Effects of scattering on wave-packet structure

E. A. Olszewski
Department of Chemical and Physical Sciences, University of North Carolina at Wilmington, Wilmington, North Carolina 28403-3297
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We consider a general reaction process in which two entrance-channel particles, the beam and target particles, interact off-resonance and produce two exit-channel particles. In the c.m. frame we derive a general expression relating the probability density of the exit-channel particles to that of the entrance-channel particles. Furthermore, we show that whenever the coherence length, w_B, of the beam particle is much larger than the coherence length, w_T, of the target particle, the wave function of each exit-channel particle may be expressed explicitly in terms of the wave function of the beam particle. We also derive expressions for the coherence time and coherence length of each exit-channel particle. In addition, whenever the speed of the target particle is much less than the speed v_i $(i=1,2)$ of an exit-channel particle, we show that a simple relationship exists between the coherence length, w_{ci}, of the exit-channel particle and the beam particle: $w_{ci}=v_i(w_B/|\mathbf{v}_B-\mathbf{v}_T|)\{1-[(\mathbf{v}_T\cdot\hat{\mathbf{e}}_3)/v_i](\cos\theta')\}$, where the velocity of the beam particle is $\mathbf{v}_B$ $(\mathbf{v}_B=v_B\hat{\mathbf{e}}_3)$, and the velocity of the target particle is $\mathbf{v}_T$ $(\mathbf{v}_T=v_T\hat{\mathbf{e}}_3)$. The angle θ' is the spherical polar angular coordinate, measured with respect to the unit vector $\hat{\mathbf{e}}_3$, of the point at which the coherence length w_{ci} is to be determined. The above relationship is applied in the case of photoionization of the hydrogen atom at low energies to obtain realistic estimates for the coherence lengths of the ionized electron and proton. The coherence length of the electron is shown to be of nearly macroscopic dimensions.

I. INTRODUCTION

In studying intensity correlations of radio waves, Hanbury-Brown and Twiss showed that intensity correlations could be observed between incoherent sources of photons.[1] Subsequently, the theory, underlying not only photon beams but also particle beams, in general, was formulated using quantum-mechanical principles.[2–4]

Goldberger, Lewis, and Watson (GLW) derived an expansion for the correlated counting rate of two detectors at arbitrary locations and for arbitrary time delay. The basis for their derivation was the wave-packet formalism which they developed. Specifically, they constructed the wave function of a beam of particles using an appropriately symmetrized product of wave packets, each one being associated with a different beam particle. After making some assumptions about the statistical independence of the beam particles, they derived the correlated counting rate of two detectors.

Bénard, applying the wave-packet formalism of GLW, extended their work and derived an expression relating to the correlated counting rate of an arbitrary number of detectors.[4] Specifically, she derived the pth-order coincident probability density (CPD), which is defined as the probability of detecting p particles at p arbitrary locations and at p arbitrary times. As an application of the formalism that she developed she showed how the effects of bunching and antibunching attributed to bosons and fermions, respectively, were resulting from the detection of indistinguishable particles.

The correlated two-detector counting rate derived by GLW and the CPD derived by Bénard are dependent upon the size and shape of the wave-packet associated with the individual beam particles. This being the case, we have attempted to answer, within certain limitations, the following questions: how big is a wave packet, and what is its shape? Apart from the effect of wave-packet spreading, the size and shape of a wave packet are determined during some reaction process such as elastic scattering, an absorption-emission process, or a decay process, etc. Consequently, we have investigated how the structure of a wave packet is determined during a reaction process. However, we have restricted our investigation to reaction processes in which two particles interact to produce only two other particles (though not necessarily the same as the two initially interacting particles).

