alpha+\ell_\alpha+1)}{\Gamma(n_\alpha-\ell_\alpha)\Gamma(2\ell_\alpha+2)} \\
& \times \frac{\Gamma(n_\beta+\ell_\beta+1)}{\Gamma(n_\beta-\ell_\beta)\Gamma(2\ell_\beta+2)} [(2\ell_\alpha+1)(\ell_\alpha+m_\alpha)!(\ell_\alpha-m_\alpha)!]^{1/2} \\
& \times \left[(2\ell_\beta+1)(\ell_\beta+m_\beta)!(\ell_\beta-m_\beta)!\right]^{1/2} (-1)^{m_\beta+(|\Delta m|-\Delta m)/2} \\
& \times \sum_{k_\alpha=0}^{n_\alpha-\ell_\alpha-1} a_{k_\alpha}(n_\alpha,\ell_\alpha) \sum_{k_\beta=0}^{n_\beta-\ell_\beta-1} a_{k_\beta}(n_\beta,\ell_\beta) \frac{\Gamma(N_\alpha+N_\beta)}{\Gamma(N_\alpha)\Gamma(N_\beta)} \\
& \times \sum_{\lambda_\alpha=|m_\alpha|}^{\ell_\alpha} v^{\ell_\alpha-\lambda_\alpha} \left[(\ell_\alpha-\lambda_\alpha)![(\lambda_\alpha+m_\alpha)!(\lambda_\alpha-m_\alpha)!]^{1/2}\right]^{-1} \\
& \times \sum_{\lambda_\beta=|m_\beta|}^{\ell_\beta} (-v)^{\ell_\beta-\lambda_\beta} \left[(\ell_\beta-\lambda_\beta)![(\lambda_\beta+m_\beta)!(\lambda_\beta-m_\beta)!]^{1/2}\right]^{-1} \\
& \times \sum_{\ell} \mathrm{i}^\ell (\lambda_\alpha 0 \lambda_\beta 0|\ell 0)(\lambda_\alpha m_\alpha \lambda_\beta - m_\beta|\ell m)[(\ell+m)!(\ell-m)!]^{1/2} \\
& \times \sum_{\lambda=|m|}^{\ell} \frac{P_\lambda^{|m|}(0)}{(\ell-\lambda)!(\lambda+|m|)} b^\lambda \int_{-\infty}^{+\infty} \mathrm{d}Z \mathrm{e}^{\mathrm{i}(v/2-\Delta E/v)Z} Z^{\ell-\lambda}(R+Z)^{-\mathrm{i}\xi} \\
& \times R^{2N_\alpha+2N_\beta-L-\ell-5/2} \int_0^1 \mathrm{d}x\, x^{N_\alpha+\ell_\beta-\lambda_\beta-1}(1-x)^{N_\beta+\ell_\alpha-\lambda_\alpha-1} \\
& \times \mathrm{e}^{-\mathrm{i}vZx} I_{N_\alpha+N_\beta,L,\ell+1/2}(\kappa(x)R)
\end{aligned} \tag{73}$$

where

$$N_\alpha = \ell_\alpha + k_\alpha + 1, \quad N_\beta = \ell_\beta + k_\beta + 2 \qquad L = \lambda_\alpha + \lambda_\beta + \tfrac{1}{2} \tag{74}$$

$$P_\lambda^{|m|}(0) = \frac{2^{|m|}\pi^{1/2}}{\Gamma(1+(\lambda-|m|)/2)\Gamma(\frac{1}{2}-(\lambda+|m|)/2)} \tag{75}$$

$\Delta m = m_\alpha - m_\beta$, $\lambda + |m|$ being an integer, and

$$\kappa^2(x) = v^2 x(1-x) + \frac{e_\alpha^2}{n_\alpha^2}x + \frac{e_\beta^2}{n_\beta^2}(1-x). \tag{76}$$

As before, $R = (b^2 + Z^2)^{1/2}$. The symbols $(a\alpha b\beta|c\gamma)$ denote Clebsch–Gordan coefficients. The function $I_{N_\alpha+N_\beta,L,\ell+1/2}(\kappa(x)R)$ has been calculated analytically in I:

$$I_{N,L,\ell+1/2}(y) = \sum_{j=0}^{Q}(-1)^j 2^{Q-j} C_Q^j \frac{\Gamma(\ell+\frac{1}{2}+Q+1)}{\Gamma(\ell+\frac{1}{2}+j+1)} I_{N,M,M}(y) \tag{77}$$

where $Q = \frac{1}{2}(L-\ell-\frac{1}{2})$, $N = N_\alpha + N_\beta$, $C_Q^j = Q!/j!(Q-j)!$, and $M = \frac{1}{2}(L+\ell+\frac{1}{2})+j$. For $I_{N,M,M}(y)$ we can use (Gradshtein and Ryzhik 1965):

$$I_{N,M,M}(y) = \frac{1}{2^{N-1}\Gamma(N)y^{N-M-1}} K_{N-M-1}(y) \tag{78}$$

where $K_{N-M-1}(y)$ is the Bessel function of the third kind with half-integer index.

Thus we have obtained the effective potential as it occurs as driving term in the AGS equations.† To get the corresponding expression to be used in the kernel of these equations one only has to substitute for the form (61) of $D(R)$ the expression

$$D(R) = (Mv)^{-i(\eta_\alpha - \eta_\beta)}(R+Z)^{-i\xi}. \tag{79}$$

Note the absence of the factor $b^{2i\eta_\alpha}$.

