# $2e^{-}$ transfer and excitation formalism in ion-atom collisions at high energies

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An analytical expression for the transition amplitude is obtained by means of the continuum distorted-wave approximation of Cheshire, in order to study the double capture and excitation process. The Dodd-Greider formalism is used to provide a way of connecting the diagrams in the subseries by introducing an intermediate channel. This expression, so derived, is a rigorous first-order term of a perturbation series.

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# I. INTRODUCTION

A great deal of work on the simultaneous transfer and excitation occurring in ion-atom collisions has appeared in recent years: Shakeshaft and Spruch [1], Tanis *et al.* [2], Brandt [3], Feagin *et al.* [4], Itoh *et al.* [5], Swenson *et al.* [6], Tanis [7], Stolterfoht *et al.* [8], Hahn [9], Zouros *et al.* [10], and Gayet and Hanssen [11].

The process of transfer and excitation appears as follows: the two-electron transition in which a target electron is transferred and a projectile electron is excited at the same time.

Recently, a four-body approach is derived by means of the continuum distorted-wave treatment of resonant and nonresonant modes, where a doubly excited state is formed on the projectile, which invokes a two-electron process at the lowest order of perturbation.

In this work, we study a different approach by using the continuum distorted-wave formalism [12] which is presented at the first order of a five-body perturbation series. Threeelectron transition is necessary for transfer and excitation processes to occur in atomic collisions. A large number of observations and several reviews of transfer excitation are available (Tanis [13], Richard [14], Graham [15], and Mokler [16]).

In the sample, transfer and excitation process (Tanis *et al.* [2]) discovered a resonance in the total cross section. The observed resonance was interpreted as an inverse Auger process (or dielectronic recombination), in which the projectile electron is excited by interaction with a captured target electron. This process occurs when the kinetic energy of the projectile electron matches the transition energy, i.e., a resonant condition in the collision velocity. This process has been referred to as resonant transfer and excitation (RTE). In some cases RTE dominates the total cross section for transfer excitation. Pepmiller et al. [17] observed a nonresonant process for transfer and excitation (NTE) occurring when the transfer and excitation occur due to an independent interactions (Zerarka [18]) of the two electrons with the nuclear charges  $Z_P$ and  $Z_T$  of the projectile and the target, respectively. Thus, RTE is a process with electron correlation and NTE is an uncorrelated process. Other applications have been tested in this direction, for instance, Bachau et al. [19] have studied the transfer excitation for the case of  $S^{15+} + H$  collision, who observed the effect of the interference between RTE and NTE modes. Atomic units are used throughout unless otherwise stated.

#### **II. THEORY**

In this formalism, we consider a hydrogenlike projectile with a nuclear charge  $Z_P$  and a helium atom or a heliumlike ion target of nuclear charge  $Z_T$ , the collision may be written as follows:

$$(Z_P, e_1^-) + (Z_T, e_2^-, e_3^-) \to (Z_P, e_1^-, e_2^-, e_3^-)^{***} + Z_T,$$
(1)

where  $e_1^-$  is the electron initially bound to the projectile,  $e_2^-$  and  $e_3^-$  are the electrons initially bound to the target.

The complete Hamiltonian may be written as

$$H = H_i + V_i = H_f + V_f, (2)$$

where  $H_i$  and  $V_i$  ( $H_f$  and  $V_f$ ) are, respectively, the Hamiltonian and the perturbation interaction in the initial (final) channel.

In the entrance channel, let us write

$$H_{i} = -\sum_{j=2}^{3} \frac{1}{2m_{ij}} \nabla_{\mathbf{x}_{j}}^{2} - \frac{Z_{T}}{x_{2}} - \frac{Z_{T}}{x_{3}} + \frac{1}{r_{23}} - \frac{1}{2\mu_{1}} \nabla_{\mathbf{s}_{1}}^{2} - \frac{Z_{P}}{s_{1}} - \frac{1}{2\mu_{i}} \nabla_{\mathbf{r}_{i}}^{2} + \frac{(Z_{P} - 1)(Z_{T} - 2)}{r_{i}},$$
(3)

$$V_{i} = \frac{Z_{P}Z_{T}}{R} - \frac{Z_{T}}{x_{1}} - \frac{Z_{P}}{s_{3}} + \frac{1}{r_{12}} - \frac{Z_{P}}{s_{2}} + \frac{1}{r_{13}} - \frac{(Z_{P}-1)(Z_{T}-2)}{r_{i}}$$
(4)

