Collisional mixing among excited degenerate states in inelastic ion-atom collisions

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Stark mixing among excited degenerate states following capture or excitation by ion impact on hydrogenlike atoms is calculated at high velocities by using the perturbative formalism. For electron capture, the second-order Brinkman-Kramers approximation is found to describe the correct infinitesimal Stark rotation valid in the high-velocity regime. However, the second-order continuum distorted-wave approximation does not provide such a rotational form in that regime. It is concluded that the continuum distorted-wave amplitudes should not be Stark rotated even though a numerical coincidence is found between our formalism and the usual Stark rotation in the experimental range of interest. Finally for electron excitation, it is found that the perturbative formalism does not lead to a rotational structure. [S1050-2947(96)09305-5]

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I. INTRODUCTION

Let us begin by considering a simple charge-transfer process in an atomic collision,

$$P_{\vec{K}_i}+(T+e)_{1s}\rightarrow T+(P+e)_{\vec{K}'_f,nlm}, \tag{1}$$

where P, T, and e denote the heavy projectile, the nucleus target, and the electron, respectively. Studying this process, Burgdörfer [1] remarked that the first-order approximation for the relative l population of the final states fails since it neglects, among other effects, Stark mixing between the degenerate excited states of the projectile escaping the field of the residual target ion. Burgdörfer developed a model called post-collision interaction (PCI) [1] considering the mixing between states of the same principal shell. Besides a full PCI calculation, he developed an analytical eikonal approximation that can be expressed as follows for capture into the $n=2$ level,

$$\begin{pmatrix} a^{PCI}_{1s,2s} \\ a^{PCI}_{1s,2p_0} \end{pmatrix} = \begin{pmatrix} \cos\phi^{BK1} & i\sin\phi^{BK1} \\ i\sin\phi^{BK1} & \cos\phi^{BK1} \end{pmatrix} \begin{pmatrix} a^{BK1}_{1s,2s} \\ a^{BK1}_{1s,2p_0} \end{pmatrix}, \tag{2}$$

where $a^{BK1}_{i,f}=a^{BK1}_{i,f}(\vec{\rho})$ is the first-order Brinkman-Kramers (BK1) amplitude [2] for the transition $i\rightarrow f$, $a^{PCI}_{i,f}=a^{PCI}_{i,f}(\vec{\rho})$ is the corresponding amplitude including the PCI mixing, and $\vec{\rho}$ is the impact parameter. The matrix equation (2) represents a unitary rotation where the angle ϕ^{BK1} was calculated in an eikonal approximation [1] to give

$$\phi^{BK1}\simeq\phi_B=-\frac{1}{v}\int_{R_0}^{\infty}H_{2s,2p_0}(Z,\vec{\rho}=0)dZ, \tag{3}$$

with

$$H_{2s,2p_0}(Z,\vec{\rho})=\langle 2s|-\frac{Z_T}{|\vec{R}+\vec{r}'|}|2p_0\rangle. \tag{4}$$

Here, Z_T (Z_P) is the target (projectile) charge, $\vec{R}=\vec{\rho}+\vec{Z}$ is the projectile position with respect to the target, $\vec{Z}=\vec{v}t$, $\vec{v}$ is the projectile velocity, t represents the time, and $\vec{r}'$ is the electron coordinate with respect to the projectile. Atomic units are used and heavy projectiles are assumed.

The integral (3) is simple and it gives the evolution phase as a function of the lower bound R_0,

$$\phi_B=\frac{Z_T}{v}\left[\frac{3}{x_0}-\exp(-x_0)\left(\frac{x_0^2}{8}+\frac{3x_0}{4}+\frac{9}{4}+\frac{3}{x_0}\right)\right], \tag{5}$$

where $x_0=Z_PR_0$. The parameter R_0, which divides the internal collisional and the post-collisional regions, is not uniquely defined. It was set equal to the smallest $n=2$ radius ($x_0=5$) by comparison between the analytical approximation and the full PCI calculation at moderate velocities. This choice of the starting point of the PCI gives $\phi_B=0.534Z_T/v$ [1]. Later works have taken this value for granted, even when transition amplitudes were calculated using other distorted-wave methods such as the continuum-distorted-wave (CDW) method [3–7] or the eikonal approximation [8] instead of the first-order Brinkman-Kramers (BK1) method.

The *first* question we pose here is the following: is it possible to find the value of ϕ^{BK1}, at least in the high velocity limit, without invoking R_0? The answer is *yes*; in Sec. II A we obtain this value of ϕ^{BK1} corresponding to an infinitesimal Stark rotation in the high-energy limit from the perturbative formalism.