The paper is organized as follows. In Sec. II we consider a reaction process in which two particles in the entrance channel interact and produce two particles in the exit channel. For the situation of off-resonance scattering we derive the exit-channel wave function in terms of the wave packet describing the particles in the entrance channel. In Sec. III we consider the situation when the wave-packet size of the target particle is much smaller than that of the beam particle and derive the probability density of each exit-channel particle in terms of the wave packet describing the beam particle. In addition, we obtain explicit relationships for the coherence time and the coherence length of each exit-channel particle. In Sec. IV we apply the formalism derived in Sec. III to photoionization of the hydrogen atom at low energies and obtain realistic estimates of the coherence lengths of the ionized electron and proton.

Concerning units, in Secs. II and III we set c, the speed of light, and $\hbar$ equal to 1. This serves to reduce the complexity in appearance of many of the equations presented.

However, in Sec. IV where we perform certain numerical calculations, we use a system of units in which c and $\hbar$ are exhibited explicitly in any equations.

II. REACTION PROCESSES

In our analysis of reaction processes we have applied the wave-packet formalism as set forth by Goldberger and Watson, and consequently have adhered very closely to their notation.[5] Furthermore, to simplify our discussion we have ignored wave-function symmetrization for systems of identical particles.

Consider an arbitrary reaction process in which two particles, denoted as the beam and target particles, interact in the entrance channel. Assume that after the interaction there appear in the exit channel only two particles, which may or may not be the same as those in the entrance channel. The beam and target particles, which are initially noninteracting, are prepared at time $t_0 = -|t_0|$. The reaction process is described in the c.m. frame by a coordinate system chosen so that at time $t=0$ the midpoints of the wave packets describing the two particles coincide with the origin of the coordinate system. Furthermore, since the reaction process is described in the c.m. frame, the group velocities of the beam and target particles, $\mathbf{v}_B$ and $\mathbf{v}_T$ respectively, are parallel. Thus, without any loss of generality we can assume a coordinate system in which their group velocities are parallel to the z axis of the coordinate system. Specifically,

$$\mathbf{v}_B = v_B \hat{\mathbf{e}}_3 \tag{2.1a}$$

and

$$\mathbf{v}_T = v_T \hat{\mathbf{e}}_3 , \tag{2.1b}$$

where $\hat{\mathbf{e}}_3$ is a unit vector along the z axis of the coordinate system. We also assume that the range of the potential governing the interaction between the two particles is small enough in comparison to the size of their respective wave packets so that the time during which they interact, T, is approximately given by the relationship

$$T = \frac{w_B + w_T}{v_e} , \tag{2.2}$$

where w_B (w_T) is the coherence length of the beam (target) particle, i.e., their wave-packet size in their direction of propagation, and where v_e,

$$v_e = |\mathbf{v}_B - \mathbf{v}_T| , \tag{2.3}$$

is the relative speed of the two entrance-channel particles.

We now derive the time-dependent wave function of the system after the interaction has occurred. First, we construct the wave packet of the particles in the entrance channel. We then derive the wave packet for the system of particles in the exit channel. Finally, we extract from the exit-channel wave function that part resulting from the reaction process, i.e., the scattered wave packet.

In the entrance channel for times during which the particles are noninteracting, the time-dependent two-particle wave packet may be expressed as[6]

$$\phi(t) = \exp[-iK_e(t-t_0)]X_{\bar{a}} , \tag{2.4}$$

where

$$X_{\bar{a}} = \int_{-\infty}^{\infty} d\mathbf{q}_B d\mathbf{q}_T A_B(\mathbf{q}_B - \mathbf{p}_B) A_T(\mathbf{q}_T - \mathbf{p}_T) \chi_{\bar{a}} . \tag{2.5}$$