3.2. The effective potential: scattering channel

We begin with the second term on the right-hand side of (59). Taking into account $\rho_\alpha \simeq -\rho_\beta \simeq \boldsymbol{R}$ one can write for the driving term

$$\left[\mathcal{V}^{(1)(+)}_{\alpha n,\alpha m}(q'_\alpha, q_\alpha)\right]_2 = \delta_{nm}\int d^3R\,(Mvb)^{2i\eta_\alpha} e^{i\boldsymbol{q}\cdot\boldsymbol{R}}\left(-\frac{e_\alpha}{R}\right) \tag{80}$$

where $\boldsymbol{q} = \boldsymbol{q}_\alpha - \boldsymbol{q}'_\alpha$, and the same expression but without the factor $(Mvb)^{2i\eta_\alpha}$ when it occurs in the kernel of AGS equations. It is apparent that this term which arises only in the case of elastic scattering ($\alpha \to \alpha$, $m = n$) has a singularity of the q^{-2} type. As we will see below it cancels an identical singularity occurring in the first term of (59).

Let us now consider the first term on the right-hand side of (59) which explicitly looks as

$$\left[\mathcal{V}^{(1)(+)}_{\alpha n,\alpha m}(q'_\alpha, q_\alpha)\right]_1 = \int d^3R\,d^3r_\beta\,\varphi^*_{\alpha n}(\boldsymbol{r}_\alpha)\left(-\frac{e_\alpha}{r_\beta}\right)\varphi_{\alpha m}(\boldsymbol{r}_\alpha)e^{i\boldsymbol{q}\cdot\boldsymbol{R}}D(R) \tag{81}$$

with

$$D(R) = (Mvb)^{2i\eta_\alpha}. \tag{82}$$

† After completion of the calculations the authors became aware that an efficient method to carry out the integration over Z in (73) analytically had been proposed by Belkić (1989).

It proves convenient to rewrite (81) as

$$\left[\mathcal{V}^{(1)(+)}_{\alpha n,\alpha m}(q'_\alpha, q_\alpha)\right]_1 = \int \mathrm{d}^3R\, \mathrm{e}^{\mathrm{i}q\cdot R}(Mvb)^{2\mathrm{i}\eta_\alpha} J(R) \tag{83}$$

where we have introduced

$$\begin{aligned} J(R) &= \int \mathrm{d}^3r_\beta\, \varphi^*_{\alpha n}(R+r_\beta)\left(-\frac{e_\alpha}{r_\beta}\right)\varphi_{\alpha m}(R+r_\beta) \\ &= \int \frac{\mathrm{d}^3k}{(2\pi)^3}\left(-\frac{4\pi e_\alpha}{k^2}\right)\mathrm{e}^{\mathrm{i}k\cdot R} I(k) \end{aligned} \tag{84}$$

with

$$I(k) = \int \mathrm{d}^3r \varphi^*_{\alpha n}(r)\varphi_{\alpha m}(r)\mathrm{e}^{-\mathrm{i}k\cdot r}. \tag{85}$$

The bound state wavefunction in configuration space has the form ($s = n_\alpha \ell_\alpha m_\alpha$)

$$\varphi_{\alpha s}(r) = \mathrm{i}^{\ell_\alpha}\tilde{R}_{n_\alpha\ell_\alpha}(r)Y_{\ell_\alpha m_\alpha}(\hat{r}). \tag{86}$$

Herein, the radial part is given by

$$\tilde{R}_{n_\alpha\ell_\alpha}(r) = \tilde{N}_{n_\alpha\ell_\alpha}\left(\frac{2e_\alpha r}{n_\alpha}\right)^{\ell_\alpha}\mathrm{e}^{-e_\alpha r/n_\alpha}F\left(-n_\alpha+\ell_\alpha+1, 2\ell_\alpha+2; \frac{2e_\alpha}{n_\alpha}r\right) \tag{87}$$

with the normalization

$$\tilde{N}_{n_\alpha\ell_\alpha} = \frac{1}{(2\ell_\alpha+1)!}\left(\frac{2e_\alpha}{n_\alpha}\right)^{3/2}\left[\frac{(n_\alpha+\ell_\alpha)!}{2n_\alpha(n_\alpha-\ell_\alpha-1)!}\right]^{1/2}. \tag{88}$$

Integration over the direction of r in (85) leads to

$$I(k) = \sum_{\ell m} P^{\ell m}_{\ell_\alpha m_\alpha,\ell'_\alpha m'_\alpha} Y^*_{\ell m}(\hat{k})\int_0^\infty \mathrm{d}r r^2 j_\ell(kr)\tilde{R}_{n'_\alpha\ell'_\alpha}(r)\tilde{R}_{n_\alpha\ell_\alpha}(r) \tag{89}$$

where $(n'_\alpha, \ell'_\alpha, m'_\alpha)$ denotes the set of quantum numbers of the bound electron in the final state. Here, we have introduced the abbreviation

$$P^{\ell m}_{\ell_\alpha m_\alpha,\ell'_\alpha m'_\alpha} = (-1)^{(\ell+\ell'_\alpha-\ell_\alpha)/2}\left[\frac{4\pi(2\ell_\alpha+1)(2\ell+1)}{2\ell'_\alpha+1}\right]^{1/2}(\ell_\alpha 0\ell 0|\ell'_\alpha 0)(\ell_\alpha m_\alpha \ell m|\ell'_\alpha m'_\alpha). \tag{90}$$