On the other hand, several distorted-wave methods have been extensively used in the electron transfer theory to improve the BK1 approximation in the high- and intermediate-energy regions, such as the mentioned CDW one [9]. It has been observed that the CDW approximation fails to describe the experimental density matrix elements [3]. Some authors considered that this failure could be due to the missing of the Stark mixing, and they rotated the CDW results with $\phi_B=0.534Z_T/v$ straightforwardly [3–7]. It has already been addressed that though the CDW amplitudes rotated with the

eikonal PCI model gives a perihelion velocity $(\vec{L}\times\vec{A})_z$ that agrees with the close-coupling data at intermediate energies, the particular form chosen in the analytical PCI treatment may overestimate the effect [6]. The point is that we do not know to what extent the CDW amplitudes do already contain the $2s-2p_0$ Stark mixing. Here we pose the *second* question: is it possible to find the corresponding Stark rotation angle ϕ^{CDW} using amplitudes $a^{CDW}_{i,f}(\vec{\rho})$ instead of $a^{BK1}_{i,f}(\vec{\rho})$? The answer is *yes*; in Sec. II B we obtain the value of ϕ^{CDW} in the high-energy limit and find that $\phi^{CDW}/\phi^{BK1}\to O(1/v)$ as $v\to\infty$. We will conclude that the CDW wave functions do already contain such a mixing at least in the high-energy regime. In other words, if CDW amplitudes are Stark rotated we account for the Stark mixing twice.

So far, we have circumscribed our discussions to rearrangement processes. A *third* question is posed: should we Stark rotate the first-order amplitudes when target excitation is considered? The answer is *no*; as we shall see in Sec. III, second-order amplitudes for direct processes do not present a rotational structure for large velocities.

II. METHOD FOR CAPTURE PROCESS

A. The Brinkman-Kramers approximation

Let us start considering the second-order Brinkman-Kramers approximation with the Green function including the projectile potential to all orders (BK2P). The second-order transition amplitude in the nonrelativistic quantum formalism is

$$T^{BK2P}_{if}=T^{BK1}_{if}+\langle\psi_f|V_T\frac{1}{E-H_0-V_P+i\varepsilon}V_P|\psi_i\rangle, \tag{6}$$

where $T^{BK1}_{if}=\langle\psi_f|V_P|\psi_i\rangle=\langle\psi_f|V_T|\psi_i\rangle$ is the first-order Brinkman-Kramers transition matrix element, V_T (V_P) is the T-e (P-e) potential, H_0 is the kinetic-energy operator, $\varepsilon\to0^+$ and $\psi_{(i,f)}$ satisfy $(H_0+V_{(T,P)}-E)\psi_{(i,f)}=0$. Note that the internuclear interaction was removed invoking the Wicks argument [10]. To calculate the second-order contribution, we proceed as usual in these cases [10]. Let us consider $|\psi_n\rangle=|\vec{K}'_n,a\rangle$ a complete set of unperturbed wave functions centered on the projectile, satisfying the Schrödinger equation $(H_0+V_P-E'_n)|\vec{K}'_n,a\rangle$. Then we can express the spectral representation of the projectile-based Green operator as follows:

$$\frac{1}{E-H_0-V_P+i\varepsilon}=\int d\vec{K}'_n\sum_a\frac{|\vec{K}'_n,a\rangle\langle\vec{K}'_n,a|}{E-E'_n+i\varepsilon}, \tag{7}$$

where

$$E=\frac{K_i^2}{2\nu_T}-\frac{Z_T^2}{2}=\frac{K_f'^2}{2\nu_P}-\frac{Z_P^2}{8},\quad E'_n=\frac{K_n'^2}{2\nu_P}-\frac{Z_P^2}{2n^2},$$
$$\nu_T^{-1}=(M_T+1)^{-1}+M_P^{-1},\quad \nu_P^{-1}=M_T^{-1}+(M_P+1)^{-1}, \tag{8}$$

and M_T (M_P) is the target (projectile) mass. Using the orthogonality condition

$$\langle\vec{K}'_n,a|\vec{K}'_{n'},b\rangle=\delta(\vec{K}'_n-\vec{K}'_{n'})\,\delta_{a,b} \tag{9}$$

and considering only the intermediate Stark states that play a relevant role in the Stark mixing, for $n=2$ the $2s$ and $2p_0$ states we find the following matrix expression,

$$\begin{pmatrix}T^{BK2P}_{1s,2s}\\T^{BK2P}_{1s,2p_0}\end{pmatrix}=\begin{pmatrix}1+C^{BK1}_{2s,2s} & C^{BK1}_{2p_0,2s}\\ C^{BK1}_{2s,2p_0} & 1+C^{BK1}_{2p_0,2p_0}\end{pmatrix}\begin{pmatrix}T^{BK1}_{1s,2s}\\T^{BK1}_{1s,2p_0}\end{pmatrix}, \tag{10}$$

where

$$C^{BK1}_{a,b}=\int\frac{T^{BK1}_{1s,a}(\vec{K}_i,\vec{K}'_n)T^{B1}_{a,b}(\vec{K}'_n,\vec{K}'_f)}{T^{BK1}_{1s,a}(\vec{K}_i,\vec{K}'_f)(E-E'_n+i\varepsilon)}d\vec{K}'_n. \tag{11}$$