and for the exit channel,

$$H_{f} = -\sum_{j=1}^{3} \left( \frac{1}{2m_{fj}} \nabla_{\mathbf{S}_{j}}^{2} + \frac{Z_{P}}{s_{j}} \right) + \frac{1}{r_{12}} + \frac{1}{r_{13}} + \frac{1}{r_{23}} - \frac{1}{2\mu_{f}} \nabla_{\mathbf{r}_{f}}^{2} + \frac{(Z_{P} - 3)Z_{T}}{r_{f}},$$
(5)

$$V_f = \frac{Z_P Z_T}{R} - \frac{Z_T}{x_1} - \frac{Z_T}{x_2} - \frac{Z_T}{x_3} - \frac{(Z_P - 3)Z_T}{r_f}.$$
 (6)

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FIG. 1. P(T) is the projectile (target) nucleus.  $e_1^-$  is the electron initially bound to the projectile nucleus.  $e_2^-$  and  $e_3^-$  are the electrons initially bound to the target nucleus.

The coordinates are represented in Figs. 1 and 2:

$$\mathbf{s}_1 = \mathbf{S}_1,$$

$$\mathbf{s}_2 = \mathbf{S}_2 + O(1/M_P),$$

$$\mathbf{s}_3 = \mathbf{S}_3 + O(1/M_P),$$

$$\mathbf{x}_1 = \mathbf{X}_1,$$

$$\mathbf{x}_2 = \mathbf{X}_2,$$

$$\mathbf{x}_3 = \mathbf{X}_3 + O(1/M_T),$$

$$\mathbf{R} = \mathbf{r}_i + O(1/M_T) = -\mathbf{r}_f + O(1/M_P).$$

In expressions (3) and (5),

$$m_{ij} = \frac{M_T + j - 2}{M_P + j - 1}, \quad j = 2, 3,$$
$$\mu_1 = \frac{M_P}{M_P + 1},$$
$$\mu_i = (M_P + 1)(M_T + 2)/M,$$



FIG. 2. Representation of coordinates  $S_2$ ,  $S_3$ ,  $X_3$ ,  $\mathbf{r}_i$  and  $\mathbf{r}_f$  with respect to the center of mass (CDM).

$$m_{fj} = \frac{M_P + j - 1}{M_P + j}, \ j = 1, 2, 3,$$
  
 $\mu_f = (M_P + 3)M_T/M,$ 

where  $M = M_T + M_P + 3$ .

We introduce two versions of the kinetic-energy operator for the relative motion of particles:

$$T = \begin{cases} -\frac{1}{2\mu_{i}} \nabla_{\mathbf{r}_{i}}^{2} - \frac{1}{2\mu_{1}} \nabla_{\mathbf{s}_{1}}^{2} - \sum_{j=2}^{3} \frac{1}{2m_{ij}} \nabla_{\mathbf{X}_{j}}^{2} \\ -\frac{1}{2\mu_{f}} \nabla_{\mathbf{r}_{f}}^{2} - \sum_{j=1}^{3} \frac{1}{2m_{fj}} \nabla_{\mathbf{S}_{j}}^{2}. \end{cases}$$
(7)

In the configuration space, the wave function of the  $H_i$  $(H_f)$  in the initial (resp final) channel is  $\Phi_i$   $(\Phi_f)$ , thus one has

$$H_i \Phi_i = E \Phi_i \,, \tag{8}$$

$$H_f \Phi_f = E \Phi_f, \tag{9}$$

where

$$\Phi_i(\mathbf{r}_i, \mathbf{s}_1, \mathbf{x}_2, \mathbf{x}_3) = \varphi_P(\mathbf{s}_1) \varphi_T(\mathbf{x}_2, \mathbf{x}_3) \mathcal{F}^+_{+k_i}(\mathbf{r}_i), \quad (10)$$

$$\Phi_f(\mathbf{r}_f, \mathbf{s}_1, \mathbf{s}_2, \mathbf{s}_3) = \Psi_f(\mathbf{s}_1, \mathbf{s}_2, \mathbf{s}_3) \mathcal{F}_{-k_f}^{-}(\mathbf{r}_f), \qquad (11)$$

$$E = \frac{k_i^2}{2\mu_i} + \varepsilon_i = \frac{k_f^2}{2\mu_f} + \varepsilon_f.$$
(12)

In the frame of the center of mass of the whole system,  $k_i$   $(k_f)$  is the momentum of the reduced particle in the entrance (exit) channel.