Inserting (89) into (84) one obtains

$$J(R) = -\frac{2e_\alpha}{\pi}\sum_{\ell m}\mathrm{i}^\ell P^{\ell m}_{\ell_\alpha m_\alpha,\ell'_\alpha m'_\alpha} Y^*_{\ell m}(\hat{R})\int_0^\infty \mathrm{d}r\, r^2\tilde{R}_{n'_\alpha\ell'_\alpha}(r)\tilde{R}_{n_\alpha\ell_\alpha}(r)\int_0^\infty \mathrm{d}k j_\ell(kr)j_\ell(kR). \tag{91}$$

The integral over k can be evaluated yielding

$$\int_0^\infty \mathrm{d}k j_\ell(kr)j_\ell(kR) = \frac{\pi}{2(2\ell+1)\sqrt{Rr}}\times\begin{cases}\left(\dfrac{r}{R}\right)^{\ell+1/2} & \text{for } r<R \\ \left(\dfrac{R}{r}\right)^{\ell+1/2} & \text{for } r>R.\end{cases} \tag{92}$$

Thus, for $J(\boldsymbol{R})$ we arrive at

$$J(\boldsymbol{R}) = -e_\alpha \sum_{\ell m} \frac{\mathrm{i}^\ell}{2\ell+1} P^{\ell m}_{\ell_\alpha m_\alpha, \ell'_\alpha m'_\alpha} Y^*_{\ell m}(\hat{R}) \left\{ \frac{1}{R^{\ell+1}} \int_0^\infty dr\, r^{\ell+2} \tilde{R}_{n'_\alpha \ell'_\alpha}(r) \tilde{R}_{n_\alpha \ell_\alpha}(r) \right.$$
$$\left. - R^\ell \int_R^\infty \mathrm{d}r\, r^{1-\ell} \left(\left(\frac{r}{R} \right)^{2\ell+1} - 1 \right) \tilde{R}_{n'_\alpha \ell'_\alpha}(r) \tilde{R}_{n_\alpha \ell_\alpha}(r) \right\}. \tag{93}$$

For purely elastic scattering ($n'_\alpha = n_\alpha$, $\ell'_\alpha = \ell_\alpha$) and $\ell = 0$, expression (93) simplifies to

$$J(\boldsymbol{R}) = -\frac{e_\alpha}{R} + e_\alpha \int_R^\infty \mathrm{d}r\, r \left(\frac{r}{R} - 1 \right) \tilde{R}^2_{n_\alpha \ell_\alpha}(r). \tag{94}$$

We recall that according to (30) one has $-e_\alpha/R \simeq v'_\alpha(\rho_\alpha)$ because of $\rho_\alpha \simeq R$. The first term on the right-hand side of (94) leads to a singularity $\sim q^{-2}$ in the effective potential part $\left[\mathcal{V}^{(1)(+)}_{\alpha n,\alpha m}(\boldsymbol{q}'_\alpha, \boldsymbol{q}_\alpha)\right]_1$ which, however, as was mentioned above cancels against the same term in $\left[\mathcal{V}^{(1)(+)}_{\alpha n,\alpha m}(\boldsymbol{q}'_\alpha, \boldsymbol{q}_\alpha)\right]_2$, so that the full effective potential $\mathcal{V}^{(1)(+)}_{\alpha n,\alpha m}(\boldsymbol{q}'_\alpha, \boldsymbol{q}_\alpha)$, equation (59), does not have this dangerous singularity.

The integrals appearing in (93) can easily be evaluated after insertion of (87) for $\tilde{R}_{n_\alpha \ell_\alpha}(r)$. For the first integral we find

$$I_0 = \tilde{N}_{n_\alpha \ell_\alpha} \tilde{N}_{n'_\alpha \ell'_\alpha} \left(\frac{2e_\alpha}{n_\alpha} \right)^{\ell_\alpha} \left(\frac{2e_\alpha}{n'_\alpha} \right)^{\ell'_\alpha} \sum_{k=0}^{n_\alpha - \ell_\alpha - 1} b_k(n_\alpha, \ell_\alpha) \left(\frac{2e_\alpha}{n_\alpha} \right)^k$$
$$\times \sum_{k'=0}^{n'_\alpha - \ell'_\alpha - 1} b_{k'}(n'_\alpha, \ell'_\alpha) \left(\frac{2e_\alpha}{n'_\alpha} \right)^{k'} \frac{L!}{a^{L+1}} \tag{95}$$

where

$$a = \frac{e_\alpha}{n_\alpha} + \frac{e_\alpha}{n'_\alpha} \qquad L = \ell_\alpha + \ell'_\alpha + \ell + k + k' + 2. \tag{96}$$

The coefficients $b_k(n, \ell)$ can be calculated from the recurrence relation

$$b_k = b_{k-1} \cdot \frac{(-n + \ell + k)}{k(2\ell + k + 1)} \qquad b_0 = 1. \tag{97}$$

The second integral in (93) gives

$$I_R = \tilde{N}_{n_\alpha \ell_\alpha} \tilde{N}_{n'_\alpha \ell'_\alpha} \left(\frac{2e_\alpha}{n_\alpha} \right)^{\ell_\alpha} \left(\frac{2e_\alpha}{n'_\alpha} \right)^{\ell'_\alpha} \mathrm{e}^{-aR}$$
$$\times \sum_{k=0}^{n_\alpha - \ell_\alpha - 1} b_k(n_\alpha, \ell_\alpha) \left(\frac{2e_\alpha}{n_\alpha} \right)^k \sum_{k'=0}^{n'_\alpha - \ell'_\alpha - 1} b_{k'}(n'_\alpha, \ell'_\alpha) \left(\frac{2e_\alpha}{n'_\alpha} \right)^{k'}$$
$$\times \left\{ \frac{L!}{R^{2\ell+1} a^{L+1}} \sum_{i=0}^{L} \frac{(aR)^i}{i!} - \frac{(L - 2\ell - 1)!}{a^{L-2\ell}} \sum_{i=0}^{L-2\ell-1} \frac{(aR)^i}{i!} \right\}. \tag{98}$$