The momentum distributions of the beam and target particles are A_B and A_T. The quantities $\mathbf{p}_B$ and $\mathbf{p}_T$ are the average momenta of the beam and target particles. The operator K_e is the noninteraction part of the Hamiltonian, H, for the two-particle system so that

$$K_e = H - V_e , \tag{2.6}$$

V_e being the interaction part of the Hamiltonian in the entrance channel. The function $\chi_{\bar{a}}$, representing a state of energy $\epsilon_{\bar{a}}$, is an eigenfunction of the operator K_e, i.e.,

$$K_e \chi_{\bar{a}} = \epsilon_{\bar{a}} \chi_{\bar{a}} . \tag{2.7}$$

Explicitly,

$$\chi_{\bar{a}} = \frac{\exp(i\mathbf{q}_B \cdot \mathbf{r}_B)}{(2\pi)^{3/2}} g_{B\bar{a}} \frac{\exp(i\mathbf{q}_T \cdot \mathbf{r}_T)}{(2\pi)^{3/2}} g_{T\bar{a}} , \tag{2.8}$$

where $\mathbf{r}_B$, $[\mathbf{r}_B = (x_B, y_B, z_B)]$ and $\mathbf{r}_T$ $[\mathbf{r}_T = (x_T, y_T, z_T)]$ are the positions of the beam and target particles, and $\mathbf{q}_B$ and $\mathbf{q}_T$ are their momenta. The functions $g_{B\bar{a}}$ and $g_{T\bar{a}}$ are the most probable internal wave functions of the beam and target particles. Equation (2.5) may be reexpressed in a form which explicitly exhibits its coordinate dependence as

$$X_{\bar{a}} = \frac{\exp(i\mathbf{p}_B \cdot \mathbf{r}_B)}{(2\pi)^{3/2}} \frac{\exp(i\mathbf{p}_T \cdot \mathbf{r}_T)}{(2\pi)^{3/2}} \times G_B(x_B, y_B, z_B/w_B) G_T(x_T, y_T, z_T/w_T) . \tag{2.9}$$

The functions G_I ($I = B, T$) are defined as

$$G_I(x_I, y_I, z_I/w_I) = \frac{1}{(2\pi)^{3/2}} \int d\mathbf{q}_I A_I(\mathbf{q}_I - \mathbf{p}_I) \exp(i\mathbf{q}_I \cdot \mathbf{r}_I) \tag{2.10a}$$

and normalized so that

$$\int d\mathbf{r}_I \, |G_I(x_I, y_I, z_I/w_I)|^2 = (2\pi)^{3/2} . \tag{2.10b}$$

The total energy of the entrance-channel particles is

$$\epsilon_{\bar{a}} = \epsilon_B + \epsilon_T , \tag{2.11}$$

where the energies of the beam and target particles are

$$\epsilon_B = (\mathbf{q}_B \cdot \mathbf{q}_B + m_B^2)^{1/2} \tag{2.12}$$

and

$$\epsilon_T = (\mathbf{q}_T \cdot \mathbf{q}_T + m_T^2)^{1/2} . \tag{2.13}$$

The quantities m_B and m_T are those masses of the beam and target particles associated with their internal wave functions $g_{B\bar{a}}$ and $g_{T\bar{a}}$. If we neglect the spreading of the wave packets in the entrance channel, we can perform the integration in Eq. (2.4) to obtain[7]

$$\phi(t)=G_B\left[x_B,y_B,\frac{z_B-v_Bt}{w_B}\right]G_T\left[x_T,y_T,\frac{z_T-v_Tt}{w_T}\right]$$
$$\times\exp[-i(\langle\epsilon_{\bar a}\rangle_{av}t-\mathbf{p}_B\cdot\mathbf{r}_B-\mathbf{p}_T\cdot\mathbf{r}_T)]$$
$$\times\frac{g_{B\bar a}}{(2\pi)^{3/2}}\frac{g_{T\bar a}}{(2\pi)^{3/2}}\ . \tag{2.14}$$

The total average energy of the beam and target particles is

$$\langle\epsilon_{\bar a}\rangle_{av}=\langle\epsilon_B\rangle_{av}+\langle\epsilon_T\rangle_{av}\ . \tag{2.15}$$

Here the average energy, $\langle\epsilon_B\rangle_{av}$, of the beam particle is

$$\langle\epsilon_B\rangle_{av}=(\mathbf{p}_B\cdot\mathbf{p}_B+m_B^2)^{1/2}\ , \tag{2.16}$$

and the average energy, $\langle\epsilon_T\rangle_{av}$, of the target particle is

$$\langle\epsilon_T\rangle_{av}=(\mathbf{p}_T\cdot\mathbf{p}_T+m_T^2)^{1/2}\ . \tag{2.17}$$