Here $T^{B1}_{a,b}(\vec{K}'_n,\vec{K}'_f)=\langle\psi_f|V_T|\psi_n\rangle$ denotes the first-order Born approximation to the transition matrix element for the direct process (excitation),

$$T+(P+e)_{\vec{K}'_n,a}\to T+(P+e)_{\vec{K}'_f,b}. \tag{12}$$

In (10) we restrain the set of intermediate states to the relevant Stark states $2s$ and $2p_0$ ($2p_1$ is missing). This is a limitation of our calculation, but it will permit us a direct comparison with the eikonal PCI formulation.

We will concentrate on the nondiagonal elements. From a physical point of view, these elements represent very simple mechanisms. The first-order amplitude considers a single transition $1s\to2s$ ($1s\to2p_0$), while the second-order amplitude considers a typical two-step process $1s\to2p_0\to2s$ ($1s\to2s\to2p_0$). In a similar form, the third order gives three-step contributions, and so on.

We can find in the literature [17] the closed forms for the elements $T^{BK1}_{1s,a}(\vec{K}_i,\vec{K}'_n)$ and $T^{B1}_{a,b}(\vec{K}'_n,\vec{K}'_f)$, for any states a and b, in terms of Feynman integrals [11,12]. Figure 1 shows the numerical results of $C^{BK1}_{2p_0,2s}$ and $C^{BK1}_{2s,2p_0}$ normalized to their value in the high-velocity limit, for different values of Z_T/Z_P. Two main features can be drawn: first, $C^{BK1}_{2p_0,2s}$ and $C^{BK1}_{2s,2p_0}$ are purely imaginary; second, for large velocities both elements tend to the *same* limit, $i\phi^{BK1}=i3Z_T/(4v)$, independent of the ratio Z_T/Z_P. The ejection angle of the rearranged atom, θ', is considered equal to zero (forward direction, corresponding to the large impact parameter). Similar limits are observed for $\theta'>0$ as $v\to\infty$, except in a narrow region around the critical angle $\theta'=\sqrt{3}(M_T+M_P)/(2M_TM_P)$ [13].

In the high-energy limit, $C^{BK1}_{2s,2p_0}$ and $C^{BK1}_{2p_0,2s}$ have analytical expressions that can be obtained using the peak approximation [13]. It consists of evaluating $T^{BK1}_{1s,a}(\vec{K}_i,\vec{K}'_n)\simeq T^{BK1}_{1s,a}(\vec{K}_i,\vec{K}'_f)$, that is where $T^{B1}_{a,b}(\vec{K}'_n,\vec{K}'_f)$ peaks. We then obtain

$$C^{BK1}_{a,b}\simeq\int\frac{T^{B1}_{a,b}(\vec{K}'_n,\vec{K}'_f)}{E-E'_n+i\varepsilon}d\vec{K}'_n. \tag{13}$$

Since $T^{B1}_{2s,2p_0}=T^{B1}_{2p_0,2s}$, the nondiagonal elements of the matrix (10) evaluated in the forward direction tend to the same value for large velocities, given by

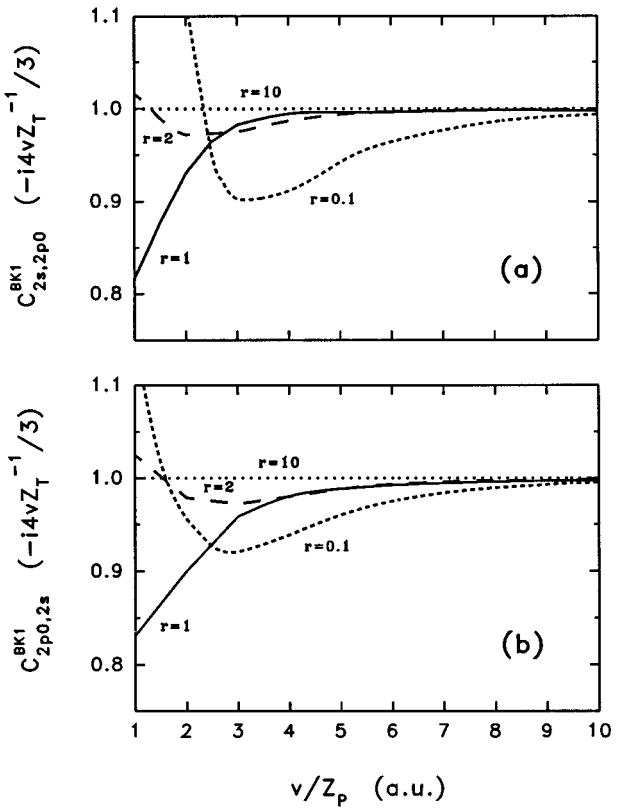

FIG. 1. Numerical values for (a) $C^{BK1}_{2s,2p_0}/i\phi^{BK1}$ and (b) $C^{BK1}_{2p_0,2s}/i\phi^{BK1}$ with $\phi^{BK1}=3Z_T/(4v)$, as a function of the scaled velocity in atomic units, for different values of $r=Z_T/Z_P$. The system under consideration is $P^{Z_P+}+T^{(Z_T-1)+}(1s)\rightarrow P^{(Z_P-1)+}(n=2)+T^{Z_T+}$, at $\theta'=0$.