Using (93) with (95) and (98) in (83) and going over via (72) to the impact parameter representation we obtain the expression for the effective potential $\left[\tilde{\mathcal{V}}^{(1)(+)}_{\alpha n,\alpha m}(b)\right]_1$:

$$\left[\tilde{\mathcal{V}}^{(1)(+)}_{\alpha n,\alpha m}(b)\right]_1 = 2\pi (Mvb)^{2\mathrm{i}\eta_\alpha} \int_{-\infty}^{+\infty} \mathrm{d}Z \mathrm{e}^{\mathrm{i}q_\perp Z} J(\boldsymbol{R}) \tag{99}$$

where $q_\parallel = -\Delta E/v$ is the longitudinal component of the momentum transfer q. The phase factor $(Mvb)^{2i\eta_\alpha}$ is absent in the effective potential $\tilde{V}^{(1)(-)}_{\alpha n,\alpha m}(b)$, i.e., one has

$$\left[\tilde{V}^{(1)(-)}_{\alpha n,\alpha m}(b)\right]_1 = 2\pi \int_{-\infty}^{+\infty} \mathrm{d}Z \mathrm{e}^{\mathrm{i}q_\parallel Z} J(\boldsymbol{R}). \tag{100}$$

It is easy to check that the absence of $(Mvb)^{2i\eta_\alpha}$ is equivalent to switching off the interaction v'_α (i.e., $\eta_\alpha = 0$), leading to $V_3 + v'_\alpha = 0$. For this case the first term of the effective potential in the momentum representation is given by

$$\left[V^{(1)(-)}_{\alpha n,\alpha m}(q'_\alpha, q_\alpha)\right]_1 = -\frac{4\pi e_\alpha}{q^2} \int \mathrm{d}^3 r \varphi^*_{\alpha n}(r) \varphi_{\alpha m}(r) \mathrm{e}^{\mathrm{i}q\cdot r}. \tag{101}$$

It corresponds to the triangle diagram involving scattering of the electron off particle α in Born approximation (for a diagrammatic representation see figure 2(*c*) of I).

4. Calculation of charge exchange in collisions of fully stripped ions with atomic hydrogen

In this section we present the results of our calculations of total cross sections of electron transfer reactions in collisions of the fully stripped ions H^+, He^{2+} and Li^{3+} with atomic hydrogen.

The amplitude describing the transition from an initial state with a set of quantum numbers $i = (n_i\, \ell_i\, m_i)$ to the final state characterized by quantum numbers $n\,\ell\,m$ at a fixed impact parameter, $\tilde{T}^{(0)}_{n\ell m,i}(b)$, is found by numerically solving the set of coupled linear equations (39). In principle, it contains infinite sums over all possible quantum numbers of the bound electron. In concrete calculations these sums must be truncated, keeping states up to some maximal principal quantum number $n = n_{\max}$ chosen such as to ensure the desired degree of accuracy of the calculated cross sections. For a given value of $n_{\max}$ the number of coupled algebraic equations is then $n_{\max}(n_{\max}+1)(2n_{\max}+1)/3$.

Partial cross sections for electron capture into a state with quantum numbers $n\ell m$ are determined via

$$\sigma^i_{n\ell m} = 2\pi \int_0^\infty \mathrm{d}b\, b\, P^i_{n\ell m}(b) \tag{102}$$

where the transition probability $P^i_{n\ell m}(b)$ is related to the amplitude by

$$P^i_{n\ell m}(b) = \frac{1}{(2\pi v)^2} |\tilde{T}^{(0)}_{n\ell m,i}(b)|^2. \tag{103}$$

The total transfer cross section is the sum of the partial cross sections over all final states:

$$\sigma^i = \sum_{n\ell m} \sigma^i_{n\ell m}. \tag{104}$$

Table 1. Total cross sections $\sigma^i(E)$ (10^{-16} cm^2) calculated for different values of n_{max} for the process (*a*) $H^+ + H(1s) \longrightarrow H + H^+$, and for the process (*b*) $H^+ + H(2s) \longrightarrow H + H^+$.

	n_{max}				
E (keV)	1	2	3	4	5
(*a*)					
1(−1)	2.64(+1)	2.64(+1)	2.64(+1)	2.64(+1)	2.64(+1)
1	2.07(+1)	2.07(+1)	2.07(+1)	2.07(+1)	2.07(+1)
1(+1)	1.23(+1)	1.13(+1)	1.12(+1)	1.12(+1)	1.13(+1)
1(+2)	3.09(−1)	4.18(−1)	4.59(−1)	4.77(−1)	4.84(−1)
1(+3)	6.65(−6)	7.81(−6)	8.15(−6)	8.28(−6)	8.35(−6)
(*b*)					
1(−1)	—	1.22(+2)	1.22(+2)	1.22(+2)	1.22(+2)
1	—	9.91(+1)	1.04(+2)	1.03(+2)	1.03(+2)
1(+1)	—	1.44(+1)	2.38(+1)	2.56(+1)	2.69(+1)
1(+2)	—	8.17(−2)	9.24(−2)	9.74(−2)	9.93(−2)
1(+3)	—	1.10(−6)	1.15(−6)	1.17(−6)	1.18(−6)

4.1. Electron capture by protons from the ground and low-lying excited states of atomic hydrogen

Here we present a comprehensive analysis of the electron capture by protons from the ground and the low-lying excited states of hydrogen at intermediate and high collision energies. The capture from excited states is of considerable interest, e.g., in high density thermonuclear plasma where the electrons of the hydrogen atoms may, as a result of various processes, occupy excited states. Hence the question arises how this fact affects the capture dynamics. The results of our calculations show that, indeed, interesting effects take place.