After the interaction has occurred, i.e., for times $t>|T|$, the wave function for the system, describing both incident particles and reaction products, is[8]

$$\psi(t)=\exp[-iH(t-t_0)]\exp(-iK_et_0)X_{\bar a}\ . \tag{2.18}$$

Equation (2.18) can be expressed in a form which more clearly exposes its physical content. In order to do so we require some additional definitions. In the exit channel the noninteraction part of the Hamiltonian for the two-particle system is

$$K_x=H-V_x\ , \tag{2.19}$$

V_x being the interaction part. The eigenfunctions of K_x are denoted X_d and satisfy the equation

$$K_xX_d=\epsilon_dX_d\ . \tag{2.20}$$

Explicitly,

$$X_d=\frac{\exp(i\mathbf{q}_1\cdot\mathbf{r}_1)}{(2\pi)^{3/2}}g_{d1}\frac{\exp(i\mathbf{q}_2\cdot\mathbf{r}_2)}{(2\pi)^{3/2}}g_{d2}\ , \tag{2.21}$$

where $\mathbf{r}_1$ $[\mathbf{r}_1=(x_1,y_1,z_1)]$ and $\mathbf{r}_2$ $[\mathbf{r}_2=(x_2,y_2,z_2)]$ are the positions of the particles; $\mathbf{q}_1$ and $\mathbf{q}_2$ are their momenta. The functions g_{d1} and g_{d2} are the internal wave functions of the exit-channel particles. The total energy of the exit-channel particles is

$$\epsilon_d=\epsilon_1+\epsilon_2\ , \tag{2.22}$$

where the energy of each exit-channel particle is

$$\epsilon_1=(\mathbf{q}_1\cdot\mathbf{q}_1+m_1^2)^{1/2} \tag{2.23}$$

and

$$\epsilon_2=(\mathbf{q}_2\cdot\mathbf{q}_2+m_2^2)^{1/2}\ , \tag{2.24}$$

m_1 and m_2 being their masses. To simplify the discussion we are assuming the values of the masses are independent of the internal wave functions. Using results from standard scattering theory we can reexpress Eq. (2.18) for times $t\gg|T|$, as[9]

$$\psi(t)=\int d\mathbf{q}_Bd\mathbf{q}_TA_B(\mathbf{q}_B-\mathbf{p}_B)A_T(\mathbf{q}_T-\mathbf{p}_T)$$
$$\times\exp(-i\epsilon_{\bar a}t)\psi_{\bar a}^+\ , \tag{2.25}$$

where

$$\psi_{\bar a}^+=X_{\bar a}+\int d\mathbf{q}_1d\mathbf{q}_2\sum_d X_d\frac{1}{\epsilon_{\bar a}+i\eta-\epsilon_d}\langle X_d|\mathcal{T}|X_{\bar a}\rangle\ , \tag{2.26}$$

η being a small positive constant associated with those solutions which propagate forward in time. The scattering matrix $\mathcal{T}$ is given by

$$\langle X_d|\mathcal{T}|X_{\bar a}\rangle=\left\langle X_d\left|\left[V_e+V_x\frac{1}{\epsilon_{\bar a}+i\eta-H}V_e\right]\right|X_{\bar a}\right\rangle\ . \tag{2.27}$$