$$C^{BK1}_{2s,2p_0}\simeq\int\frac{T^{B1}_{2s,2p_0}(\vec{K}'_n,\vec{K}'_f)}{E-E'_n+i\varepsilon}d\vec{K}'_n\rightarrow i\frac{3Z_T}{4v}=i\phi^{BK1}. \quad (14)$$

The terms $C^{BK1}_{2s,2s}$ and $C^{BK1}_{2p_0,2p_0}$ represent the elastic contribution, so we can neglect them in comparison with unity [20]. Then, in the high-energy regime, the matrix equation (10) can be written as follows:

$$\begin{pmatrix} T^{BK2P}_{1s,2s} \\ T^{BK2P}_{1s,2p_0}\end{pmatrix}=\begin{pmatrix} 1 & i\phi^{BK1} \\ i\phi^{BK1} & 1\end{pmatrix}\begin{pmatrix} T^{BK1}_{1s,2s} \\ T^{BK1}_{1s,2p_0}\end{pmatrix}. \quad (15)$$

In comparison with (2), it is concluded that the second order provides an infinitesimal rotation corresponding to the leading $1/v$ term of the Stark mixing. By infinitesimal rotation we mean $\phi^{BK1}\ll 1$, then $\sin\phi^{BK1}\simeq\phi^{BK1}\simeq 3Z_T/4v$, and $\cos\phi^{BK1}\simeq 1$.

At this stage, we can make a link with the result of Burgdörfer [1]. Let us start with the peak approximation of $C^{BK1}_{2s,2p_0}$ given in (14) and perform the following Fourier transforms:

$$T^{B1}_{2s,2p_0}(\vec{K}'_n,\vec{K}'_f)=\int d\vec{R}\frac{\exp(i\vec{q}\cdot\vec{R})}{(2\pi)^3}H_{2s,2p_0}(\vec{R}) \quad (16)$$

and

$$\frac{1}{E-E'_n+i\varepsilon}\simeq\frac{1}{-(\vec{K}'_n-\vec{K}'_f)\cdot\vec{v}+i\varepsilon}=-i\int_0^\infty dt\,\exp(-\varepsilon t)\exp(-i\vec{q}\cdot\vec{v}t), \quad (17)$$

where $\vec{q}=\vec{K}'_n-\vec{K}'_f$. After simple algebra, we find

$$C^{BK1}_{2s,2p_0}\simeq -i\int_0^\infty dt\int d\vec{R}d\vec{q}\frac{\exp[i\vec{q}\cdot(\vec{R}-\hat{\vec{v}}\,Z)]}{(2\pi)^3}H_{2s,2p_0}(\vec{R})$$

$$=-i\int_0^\infty dt\int d\vec{R}\,\delta(\vec{R}-Z\hat{\vec{v}})H_{2s,2p_0}(\vec{R})$$

$$=-\frac{i}{v}\int_0^\infty dZ\,H_{2s,2p_0}(Z,\vec{\rho}=\vec{0}). \quad (18)$$

This expression is equal to that of Burgdörfer as given in (3), except in the lower bound. Eq. (18) starts the integration from zero, while Eq. (3) starts from $R_0=\langle r\rangle_{n=2}$. In the PCI model R_0 is evaluated for moderately high velocities (i.e., $v=2$, for the electron capture $H^++H(1s)\rightarrow H(n=2)+H^+$, see Fig. 1 of [1]). From (18) we can say that this bound tends to zero in the asymptotic limit. The Stark rotation angle ϕ^{BK1} is obtained in the high velocity limit from the perturbative formalism and it is exact in the nonrelativistic limit. The performance of the density matrix elements using ϕ^{BK1} is, of course, similar to that using ϕ_B [1] since the difference in the angles is not very significant.

B. The continuum distorted-wave approximation

We follow the same pattern as before. The second order in the CDW series to the transition matrix element reads

$$T^{CDW2}_{if}=T^{CDW1}_{if}+\langle\chi^-_f|W_f\frac{1}{E-H+W_f+i\varepsilon}W_i|\chi^+_i\rangle, \quad (19)$$

where $T^{CDW1}_{if}=\langle\chi^-_f|W_i|\chi^+_i\rangle=\langle\chi^-_f|W_f|\chi^+_i\rangle$ is the first-order CDW element, and χ^+_i and χ^-_f are CDW wave functions satisfying $(E-H+W_{i,f})\chi^{+,-}_{i,f}=0$. As found in (6) for BK2P, we expect that Eq. (19) contains the infinitesimal Stark rotation corresponding to the CDW, if any [14].