Table 1 lists the values of the total cross sections for the electron capture from $i = 1s$ and 2s states, calculated in three-body eikonal approach (TBEA) developed above, for $n_{max} = 1$, 2, 3, 4 and 5, at different collision energies (the corresponding data for $i = 2p_0$ and $2p_1$ states are similar to those for the 2s state. Here, the subscript denotes the absolute value of the magnetic quantum number of the bound electron.) Inspection reveals that with $n_{max} = 5$ the cross sections σ^{1s} and σ^{2s} have practically converged to good accuracy in the whole energy range under consideration, i.e., from 0.1 to 1000 keV. The largest change when increasing n_{max} from 4 to 5 occurs for σ^{1s} at 100 keV and amounts to 1.4%, while for σ^{2s} it is 5% at 10 keV. Hereafter, all calculations shown are made with $n_{max} = 5$.

In figure 2 we present total cross sections for electron capture by protons from 1s, 2s, $2p_0$ and $2p_1$ states of the hydrogen atom, as functions of the collision energy. Experimental data for the capture from the ground state are included. The calculations show that in the region of high collision energies the ground state capture cross section dominates over those for the capture from excited states. For fixed principal quantum number n, the larger the orbital quantum number ℓ and its projection $|m|$, the smaller is the capture cross section. The observed dependence of the total cross section on the initial state principal quantum number can be qualitatively understood by the Oppenheimer $\sigma_{n_i} \sim n_i^{-3}$ rule, which is applicable at high energies.

When the collision energy decreases down to 10–20 keV the cross sections for the capture from the ground and from the excited states become comparable in magnitude; but if the energy decreases further the capture from excited states begins to dominate. In fact, the cross section for the capture from $2p_0$ reaches its maximum in the region of 1 keV and then decreases with decreasing energy, becoming smaller than σ^{1s} at 0.1 keV. However, σ^{2s} and σ^{2p_1} continue to exceed σ^{1s} even at low energies. A rough classical explanation

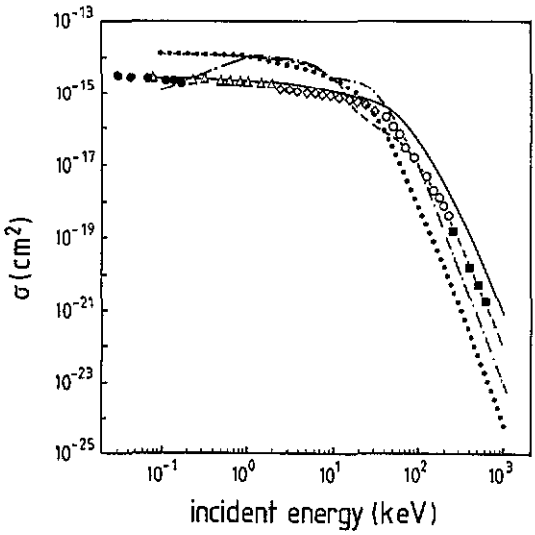

Figure 2. Total cross sections for the process $H^+ + H \rightarrow H + H^+$. TBEA: full curve, capture from the ground state; broken curve, capture from the 2s state; chain curve, capture from the $2p_0$ state; dotted curve, capture from the $2p_1$ state. Experimental data for the capture from the 1s state: full circles, Newman *et al* (1982); triangles, Fite *et al* (1962); diamonds, McClure (1966); open circles, Wittkower *et al* (1966); full squares, Hvelplund and Andersen (1982).

of this dependence of the total cross section on the initial state principal quantum number n_i at low energies ($E = 1$–10 keV) can be given in the framework of the Bohr–Linhard approach. Indeed, following the work of Knudsen *et al* (1981) one can see that the total cross section ratio for two different principal quantum numbers $n_2 = 2$ and $n_1 = 1$ is given by

$$\frac{\sigma^2}{\sigma^1} = \left(\frac{n_2}{n_1}\right)^4 = 16. \tag{105}$$

We obtain, in fact, cross section ratios of this order of magnitude. For instance, for $E = 1$ keV we find $\sigma^{2s}/\sigma^{1s} \approx 5$.

Note that the TBEA results for σ^{1s} are in rather good agreement with experimental data. We mention that they differ only slightly from those obtained in IPFA. It should be recalled that in IPFA the effective potential in the scattering channel has been neglected while in TBEA its contribution is taken into account at least approximately.

Figures 3 and 4 show the dependence of the partial cross section on the final state principal quantum number n, at four different values of the collision energy $E = 0.1$, 1, 10 and 100 keV, for the capture from the ground and the excited $2p_0$ state. Inspection of figure 3 reveals that at all energies considered σ^{1s} is dominated by transitions into the final $n = 1$ shell. At energies below 1 keV the capture displays a strong resonance character. This pattern changes at intermediate energies if the capture from excited states takes place. So, for example, if the incoming proton captures the electron from the $2p_0$ state then at $E = 100$ keV the $n = 1$ shell is preferred; when E decreases down to 10 keV the dominant role is taken over by the $n = 2$ shell; and at an energy of 1 keV the contribution from the $n = 3$ shell becomes the largest. Finally, in the region of $E = 0.1$ keV the capture is resonant. We only mention that the latter effect takes place also in the case of the capture from the 2s state but there it is not so pronounced.