Because of momentum conservation we can define the reduced matrix $T_{d\bar a}$,

$$\delta(Q-Q_{\bar a})T_{d\bar a}(\mathbf{q}_B,\mathbf{q}_T),\mathbf{q}_1,\mathbf{q}_2)=\langle X_d|\mathcal{T}|X_{\bar a}\rangle\ , \tag{2.28}$$

where the total momentum of the incident particles is

$$\mathbf{Q}_{\bar a}=\mathbf{q}_B+\mathbf{q}_T \tag{2.29a}$$

and the total momentum of the reaction products is

$$\mathbf{Q}=\mathbf{q}_1+\mathbf{q}_2\ . \tag{2.29b}$$

Substituting Eqs. (2.26) and (2.28) into Eq. (2.25) we obtain

$$\psi(t)=\int d\mathbf{q}_Bd\mathbf{q}_TA_B(\mathbf{q}_B-\mathbf{p}_B)A_T(\mathbf{q}_T-p_T)$$
$$\times\left[\exp(-i\epsilon_{\bar a}t)X_{\bar a}+\int d\mathbf{q}_1d\mathbf{q}_2\sum_d\exp(-i\epsilon_dt)X_d\frac{\exp[i(\epsilon_d-\epsilon_{\bar a})t]}{\epsilon_{\bar a}+i\eta-\epsilon_d}\delta(\mathbf{Q}-\mathbf{Q}_{\bar a})T_{d\bar a}\right]\ . \tag{2.30}$$

Using Eq. (2.14) and the fact that

$$\lim_{t\to\infty}\frac{\exp[i(\epsilon_d-\epsilon_{\bar a})t]}{\epsilon_{\bar a}+i\eta-\epsilon_d}=-2\pi i\delta(\epsilon_d-\epsilon_{\bar a})\ , \tag{2.31}$$

we can reexpress Eq. (2.30) as

$$\psi(t)=\phi(t)+\phi'(t)\ , \tag{2.32}$$

where

$$\phi'(t)=-2\pi i\int d\mathbf{q}_B d\mathbf{q}_T A_B(\mathbf{q}_B-\mathbf{p}_B)A_T(\mathbf{q}_T-\mathbf{p}_T)$$
$$\times\int d\mathbf{q}_1 d\mathbf{q}_2\sum_d \exp(-i\epsilon_d t)\chi_d\delta(\epsilon_d-\epsilon_{\bar a})\delta(\mathbf{Q}-\mathbf{Q}_{\bar a})T_{d\bar a}(\mathbf{q}_B,\mathbf{q}_T,\mathbf{q}_1,\mathbf{q}_2)\ . \tag{2.33}$$

To evaluate the integrals in Eq. (2.33) we transform the coordinates of the reaction products to c.m. coordinates, $\mathbf{R}$ $[\mathbf{R}=(X,Y,Z)]$, where

$$\mathbf{R}=\frac{\langle\epsilon_1\rangle_{\rm av}\mathbf{r}_1+\langle\epsilon_2\rangle_{\rm av}\mathbf{r}_2}{\langle\epsilon_d\rangle_{\rm av}}\ , \tag{2.34}$$

and reduced-mass (r.m.) coordinates, $\mathbf{r}$ $[\mathbf{r}=(x,y,z)]$, where

$$\mathbf{r}=\mathbf{r}_1-\mathbf{r}_2\ . \tag{2.35}$$

By energy conservation the total average energy, $\langle\epsilon_d\rangle_{\rm av}$, of the exit-channel particles satisfies the relationship

$$\langle\epsilon_d\rangle_{\rm av}=\langle\epsilon_{\bar a}\rangle_{\rm av}\ . \tag{2.36}$$

The average energy of each exit-channel particle is

$$\langle\epsilon_1\rangle_{\rm av}=\frac{\langle\epsilon_d\rangle_{\rm av}^2+m_1^2-m_2^2}{2\langle\epsilon_d\rangle_{\rm av}} \tag{2.37}$$

and

$$\langle\epsilon_2\rangle_{\rm av}=\frac{\langle\epsilon_d\rangle_{\rm av}^2+m_2^2-m_1^2}{2\langle\epsilon_d\rangle_{\rm av}}\ . \tag{2.38}$$