 $\mathcal{F}_{\pm k_{i,f}}^{\pm}$  are the Coulomb functions normalized to  $(2\pi)^3 \delta(\mathbf{k}-\mathbf{k}')$ , expressed by

$$\mathcal{F}_{+k_i}^+(\mathbf{r}_i) = N_{\lambda_i}^+ \exp(+i\mathbf{k}_i \cdot \mathbf{r}_i) {}_1F_1(-i\lambda_i; 1; +ik_ir_i - i\mathbf{k}_i \cdot \mathbf{r}_i),$$
(13)

$$\mathcal{F}_{-k_f}^{-}(\mathbf{r}_f) = N_{\lambda_f}^{-} \exp(-i\mathbf{k}_f \cdot \mathbf{r}_f)_1 F_1(+i\lambda_f; 1; -ik_f r_f + i\mathbf{k}_f \cdot \mathbf{r}_f),$$
(14)

where

$$N_{\lambda_{i,f}}^{\pm} = \Gamma(1 \pm i\lambda_{i,f}) \exp\left(-\frac{\pi}{2}\lambda_{i,f}\right)$$
$$\lambda_i = (Z_P - 1)(Z_T - 2)/v,$$
$$\lambda_f = (Z_P - 3)Z_T/v,$$

v is the relative velocity of P and T.

In the initial channel,  $\varphi_T (\varphi_P)$  is the target (projectile) bound state with the energy  $\varepsilon_T (\varepsilon_P)$ . In the final channel,  $\Psi_f$ are the excited states on the projectile.

It appears clearly that in the Dodd-Greider [20] formalism post and prior forms of matrix elements are

$$T_{if}^{+} = \langle \Phi_f | U_{if}^{+} | \Phi_i \rangle, \qquad (15)$$

$$T_{if}^{-} = \langle \Phi_f | U_{if}^{-} | \Phi_i \rangle \tag{16}$$

and one has to first order of perturbation,

$$U_{if}^{+} \simeq \omega_{f}^{-\dagger} (V_{f} - W_{f}^{\dagger}) (1 + g_{x}^{+} V_{i}), \qquad (17)$$

$$U_{if}^{-} \simeq (1 + g_x^{-} V_f)^{\dagger} (V_i - W_i) \omega_i^{+}, \qquad (18)$$

where the Green functions  $g_x^{\pm}$  are given by

$$g_x^{\pm} = (E - H + v_x \pm i\varepsilon)^{-1}.$$

Here,  $v_x$  is an intermediate potential,  $W_i$  and  $W_f$  are distorting potentials,

$$\omega_i^+ = 1 + g_i^+ W_i,$$
  
$$\omega_f^- = 1 + g_f^- W_f,$$

where  $g_{i,f}^{\pm}$  are defined by the following expressions:

$$g_{i,f}^{\pm} = (E - H_{i,f} - W_{i,f} \pm i\varepsilon)^{-1}$$

We may see that for obtaining the transition amplitude expression, we have the liberty to choose form (17) or (18). The electronic interactions always appear in the distorted-wave equation for the initial channel in the integral equation  $U_{if}^+$ .

In order to avoid the mathematical difficulties, it is important to take form (18) in which the electronic interactions term is introduced in the equation of the final excited state.

In order to calculate  $T_{if}^-$  given by expression (16), let us set

$$\left|\zeta_{f}^{-}\right\rangle = (1 + g_{x}^{-} V_{f}) \left|\Phi_{f}\right\rangle. \tag{19}$$

In the limit  $\varepsilon = 0$  and from Eq. (2) and  $g_x^{\pm}$ ,  $\zeta_f^-$  and  $\Phi_f$  satisfy the equation

$$(E-H+v_x)|\zeta_f^-\rangle = v_x|\Phi_f\rangle.$$

We choose  $v_x$  an operator such that

$$v_x |\Phi_f\rangle = 0 \tag{20}$$

and for  $|\zeta_f^-\rangle$  the form

$$\left|\zeta_{f}^{-}\right\rangle = \left|\Psi_{f}(\mathbf{s}_{1},\mathbf{s}_{2},\mathbf{s}_{3})h_{f}^{-}\right\rangle.$$

$$(21)$$

From choices (20) and (21), Eq. (19) may be written as

$$\Psi_{f} \bigg[ E - T - \varepsilon_{f} - \frac{Z_{T} Z_{P}}{R} + Z_{T} \bigg( \frac{1}{x_{1}} + \frac{1}{x_{2}} + \frac{1}{x_{3}} \bigg) \bigg] h_{f}^{-} + v_{x} (\Psi_{f} h_{f}^{-})$$
  