To calculate the second order we consider a complete set of eigenfunctions χ^-_n of $(H-W_f)$ and proceed as in the previous section. After simple algebra, we find a matrix expression for $T^{CDW2}_{1s,2s}$ and $T^{CDW2}_{1s,2p_0}$ similar to (10) with

$$C^{CDW}_{a,b}=\int\frac{T^{CDW1}_{1s,a}(\vec{K}_i,\vec{K}'_n)\langle\chi^-_b|W_f|\chi^-_a\rangle}{T^{CDW1}_{1s,a}(\vec{K}_i,\vec{K}'_f)(E-E'_n+i\varepsilon)}d\vec{K}'_n \quad (20)$$

instead of $C^{BK1}_{a,b}$. With the help of the Nordsieck integrals [16] we can write

$$\langle\chi^-_b|W_f|\chi^-_a\rangle=T^{B1}_{a,b}(\vec{K}'_n,\vec{K}'_f)Y_{a,b}(\vec{K}'_n,\vec{K}'_f), \quad (21)$$

where $T^{B1}_{a,b}(\vec{K}'_n,\vec{K}'_f)$ is the first-order Born transition matrix element for the direct excitation as in (11), and the factor $Y_{a,b}(\vec{K}'_n,\vec{K}'_f)$ reads as follows:

$$Y_{2s,2p_0}(\vec{K}'_n,\vec{K}'_f)=\frac{\gamma^-(a_1,A_1)\gamma^+(a_2,A_2)q^4}{D^2A_1A_2}L(\vec{q}) \quad (22)$$

with

$$\gamma^{\pm}(a,A)=\exp(\pi a/2)\Gamma(1\pm ia)A^{-ia}, \quad (23a)$$

$$L(\vec{q})=F_1-(1+ia_2)\frac{(A_2-A_3)}{A_1A_2}F_2, \quad (23b)$$

$$a_i=\frac{M_T}{M_T+1}\frac{Z_T}{p_i}, \quad (23c)$$

$$\eta=1-\frac{M_TM_P}{(M_T+1)(M_P+1)}, \quad (23d)$$

$$\vec{p}_1=\eta\vec{K}'_f, \quad \vec{p}_2=\eta\vec{K}'_n, \quad (23e)$$

$$\vec{q}=\vec{K}'_n-\vec{K}'_f, \quad \vec{Q}=\vec{q}-\vec{p}_2, \quad (23f)$$

$$z=\epsilon+ip_2, \quad \epsilon\rightarrow 0^+, \quad (23g)$$

$$D=z^2+Q^2, \quad A_j=1+2S_j/D, \quad (23h)$$

$$S_j=\vec{p}_j.\vec{Q}-izp_j, j=1,2, \quad (23i)$$

$$S_3=p_1p_2-\vec{p}_1\cdot\vec{p}_2, \quad (23j)$$

$$Fj={}_2F_1(j-1+ia_1;j+ia_2;j;X_0), \quad (23k)$$

$$X_0=1-\frac{A_1+A_2-A_3}{A_1A_2}, \quad (23l)$$

and $Y_{2p_0,2s}(\vec{K}'_n,\vec{K}'_f)=Y_{2s,2p_0}(\vec{K}'_n,\vec{K}'_f)$.

As in the preceding section, we will concentrate on the nondiagonal elements $C^{CDW}_{2s,2p_0}$ and $C^{CDW}_{2p_0,2s}$. Following Crothers [15], we can express the elements $T^{CDW1}_{1s,a}(\vec{K}_i,\vec{K}'_n)$ in terms of the Nordsieck integrals [16]. Afterward, we compute a three-dimensional integral over the variable $\vec{K}'_n$. Figure 2 shows the values of $C^{CDW}_{2s,2p_0}$ and $C^{CDW}_{2p_0,2s}$ normalized to their value in the high-velocity limit. Again we evaluate it for $\theta'=0$, while $Z_T/Z_P=1,2$. In the high-energy limit, $C^{CDW}_{2s,2p_0}$ and $C^{CDW}_{2p_0,2s}$ have analytical expressions that can be derived from the peak approximation to obtain

$$C^{CDW}_{a,b}\simeq\int d\vec{K}'_nY_{a,b}(\vec{K}'_n,\vec{K}'_f)\frac{T^{B1}_{a,b}(\vec{K}'_n,\vec{K}'_f)}{(E-E'_n+i\varepsilon)}. \quad (24)$$