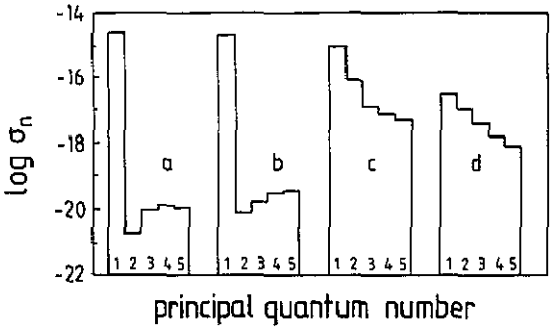

Figure 3. Partial cross sections σ_n for the process $H^+ + H(1s) \rightarrow H(n) + H^+$, against the principal quantum number n of the final state, for collision energies (a) $E = 0.1$ keV; (b) $E = 1$ keV; (c) $E = 10$ keV; (d) $E = 100$ keV.

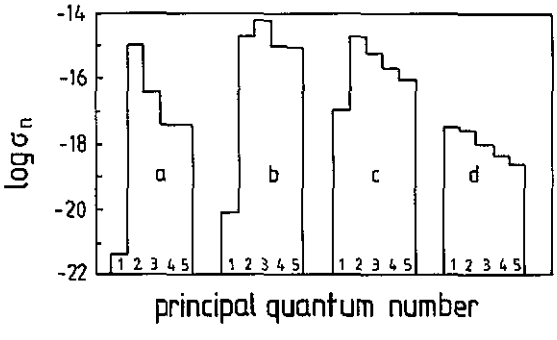

Figure 4. *The same as in figure 3 but for the process* $H^+ + H(2p_0) \rightarrow H(n) + H^+$.

Table 2. Partial cross sections σ_{nl}^{i} (10^{-16} cm^2) for the process $H^+ + H(i) \longrightarrow H(nl) + H^+$, calculated at the collision energy $E = 10$ keV.

	i			
nl	1s	2s	$2p_0$	$2p_1$
10	1.01(+1)	5.53(−1)	1.10(−1)	3.04(−2)
20	7.00(−1)	5.33(−1)	8.71(−1)	6.68(−1)
21	1.82(−1)	2.09	1.81(+1)	9.10
30	7.37(−2)	7.32(−2)	1.28(−1)	3.35(−1)
31	1.82(−2)	4.06	2.07	4.99
32	3.58(−2)	5.03	3.87	3.63
40	1.37(−2)	2.06(−2)	7.57(−2)	1.39(−1)
41	8.22(−3)	2.75	5.39(−1)	2.47
42	3.63(−2)	4.30	8.57(−1)	2.02
43	1.70(−2)	1.44	5.69(−1)	6.27(−1)
50	4.12(−3)	1.08(−2)	4.56(−2)	6.84(−2)
51	5.50(−3)	1.69	2.02(−1)	1.36
52	2.52(−2)	2.90	3.18(−1)	1.18
53	1.52(−2)	1.28	2.79(−1)	4.38(−1)
54	1.66(−3)	1.84(−1)	6.62(−2)	7.76(−2)

Partial cross sections σ_{nl} calculated in TBEA for the capture from different initial states

Table 3. Partial cross sections σ_{nl}^{i} (10^{-16} cm^2) for the process $H^+ + H(i) \longrightarrow H(nl) + H^+$, calculated at the collision energy $E = 100$ keV.

	i			
nl	1s	2s	$2p_0$	$2p_1$
10	3.11(−1)	5.77(−2)	3.52(−2)	3.58(−3)
20	6.97(−2)	1.38(−2)	1.23(−2)	1.54(−3)
21	4.16(−2)	1.24(−2)	1.33(−2)	1.30(−3)
30	1.94(−2)	3.86(−3)	3.77(−3)	4.90(−4)
31	1.61(−2)	4.75(−3)	5.53(−3)	5.58(−4)
32	1.61(−3)	6.63(−4)	8.31(−4)	7.04(−5)
40	7.74(−3)	1.55(−3)	1.57(−3)	2.08(−4)
41	7.22(−3)	2.13(−3)	2.56(−3)	2.62(−4)
42	9.67(−4)	3.97(−4)	5.15(−4)	4.44(−5)
43	3.04(−5)	1.72(−5)	2.34(−5)	1.74(−6)
50	3.93(−3)	7.85(−4)	8.07(−4)	1.08(−4)
51	3.87(−3)	1.14(−3)	1.38(−3)	1.42(−4)
52	5.67(−4)	2.33(−4)	3.06(−4)	2.67(−5)
53	2.58(−5)	1.46(−5)	2.02(−5)	1.51(−6)
54	3.59(−7)	2.76(−7)	3.95(−7)	2.35(−8)

Table 4. Partial cross sections σ_{nl}^{i} (10^{-16} cm^2) for the process $H^+ + H(i) \longrightarrow H(nl) + H^+$, calculated at the collision energy $E = 1000$ keV.