+ 
$$\sum_{j=1}^{3} \frac{1}{m_{fj}} \nabla_{\mathbf{S}_{j}} \Psi_{f} \cdot \nabla_{\mathbf{S}_{j}} h_{f}^{-} = 0.$$
(22)

Let us now choose  $v_x$  as an operator, when it is applied to an arbitrary function f, one has

$$\boldsymbol{v}_{x}f = -\sum_{j=1}^{3} \frac{1}{m_{fj}} \boldsymbol{\nabla}_{\mathbf{S}_{j}} \boldsymbol{\Psi}_{f} \cdot \boldsymbol{\nabla}_{\mathbf{S}_{j}} \left(\frac{f}{\boldsymbol{\Psi}_{f}}\right)$$
(23)

and  $h_f^-$  an independent function of the coordinates of the electron 1.

Note also that only small values of  $s_1$  contribute significantly to the amplitude since the electron  $(e_1)$  stays on the projectile. Therefore, we can write

$$x_1 = |\mathbf{R} - \mathbf{s}_1| \simeq R.$$

These two choices, associated with the approximation of  $x_1$ , Eq. (22), become

$$\left[E - T - \varepsilon_f - \frac{Z_T(Z_P - 1)}{R} + \sum_{j=2}^3 \frac{Z_T}{x_j}\right] h_f^- = 0.$$
(24)

We take the first form of Eq. (7) for T, then the solution is a product of three Coulomb wave functions.

$$h_{f}^{-} = N_{\lambda_{k}}^{-} N_{\lambda_{2}}^{-} N_{\lambda_{3}}^{-} \exp(i\mathbf{k} \cdot \mathbf{r}_{i} + i\mathbf{k}_{2} \cdot \mathbf{x}_{2} + i\mathbf{k}_{3} \cdot \mathbf{x}_{3})$$

$$\times_{1} F_{1}(i\lambda_{k}; 1; -ikr_{i} - i\mathbf{k} \cdot \mathbf{r}_{i})$$

$$\times_{1} F_{1}(i\lambda_{2}; 1; -ik_{2}X_{2} - i\mathbf{k}_{2} \cdot \mathbf{X}_{2})$$

$$\times_{1} F_{1}(i\lambda_{3}; 1; -ik_{3}X_{3} - i\mathbf{k}_{3} \cdot \mathbf{X}_{3}), \qquad (25)$$

where the wave vectors  $\mathbf{k}$ ,  $\mathbf{k}_2$ , and  $\mathbf{k}_3$  are entirely determined by the asymptotic conditions (see the Appendix).

For  $\mathbf{X}_2$ ,  $\mathbf{X}_3$ , and  $r_i$  simultaneously large,  $h_f^-$  must have the asymptotic behavior of  $\mathcal{F}_{-k_f}^-(\mathbf{r}_f)$  and the energy must be conserved.

These conditions transform expression (25) as follows:

$$h_{f}^{-} \approx N_{N}^{-} (N_{T}^{-})^{2} e_{1}^{-i\mathbf{k}_{f} \cdot \mathbf{r}_{f}} F_{1}(i\lambda_{N};1;-ik_{f}r_{i}-i\mathbf{k}_{f}\cdot\mathbf{r}_{i})_{1}F_{1}$$

$$(-i\lambda_{T};1;-ivx_{2}-i\mathbf{v}\cdot\mathbf{x}_{2})_{1}F_{1}(-i\lambda_{T};1;-ivx_{3}$$