Using Eqs. (2.34) and (2.35), we can reexpress Eq. (2.33) as

$$\phi'(t)=-2\pi i\int d\mathbf{q}_B d\mathbf{q}_T A_B(\mathbf{q}_B-\mathbf{p}_B)A_T(\mathbf{q}_T-\mathbf{p}_T)$$
$$\times\int d\mathbf{Q}\,d\mathbf{q}\exp[-i(\epsilon_d t-\mathbf{Q}\cdot\mathbf{R}-\mathbf{q}\cdot\mathbf{r})]$$
$$\times\delta(\mathbf{Q}-\mathbf{Q}_{\bar a})\delta(\epsilon_d-\epsilon_{\bar a})$$
$$\times\sum_d\frac{g_{d1}}{(2\pi)^{3/2}}\frac{g_{d2}}{(2\pi)^{3/2}}T'_{d\bar a}(\mathbf{Q},\mathbf{q})\ , \tag{2.39}$$

where

$$\mathbf{q}=\frac{\langle\epsilon_2\rangle_{\rm av}\mathbf{q}_1-\langle\epsilon_1\rangle_{\rm av}\mathbf{q}_2}{\langle\epsilon_d\rangle_{\rm av}} \tag{2.40}$$

and

$$T'_{d\bar a}(\mathbf{Q},\mathbf{q})=T'_{d\bar a}(\mathbf{q}_B,\mathbf{q}_T,\mathbf{Q},\mathbf{q})$$
$$=T_{d\bar a}(\mathbf{q}_B,\mathbf{q}_T,\mathbf{q}_1,\mathbf{q}_2)\ . \tag{2.41}$$

The energy ϵ_d can be expressed as a function of the integration variables $\mathbf{Q}$ and $\mathbf{q}$ as follows:

$$\epsilon_d=\sum_{i=1}^{2}\left[\left|\frac{\langle\epsilon_i\rangle_{\rm av}}{\langle\epsilon_d\rangle_{\rm av}}\mathbf{Q}+\mathbf{q}\right|^2+m_i^2\right]^{1/2}\ . \tag{2.42}$$

Using Eqs. (2.29) we integrate over the variable $\mathbf{Q}$ in Eq. (2.39) to obtain

$$\phi'(t)=-2\pi i\int\frac{d\mathbf{q}_B}{(2\pi)^{3/2}}\frac{d\mathbf{q}_T}{(2\pi)^{3/2}}A_B(\mathbf{q}_B-\mathbf{p}_B)A_T(\mathbf{q}_T-\mathbf{p}_T)$$
$$\times\exp[i(\mathbf{q}_B+\mathbf{q}_T)\cdot\mathbf{R}]S(t)\ , \tag{2.43}$$

where

$$S(t)=\int d\mathbf{q}\exp[-i(\epsilon_d t-\mathbf{q}\cdot\mathbf{r})]\delta(\epsilon_d-\epsilon_{\bar a})$$
$$\times\sum_d g_{d1}g_{d2}T'_{d\bar a}(\mathbf{Q}_{\bar a},\mathbf{q})\ . \tag{2.44}$$

To facilitate the integration of Eq. (2.44), we, first, expand ϵ_d and $\epsilon_{\bar a}$ in Taylor series. Retaining terms of first order, we obtain

$$\epsilon_{\bar a}\approx\langle\epsilon_{\bar a}\rangle_{\rm av}+\mathbf{v}_B\cdot(\mathbf{q}_B-\mathbf{p}_B)+\mathbf{v}_T\cdot(\mathbf{q}_T-\mathbf{p}_T) \tag{2.45}$$

and

$$\epsilon_d\approx\langle\epsilon_d\rangle_{\rm av}+v(q-\langle q\rangle_{\rm av})\ , \tag{2.46}$$

where

$$q=|\mathbf{q}|\ . \tag{2.47}$$

The average speed of the of the r.m. system is

$$v=\frac{\langle q\rangle_{\rm av}}{\mu}\ , \tag{2.48}$$

where

$$\langle q\rangle_{\rm av}=\frac{\langle\epsilon_2\rangle_{\rm av}}{2}\left[1-\left[\frac{m_1+m_2}{\langle\epsilon_d\rangle_{\rm av}}\right]^2\right]\left[1-\left[\frac{m_2-m_2}{\langle\epsilon_d\rangle_{\rm av}}\right]^2\right] \tag{2.49}$$

and

$$\frac{1}{\mu}=\frac{1}{\langle\epsilon_1\rangle_{\rm av}}+\frac{1}{\langle\epsilon_2\rangle_{\rm av}}\ . \tag{2.50}$$