By comparison with (13), $Y_{a,b}(\vec{K}'_n,\vec{K}'_f)$ can be considered as a correcting factor. After some algebra, which for short we skip, the correcting factor in the high-energy limit is

$$Y_{2s,2p_0}(\vec{K}'_n,\vec{K}'_f)\simeq\frac{q^2}{(\vec{q}+\vec{p}_1)^2+(\epsilon-ip_1)^2}. \quad (25)$$

$Y_{2s,2p_0}$ is unity when p_1 is zero, and this is equivalent to using Brinkman-Kramers undistorted wave functions as intermediate states. Since $T^{B1}_{2s,2p_0}=T^{B1}_{2p_0,2s}$, then $C^{CDW}_{2s,2p_0}$ and $C^{CDW}_{2p_0,2s}$ tend to the same asymptotic limit,

$$C^{CDW}_{2s,2p_0}\simeq\int d\vec{K}'_n\frac{q^2}{[(\vec{q}+\vec{p}_1)^2-(\epsilon-ip_1)^2]}\frac{T^{B1}_{2s,2p_0}}{(E-E'_n+i\varepsilon)}$$

$$\rightarrow-\frac{Z_TZ_P}{8v^2}=i\phi^{CDW}. \quad (26)$$

Neglecting the diagonal terms $C^{CDW}_{2s,2s}$ and $C^{CDW}_{2p_0,2p_0}$ in comparison with unity [20], we obtain the second-order CDW T-matrix elements in the high-energy limit,

$$\begin{pmatrix} T^{CDW2}_{1s,2s} \\ T^{CDW2}_{1s,2p_0}\end{pmatrix}=\begin{pmatrix} 1 & i\phi^{CDW} \\ i\phi^{CDW} & 1\end{pmatrix}\begin{pmatrix} T^{CDW1}_{1s,2s} \\ T^{CDW1}_{1s,2p_0}\end{pmatrix}, \quad (27)$$

with $\phi^{CDW}=iZ_TZ_P/(8v^2)$. Two important consequences should be pointed out. First, Fig. 2 shows that $C^{CDW}_{2s,2p_0}$ and $C^{CDW}_{2p_0,2s}$ are generally complex, but in the high-energy limit they tend to the same real value. This means that ϕ^{CDW} is

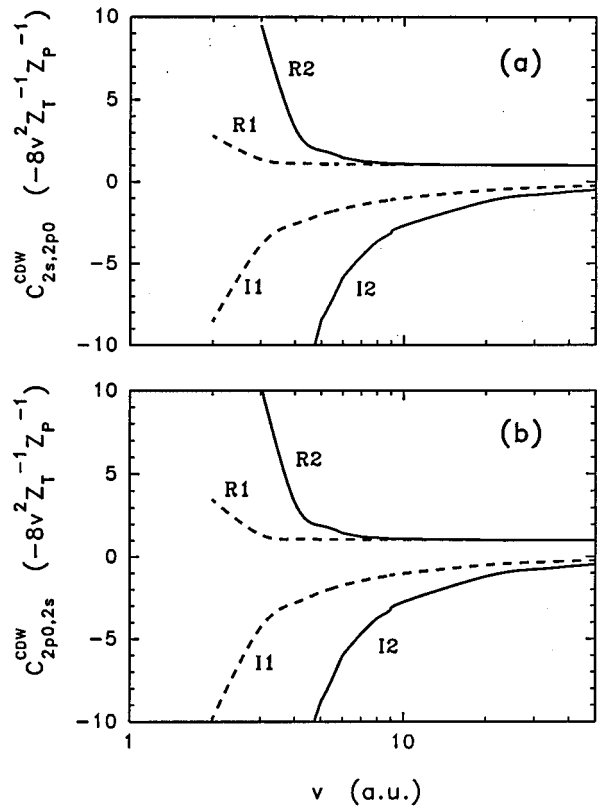

FIG. 2. Numerical values for (a) $C^{CDW}_{2s,2p_0}/i\phi^{CDW}$ and (b) $C^{CDW}_{2p_0,2s}/i\phi^{CDW}$ with $i\phi^{CDW}=-Z_TZ_P/(8v^2)$, as a function of the scaled velocity in atomic units. $R1$ and $I1$ are the real and imaginary parts for the system $H^+ + H(1s)\rightarrow H(n=2)+H^+$ at $\theta'=0$. $R2$ and $I2$ are the real and imaginary parts for the system $H^+ + He^+(1s)\rightarrow H(n=2)+He^{2+}$, at $\theta'=0$.

purely imaginary (note ϕ^{BK1} is real), so the matrix equation (27) does not have a rotational structure. Second, and more importantly, ϕ^{CDW} falls off faster than ϕ^{BK1}, i.e., $\phi^{CDW}/\phi^{BK1} \to iZ_P/(6v) = O(1/v)$, showing that in the high velocity limit the Stark mixing is embodied in the CDW wave functions [14].