$$-i\mathbf{v}\cdot\mathbf{x}_{3}), \qquad (26)$$

where

$$\lambda_N = Z_T (Z_P - 1) / v,$$
  

$$\lambda_T = Z_T / v,$$
  

$$N_N^- = \Gamma (1 - i\lambda_N) e^{-(\pi/2)\lambda_N},$$
  

$$N_T^- = \Gamma (1 + i\lambda_T) e^{+(\pi/2)\lambda_T}.$$

Let us now set

$$|\Lambda_i^+\rangle = \omega_i^+ |\Phi_i\rangle$$

In the limit  $\varepsilon = 0$ , one has

$$(E - H_i - W_i) |\Lambda_i^+\rangle = 0.$$
<sup>(27)</sup>

Let  $U_i = V_i - W_i$  and  $|\Lambda_i^+\rangle = |\varphi_P \varphi_T y_i^+\rangle$ . Expression (27) becomes A. ZERARKA, V. G. FOESTER, AND J. HANS

$$(E-H-U_i)|\Lambda_i^+\rangle = 0$$

from the first form (7) of the kinetic-energy operator T and through the two following choices:

(i) The operator  $U_i$  is such that applied to a function f, it gives

$$U_{i}f = \left(\frac{1}{r_{12}} + \frac{1}{r_{13}} - \frac{1}{s_{2}} - \frac{1}{s_{3}} - \frac{Z_{T}}{x_{1}} + \frac{Z_{T}}{R}\right)f - \sum_{j=2}^{3} \frac{1}{m_{ij}} \nabla_{\mathbf{X}_{j}} \varphi_{T} \cdot \nabla_{\mathbf{X}_{j}} \left(\frac{f}{\varphi_{T}}\right).$$
(28)

(ii) The function  $y_i^+$  is independent of coordinates of the electron 1, then it satisfies the equation:

$$\left[E - T - \varepsilon_i - \frac{Z_T(Z_P - 1)}{R} + \frac{Z_P - 1}{s_2} + \frac{Z_P - 1}{s_3}\right] y_i^+ = 0.$$
(29)

Now, the second version of Eq. (7) is introduced into Eq. (29), it appears clearly that this equation can be separated. The solution is

$$y_{i}^{+} \approx N_{N}^{+} (N_{P}^{+})^{2} e_{1}^{+i\mathbf{k}_{i}\cdot\mathbf{r}_{i}} F_{1}(-i\lambda_{N};1;ik_{i}r_{f}+i\mathbf{k}_{i}\cdot\mathbf{r}_{f})$$

$$\times_{1}F_{1}(i\lambda_{P};1;ivs_{2}+i\mathbf{v}\cdot\mathbf{s}_{2})$$

$$\times_{1}F_{1}(i\lambda_{P};1;ivs_{3}+i\mathbf{v}\cdot\mathbf{s}_{3}), \qquad (30)$$

where

$$\lambda_P = (Z_P - 1)/v,$$

$$N_P^+ = \Gamma(1 - i\lambda_P) e^{(\pi/2)\lambda_P}$$
 and  $N_N^+ = (N_N^-)^*$ .

The motion of nucleus is reduced to the term  $(\mu\rho v)^{2i\lambda_N}$ (Gayet [21]). However, in the eikonal approximation, the factor  $(\mu\rho v)^{2i\lambda_N}$ , [where  $\lambda_N = Z_T(Z_P - 1)/v$ ] also features the interaction between *T* and (P+e), and may be ignored in the evaluation of the total cross section which depends on  $|T_{ii}^-|^2$ .