	i			
nl	1s	2s	$2p_0$	$2p_1$
10	6.75(−6)	9.53(−7)	6.41(−8)	5.16(−9)
20	1.01(−6)	1.44(−7)	9.94(−9)	8.01(−10)
21	7.36(−8)	1.07(−8)	7.87(−10)	5.39(−11)
30	2.88(−7)	4.08(−8)	2.85(−9)	2.31(−10)
31	2.75(−8)	4.00(−9)	2.95(−10)	2.02(−11)
32	3.46(−10)	5.18(−11)	3.97(−12)	2.34(−13)
40	1.18(−7)	1.68(−8)	1.18(−9)	9.58(−11)
41	1.24(−8)	1.80(−9)	1.34(−10)	9.12(−12)
42	2.09(−10)	3.13(−11)	2.40(−12)	1.42(−13)
43	8.76(−13)	1.35(−13)	1.06(−14)	5.48(−16)
50	6.15(−8)	8.73(−9)	6.10(−10)	4.96(−11)
51	6.57(−9)	9.57(−10)	7.08(−11)	4.83(−12)
52	1.23(−10)	1.84(−11)	1.42(−12)	8.35(−14)
53	7.52(−13)	1.16(−13)	9.14(−15)	4.72(−16)
54	1.42(−15)	2.26(−16)	1.81(−17)	8.20(−19)

are presented in tables 2–4 at three values of the incident proton energy. It is found that at $E = 1000$ keV and for fixed values of n, transitions into the states with orbital quantum number $\ell = 0$ give the largest contribution, independently of the initial state of the target. On the other hand, for the capture from excited states of the target into excited states with $n \geqslant 3$ of the final atom, at $E = 100$ keV the transitions into the states with $\ell = 1$, and at 10 keV those into states with $\ell = 2$ (excluding the transitions to $2p_1$ states) are most probable. At smaller energies the dependence of the cross sections on ℓ is less pronounced.

4.2. Electron capture by fully stripped He^{2+} and Li^{3+} ions from hydrogen atoms.

In reactions where there is a non-vanishing Coulomb interaction between the centres of mass

of the scattered fragments in the outgoing channel the dynamics of the capture process is changed. The cross section has its maximum in the region of intermediate energies (at $\approx$ 10 keV/nucleon). As examples of such processes we consider electron transfer reactions in collisions of fully stripped He^{2+} and Li^{3+} ions with hydrogen atoms in the ground state.

Table 5. Total cross sections $\sigma(E)$ (10^{-16} cm^2) for the process $He^{2+} + H(1s) \longrightarrow He^+ + H^+$, calculated for different values of n_{max}.

	n_{max}				
E (keV)	1	2	3	4	5
1	3.17(−1)	2.03	2.12	2.13	2.13
1(+1)	1.22	1.80(+1)	1.88(+1)	1.90(+1)	1.90(+1)
1(+2)	2.83(−1)	9.39(−1)	1.22	1.35	1.42
1(+3)	8.18(−5)	1.04(−4)	1.19(−4)	1.25(−4)	1.28(−4)

The dependence of the total cross sections for the process $He^{2+} + H(1s) \rightarrow He^+ + H^+$ calculated in TBEA on the choice of n_{max} can be inferred from table 5. Inspection shows that when $n_{max} = 5$ is chosen the accuracy of the results is satisfactory. The slowest convergence is achieved at $E = 100$ keV/nucleon, but even there the change in the result when n_{max} is increased from 4 to 5 is not larger than 5%.

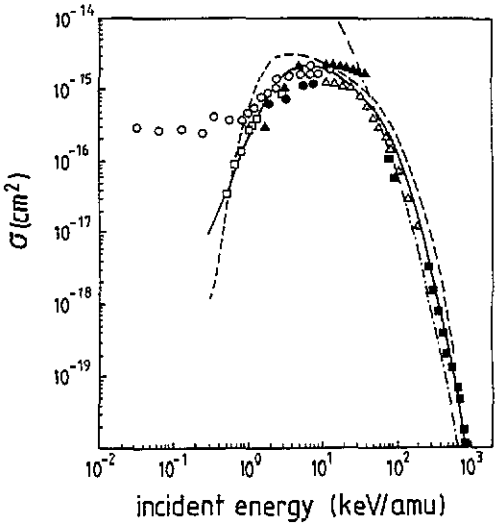

Figure 5. Total cross section for the process $He^{2+} + H(1s) \rightarrow He^+ + H^+$. Theory: full curve, TBEA; broken curve, IPFA (Avakov *et al* 1990a); chain curve, CDW (Belkić 1991). Experiment: open circles, Fite *et al* (1962); full triangles, Bayfield and Khayrallah (1975); open squares, Nutt *et al* (1978); full circles, Shah and Gilbody (1978); open triangles, Olson *et al* (1977); full squares, Hvelplund *et al* (1976) (data taken with molecular hydrogen arqe transformed to H target following Belkić and Gayet 1977).

In figure 5 we present total cross sections calculated in TBEA with $n_{max} = 5$ and compare them with the experimental data and with theoretical results obtained in IPFA (in II) and in

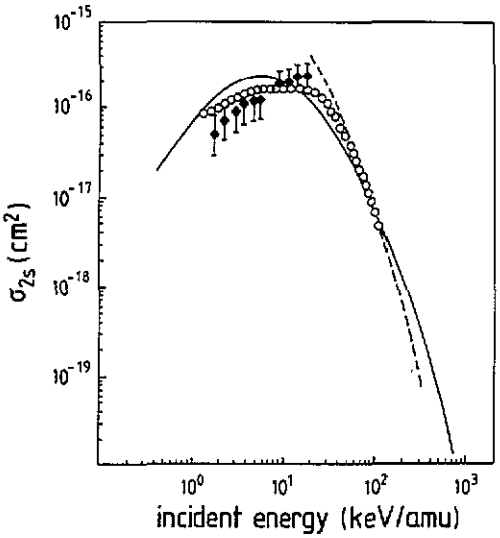

Figure 6. Partial cross section σ_{2s} for the process $He^{2+} + H(1s) \rightarrow He^+(2s) + H^+$. Theory: full curve, TBEA; broken curve, CDW (Belkić and Gayet 1977). Experiment: open circles, Shah and Gilbody (1978); diamonds, Bayfield and Khayrallah (1975).