It is noticeable that for proton on helium at $v = 2.75$ a.u. (that is in the experimental range of interest) we find the following values:

$$\phi^{CDW}_{2s,2p_0} = -iC^{CDW}_{2s,2p_0} = 0.240 + i0.066, \tag{28}$$

$$\phi^{CDW}_{2p_0,2s} = -iC^{CDW}_{2p_0,2s} = 0.260 + i0.072, \tag{29}$$

that are very close to $\phi_B = 0.262 + i0.0$. Perhaps this coincidence may elucidate the performance of the CDW with PCI in that range. It should be also noted that at lower and higher velocities than $v = 2.75$ a.u., ϕ^{CDW} disagrees with ϕ_B; for example, at $v = 4.00$ a.u.,

$$\phi^{CDW}_{2s,2p_0} = -iC^{CDW}_{2s,2p_0} = 0.051 + i0.015, \tag{30}$$

$$\phi^{CDW}_{2p_0,2s} = -iC^{CDW}_{2p_0,2s} = 0.055 + i0.015, \tag{31}$$

while $\phi_B = 0.180 + i0.0$.

III. METHOD FOR EXCITATION PROCESS

In a similar fashion to capture, we can obtain the second-order Born approximation (B2) for excitation by using a complete set of intermediate unperturbed wave functions now centered on the *target*. The process under consideration is

$$P_{\vec{K}_i} + (T+e)_{1s} \to P_{\vec{K}_f} + (T+e)_{nlm}, \tag{32}$$

and the matrix expression is

$$\begin{pmatrix} T^{B2}_{1s,2s} \\ T^{B2}_{1s,2p_0} \end{pmatrix} = \begin{pmatrix} 1 + E^{B1}_{2s,2s} & E^{B1}_{2p_0,2s} \\ E^{B1}_{2s,2p_0} & 1 + E^{B1}_{2p_0,2p_0} \end{pmatrix} \begin{pmatrix} T^{B1}_{1s,2s} \\ T^{B1}_{1s,2p_0} \end{pmatrix}, \tag{33}$$

where

$$E^{B1}_{a,b} = \int \frac{T^{B1}_{1s,a}(\vec{K}_i, \vec{K}_m) T^{B1}_{a,b}(\vec{K}_m, \vec{K}_f)}{T^{B1}_{1s,a}(\vec{K}_i, \vec{K}_f)(E - E_{mf} + i\varepsilon)} d\vec{K}_m, \tag{34}$$

and $T^{B1}_{a,b}$, $T^{B2}_{a,b}$ are the first- (B1) and second- (B2) order Born approximations to the transition element, respectively. These integrals have closed forms in terms of the Feynman integrals [11]. The numerical results are shown in Fig. 3 as a function of v/Z_T, in the forward direction, $\theta = 0$, normalized to $-3Z_P i/(4v)$. Note $E^{B1}_{2p_0,2s}$ and $E^{B1}_{2s,2p_0}$ are purely imaginary. After using the peak approximation, similar to the preceding sections, we find the following limits:

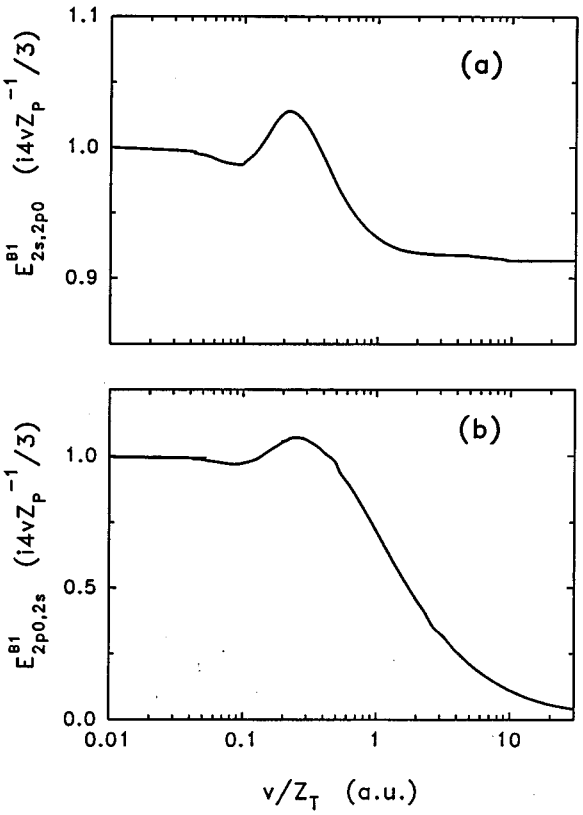

FIG. 3. Numerical values for (a) $E^{B1}_{2s,2p_0}/i\phi^{B1}$ and (b) $E^{B1}_{2p_0,2s}/i\phi^{B1}$ with $\phi^{B1} = -3Z_P/(4v)$, as a function of the scaled velocity in atomic units. The system under consideration is $P^{Z_P+} + T^{(Z_T-1)+}(1s) \to P^{(Z_P-1)+}(n=2) + T^{Z_T+}$, at $\theta = 0$.