Finally, the transition amplitude may be written as

$$T_{if}^{-} = \langle \zeta_{f}^{-} | U_{i} | \Lambda_{i}^{+} \rangle = (N_{T}^{+} N_{P}^{+})^{2} \int d\mathbf{R} d\mathbf{r}_{1} d\mathbf{r}_{2} d\mathbf{r}_{3} (\mu \rho v)^{2i\lambda_{N}} \Psi_{f}^{*}(\mathbf{s}_{1}, \mathbf{s}_{2}, \mathbf{s}_{3}) e^{+i(\mathbf{k}_{i} \cdot \mathbf{r}_{i} + \mathbf{k}_{f} \cdot \mathbf{r}_{f})} \\ \times {}_{1}F_{1}(i\lambda_{T}; 1; ivx_{2} + i\mathbf{v} \cdot \mathbf{x}_{2})_{1}F_{1}(i\lambda_{T}; 1; ivx_{3} + i\mathbf{v} \cdot \mathbf{x}_{3}) \\ \times \{ V\varphi_{P}(s_{1})\varphi_{T}(x_{1,}x_{2})_{1}F_{1}(i\lambda_{P}; 1; ivs_{2} + i\mathbf{v} \cdot \mathbf{s}_{2})_{1}F_{1}(i\lambda_{P}; 1; ivs_{3} + i\mathbf{v} \cdot \mathbf{s}_{3}) \\ - \varphi_{P}(s_{1})_{1}F_{1}(i\lambda_{P}; 1; ivs_{3} + i\mathbf{v} \cdot \mathbf{s}_{3}) \nabla_{\mathbf{x}_{2}}\varphi_{T} \nabla_{\mathbf{s}_{2}} {}_{1}F_{1}(i\lambda_{P}; 1; ivs_{2} + i\mathbf{v} \cdot \mathbf{s}_{2}) \\ - \varphi_{P}(s_{1})_{1}F_{1}(i\lambda_{P}; 1; ivs_{2} + i\mathbf{v} \cdot \mathbf{s}_{2}) \nabla_{\mathbf{x}_{3}}\varphi_{T} \nabla_{\mathbf{s}_{3}} {}_{1}F_{1}(i\lambda_{P}; 1; ivs_{3} + i\mathbf{v} \cdot \mathbf{s}_{3}) \},$$
(31)

where

$$V = \frac{1}{r_{12}} + \frac{1}{r_{13}} - \frac{1}{s_2} - \frac{1}{s_3} - \frac{Z_T}{x_1} + \frac{Z_T}{R} \quad \text{and} \quad N_T^+ = (N_T^-)^*.$$

Note that the factor  $(\mu \rho v)^{2i\lambda_N}$  may be omitted in the expression of total cross section which is not influenced by the internuclear interaction. This remark suggests that the interaction does not contribute to the double capture and excitation.

## **III. CONCLUSION**

In summary, we may conclude that expression (31) represents a transition amplitude form of a first-order perturbation for the double transfer and excitation collisions. There are other versions of  $T_{if}^-$  which are, from the computational point of view, very involved. In this work, we have only exposed the more adequate form of the transition amplitude.

We may see that result (31) of  $T_{if}^{-}$  contains coherent con-

tributions from resonant and nonresonant transfer and excitation. It is also worthwhile to mention that, according our calculations, the mode NTE can always be considered as an uncorrelated process, it could be evaluated through an independent electron model.

For the sake of completeness we would like to point out that a dominance of multiple electron capture over single capture in close collisions, which are relevant for excitation, has been reported by Andriamonje, *et al.* [22] and Schlachter, *et al.* [23]. Note that the double Auger process is a known and established phenomenon (Carlson, and Krauss [24], and Aberg, [25]), a consideration of an invariance under time reversal leads to a new process. Resonant capture of two (or more) electrons with a correlated excitation of a projectile electron, i.e., double (or multiple) RTE, was postulated by Warczak, *et al.* [26] and Liesen, *et al.* [27] as a possible explanation for the origin of structures observed in the impact parameter dependence of characteristic x-ray emission.

In a future publication, we can test this formalism, for instance, H-like  $G_e$  with  $N_e$  where the capture of two target

electrons and the simultaneous excitation of one *K*-shell electron of the projectile.

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#### APPENDIX

In this appendix we show how the solution  $h_f^-$  Eq. (25), can be reduced to form (26) and we also confirm that the energy is conserved.

The asymptotic behavior of  $h_f^-$ , that is, that of  $\mathcal{F}_{-k_f}^-(\mathbf{r}_f)$ , implies

$$h_{f}^{-} \rightarrow \mathcal{F}_{-k_{f}}^{-}(\mathbf{r}_{f}), \qquad (A1)$$
$$\mathbf{r}_{i} \rightarrow \infty,$$
$$\mathbf{X}_{2} \rightarrow \infty,$$
$$\mathbf{X}_{3} \rightarrow \infty.$$

This condition imposes the following phase conditions:

$$-\mathbf{k}_{f} \cdot \mathbf{r}_{f} = \mathbf{k} \cdot \mathbf{r}_{i} + \mathbf{k}_{2} \cdot \mathbf{X}_{2} + \mathbf{k}_{3} \cdot \mathbf{X}_{3}, \qquad (A2)$$
$$-\lambda_{f} \ln(-k_{f}r_{f} + \mathbf{k}_{f} \cdot \mathbf{r}_{f}) + c = -\lambda_{N} \ln(-k_{i}r_{i} + \mathbf{k}_{i} \cdot \mathbf{r}_{i})$$
$$+\lambda_{2} \ln(-k_{2}X_{2} - \mathbf{k}_{2} \cdot \mathbf{X}_{2})$$
$$+\lambda_{3} \ln(-k_{3}X_{3} - \mathbf{k}_{3} \cdot \mathbf{X}_{3}), \qquad (A3)$$

where *c* is a constant.