CDW (Belkić 1991). As is apparent TBEA provides better agreement with available data in the whole range of collision energies considered.

Cross sections for the process $He^{2+} + H(1s) \rightarrow He^+(2s) + H^+$ are shown in figure 6. Inspection reveals that the results obtained in TBEA are in satisfactory agreement with the experimental data, over the whole energy region. For comparison CDW calculations of this quantity (Belkič and Gayet 1977) are included. Though the latter appear to reproduce the higher energy part of the data somewhat better. At the lower energies, on the contrary, TBEA still provides a reasonable description while CDW seems not to be appropriate there.

Finally, in figure 7 we present the total cross section for the process $Li^{3+} + H(1s) \rightarrow Li^{2+} + H^+$ obtained in TBEA, as function of the collision energy. Comparison is made with the experimental data and the cross sections calculated in IPFA (II) and in CDW (Belkić 1991). On the whole, TBEA leads to better agreement with experiment than IPFA; but in the high energy region, i.e., for $E \geqslant 50$ keV/nucleon our theoretical cross sections still overestimate the experimental ones. This figure also contains the partial cross section σ_{2s} calculated in our approach. As far as we know no experimental data are available for this process.

5. Summary

The amplitudes describing scattering and charge exchange in ion–atom collisions, when written in the impact parameter representation and using the eikonal approximation, have been represented as a sum of two amplitudes. One of them describes scattering via the Coulomb potential acting between colliding heavy particles (nuclei). The second one could be factored into a product of an explicitly known factor containing all the information about the interaction V_3 between heavy particles, and a residual amplitude $\tilde{T}^{(0)}_{\beta n,\alpha m}$ which is independent of V_3. For $\tilde{T}^{(0)}_{\beta n,\alpha m}$ three-particle equations of the AGS form have been derived.

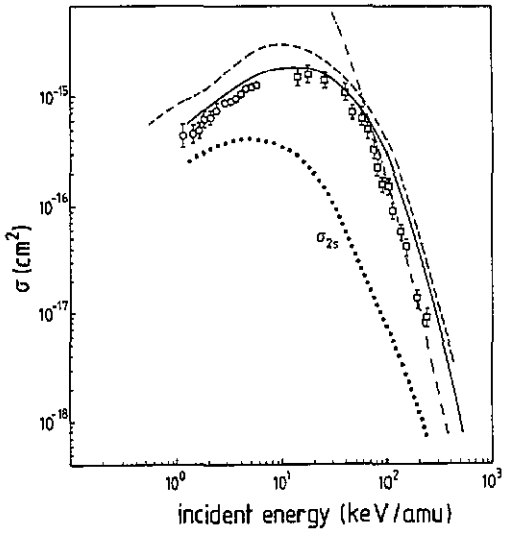

Figure 7. Total cross sections for the process $Li^{3+} + H(1s) \rightarrow Li^{2+} + H^+$. Theory: full curve, TBEA; broken curve, IPFA (Avakov *et al* 1990a); chain curve, CDW (Belkić 1991). Experiment: circles, Seim *et al* (1981); squares, Shah *et al* (1978). Also shown is the partial cross section σ_{2s} calculated in TBEA: dotted curve.

The effective potentials for both scattering and transfer channels occurring in these equations have been explicitly constructed in the lowest order quasi-Born approximation.

This three-body eikonal approach (TBEA) has been used to calculate total and partial cross sections for electron capture processes in collisions of ions H^+, He^{2+} and Li^{3+} with atomic hydrogen in the ground state. In the case of protons as projectiles the hydrogen target atoms were considered in the ground and in low-lying excited states. Some interesting features of electron transfer from excited states of the target have been presented.

When calculating total cross sections of the electron-transfer reaction, the TBEA used in the present paper differs from the IPFA employed in II in two aspects.

(i) Different approximations are used for taking into account the centre-of-mass Coulomb interaction. In the IPFA the exact centre-of-mass Coulomb wavefunctions were used but the corresponding integrals with these functions were calculated in an approximate manner. Furthermore, the accuracy of this approximation was not investigated. On the other hand, in the TBEA the much used eikonal approximation for these wavefunctions was employed, and the integrals were calculated numerically without further approximations.

(ii) In the IPFA the effective potential in the scattering channel was neglected whereas in the TBEA we take into account the contribution of the 'triangle' amplitude (the first-order quasi-Born term) to this effective potential. The results presented clearly show that the TBEA leads to a better description of the data, especially at low and intermediate energies.

The fact that the experimental cross sections at higher energies are overestimated by the TBEA is certainly not a principal drawback of the approach based on the exact AGS equations, but is rather to be attributed to the specific approximations made in the calculation of the effective potentials. Indeed, at those energies the charge-exchange amplitude in the TBEA is determined mainly by the driving term in (39), that is, by the effective potential. In the present work the effective potential in the charge-exchange channel is taken into account in the lowest order quasi-Born approximation ('pole' term) only. This contribution alone is not sufficient to ensure the correct asymptotic behaviour of the cross sections. To this end

one should take into account the next terms in the quasi-Born expansion for the effective potential, in particular the second-order term which is dominant in the high-energy limit. We plan to include these terms in the TBEA in the near future. In this context we point out that the second-order terms are present in the CDW approach, a fact which may explain the better description of the high-energy data in CDW.

Acknowledgments

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