$$E^{B1}_{2s,2p_0} \to \begin{cases} -\dfrac{3Z_P}{4v} i, & \text{as } v \to 0 \\ -\dfrac{0.685 Z_P}{v} i, & \text{as } v \to \infty \end{cases} \tag{35}$$

and

$$E^{B1}_{2p_0,2s} \to \begin{cases} -\dfrac{3Z_P}{4v} i, & \text{as } v \to 0 \\ O\left(\dfrac{1}{v^2}\right) i, & \text{as } v \to \infty. \end{cases} \tag{36}$$

The matrix equation (33) can be then written as

$$\begin{pmatrix} T^{B2}_{1s,2s} \\ T^{B2}_{1s,2p_0} \end{pmatrix} = \begin{pmatrix} 1 & O\left(\dfrac{1}{v^2}\right) i \\ -\dfrac{0.685 Z_P}{v} i & 1 \end{pmatrix} \begin{pmatrix} T^{B1}_{1s,2s} \\ T^{B1}_{1s,2p_0} \end{pmatrix}, \tag{37}$$

for large velocities and $\theta \to 0$. In contrast to capture, (37) shows that for direct processes the mixing cannot be represented by an infinitesimal rotation at high velocities.

It is interesting that the results exhibit *approximately* a Stark-rotational structure for $v < 1$, where $E^{B1}_{2p_0,2s}$

$\simeq E^{B1}_{2s,2p_0} \simeq -3Z_P i/(4v)$. Anyway, these values should not be taken seriously because the second Born approximation is not valid in the low velocity range.

We shall prove next that though $E^{B1}_{2p_0,2s} \simeq O(1/v^2)$ falls off faster than $E^{B1}_{2s,2p_0} \simeq O(1/v)$, the two-step contribution $1s-2p_0-2s$ is more important, in relative terms, than $1s-2s-2p_0$. Following Moiseiwitsch [17], we introduce the parameter $\alpha_a = T^{B1}_{1s,b} E^{B1}_{b,a} / T^{B1}_{1s,a}$ in the matrix expression (37), so that the differential cross section in the forward direction ($\theta = 0$) is represented by

$$|T^{B2}_{1s,a}|^2 = |T^{B1}_{1s,a}|^2 |1+\alpha_a|^2. \tag{38}$$

Fitting $E^{B1}_{2p_0,2s} \simeq -Z_T Z_P i/v^2$ and $E^{B1}_{2s,2p_0} \simeq -3Z_P i/(4v)$ for $v > 3$, we find that the parameters α_a have the following representation:

$$\alpha_{2s} = \frac{4v}{Z_T} i E^{B1}_{2p_0,2s} \simeq \frac{4Z_P}{v}, \tag{39a}$$

$$\alpha_{2p_0} = -\frac{Z_T}{4v} i E^{B1}_{2s,2p_0} \simeq -\frac{3Z_T Z_P}{16v^2}, \tag{39b}$$

thus

$$|T^{B2}_{1s,2s}|^2 \simeq |T^{B1}_{1s,2s}|^2 \left(1+\frac{4Z_P}{v}\right), \tag{40a}$$

$$|T^{B2}_{1s,2p_0}|^2 \simeq |T^{B1}_{1s,2p_0}|^2 \left(1-\frac{3Z_T Z_P}{16v^2}\right). \tag{40b}$$

An important conclusion is drawn: in the high-energy regime, the forbidden $1s$-$2s$ transition is also populated (note $\alpha_{2s} > 0$) via two permitted transitions $1s$-$2p_0$ (permitted) and a subsequent $2p_0$-$2s$ (permitted). In relative terms, this contribution is more relevant than the two-step $1s-2s$ transition (forbidden) and a subsequent $2s-2p_0$ (permitted) to depopulate (note $\alpha_{2p_0} < 0$) the total $1s-2p_0$ transition. This is why, for example, in the intermediate-energy regime forbidden transitions observe inherent scaling rules of the permitted transitions (such as the Janev and Presniakov scaling [18,19]).

IV. CONCLUSIONS

In summary, based on the perturbative formalism, we have answered the three questions posed in the Introduction:

(1) First, we have found the Stark rotation angle ϕ^{BK1} in the high velocity limit, and we have made a link with the one obtained by Burgdörfer for moderately high velocities [1].

(2) Second, we have found the proper value of ϕ^{CDW} and we conclude that, in the asymptotic limit, the Stark rotation is redundant when CDW amplitudes are used. For proton on helium at $v = 2.75$ a.u. (that is in the experimental range of interest) we have found a numerical coincidence between ϕ^{CDW} and the usual angle obtained from the post-collision interaction model [1] that may elucidate the performance of the CDW with PCI in that range.

(3) Third, for direct excitation the perturbative formalism does not lead to a rotational structure.

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