The energy must be conserved,

$$\frac{k_f^2}{2\mu_f} = \frac{k^2}{2\mu_i} + \frac{k_2^2}{2m_{i2}} + \frac{k_3^2}{2m_{i3}},$$
 (A4)

the vector  $\mathbf{r}_f$  may be written in a more convenient form

$$\mathbf{r}_{f} = -\frac{(M_{p}+1)}{(M_{p}+3)}\mathbf{r}_{i} - \frac{M}{(M_{p}+3)(M_{T}+1)}\mathbf{X}_{2} - \frac{M}{(M_{p}+3)(M_{T}+2)}\mathbf{X}_{3}, \qquad (A5)$$

where  $\mathbf{X}_2 = \mathbf{x}_2$  and  $\mathbf{X}_3 = \mathbf{x}_3 - [1/(M_T + 1)]\mathbf{x}_2$ .

Introducing the expression (A5) of  $\mathbf{r}_f$  into Eq. (29) and by identification, one has

$$\mathbf{k} = \frac{(M_p + 1)}{(M_p + 3)} \mathbf{k}_f \xrightarrow[M_p \to \infty]{} \mathbf{k}_f, \qquad (A6)$$

$$\mathbf{k}_2 = \frac{M_T}{(M_T + 1)} \frac{\mathbf{k}_f}{\mu_f} \xrightarrow[M_T \to \infty]{} \frac{\mathbf{k}_f}{\mu_f} = v, \qquad (A7)$$

$$\mathbf{k}_3 = \frac{M_T}{(M_T + 2)} \frac{\mathbf{k}_f}{\mu_f} \xrightarrow[M_T \to \infty]{} \frac{\mathbf{k}_f}{\mu_f} = v.$$
(A8)

In the limit  $(M_p, M_T) \rightarrow \infty h_f^-$  may be rewritten as expression (26).

In order to verify the conservation of the energy, we replace the wave vectors  $\mathbf{k}$ ,  $\mathbf{k}_2$ , and  $\mathbf{k}_3$  in Eq. (A4), we obtain

$$\frac{\mathbf{k}_{f}^{2}}{2\mu_{f}} = \frac{\mathbf{k}_{f}^{2}}{2\mu_{f}} \frac{M_{T}(M_{p}+1) + 2M}{(M_{p}+3)(M_{T}+2)} = \frac{\mathbf{k}_{f}^{2}}{2\mu_{f}}.$$

In Eq. (A3), the constant *c* may be evaluated by remarking that  $\zeta_f^-$  contains  $\Psi_f(\mathbf{s}_1, \mathbf{s}_2, \mathbf{s}_3)$ , thus only small values of  $\mathbf{s}_1$ ,  $\mathbf{s}_2$ , and  $\mathbf{s}_3$  give an appreciable quantity to the function  $\zeta_f^-$ .

Under these considerations the constant c in Eq. (A3) is given by

$$c \simeq -\frac{Z_T}{v} \ln \mu_f^2 \,.$$

In a way similar to that of the solution  $h_f^-$ , it is easy to show that the asymptotic conditions for  $y_i^+$ , i.e.,

$$y_{i}^{+} \rightarrow \mathcal{F}_{+k_{i}}^{+}(\mathbf{r}_{i}), \qquad (A9)$$
$$\mathbf{r}_{f} \rightarrow \infty,$$
$$\mathbf{S}_{2} \rightarrow \infty,$$
$$\mathbf{S}_{3} \rightarrow \infty,$$

enable us to verify the conservation of energy. In this case, it is necessary to use the following relation:

$$\mathbf{r}_{i} = -\frac{M_{T}}{M_{T}+2}\mathbf{r}_{f} - \frac{M}{M_{T}+2} \left(\frac{1}{M_{p}+2}\mathbf{S}_{2} + \frac{1}{M_{p}+3}\mathbf{S}_{3}\right).$$
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