Next, we transform the variable of integration q from Cartesian to spherical coordinates. We then make the following substitution:[10]

$$\exp(i\mathbf{q}\cdot\mathbf{r})=4\pi\sum_{l,m}i^l Y_{l,m}(\hat{\mathbf{q}})Y_{l,m}^*(\hat{\mathbf{r}})j_l(qr)\ , \tag{2.51a}$$

where the functions $Y_{l,m}$ are spherical harmonics, and the functions j_l are the spherical Bessel functions which, in the large-argument limit, $qr\gg1$, are

$$j_l(qr)\rightarrow\frac{\exp[i(qr-\pi l/2)]-\exp[-i(qr-\pi l/2)]}{2iqr}\ . \tag{2.51b}$$

The variable

$$r = |\mathbf{r}| \ . \tag{2.51c}$$

We are assuming that each of the momentum distributions A_B and A_T defines a narrow spread in momentum. Consequently, the asymptotic form of the spherical Bessel functions, Eq. (2.51b), can be used in evaluating the integrals in Eq. (2.43) whenever the condition

$$\langle q \rangle_{\rm av} r \gg 1 \tag{2.51d}$$

is satisfied. In addition, since we are considering the asymptotic condition $t \to \infty$ [see Eq. (2.31)], the second exponential in Eq. (2.51b), the incoming spherical wave, does not contribute to the integral in Eq. (2.43) and can therefore be discarded. Substituting Eqs. (2.47), (2.51a), and (2.51b) into Eq. (2.44), we obtain

$$S(t) = \frac{4\pi}{2ir} \int dq\, q^2 \frac{\exp[-i(\epsilon_d t - qr)]}{q} \delta(\epsilon_d - \epsilon_{\bar a}) \times \sum_d g_{d1} g_{d2} \int d\Omega_q \sum_{l,m} Y^*_{l,m}(\hat{\mathbf{r}}) Y_{l,m}(\hat{\mathbf{q}}) \times T'_{d\bar a}(\mathbf{Q}_{\bar a}, \mathbf{q}) \ , \tag{2.52}$$

where $q^2 dq\, d\Omega_q$ is the volume element of integration expressed in spherical coordinates. Here $\hat{\mathbf{r}}$ and $\hat{\mathbf{q}}$ are unit vectors in the directions $\mathbf{r}$ and $\mathbf{q}$, respectively. We can integrate over the spherical angles in Eq. (2.52) to obtain

$$S(t) = \frac{4\pi}{2ir} \int dq\, q \exp[-i(\epsilon_d t - qr)] \delta(\epsilon_d - \epsilon_{\bar a}) \times \sum_d g_{d1} g_{d2} T'_{d\bar a}(\mathbf{Q}_{\bar a}, q\hat{\mathbf{r}}) \ . \tag{2.53}$$

Using Eqs. (2.45) and (2.46) we perform the final integration in Eq. (2.53) and obtain

$$S(t) = \left[\frac{4\pi}{2ir}\right] \left[\frac{1}{v}\right] P \exp(-i\langle \epsilon_d \rangle_{\rm av} t) \times \exp\{-it[\mathbf{v}_B \cdot (\mathbf{q}_B - \mathbf{p}_B) + \mathbf{v}_r \cdot (\mathbf{q}_r - \mathbf{p}_r)] + irP\} \times \sum_d g_{d1} g_{d2} T'_{d\bar a}(\mathbf{Q}_{\bar a}, q\hat{\mathbf{r}}) \ , \tag{2.54a}$$

where

$$P = \langle q \rangle_{\rm av} + \frac{\mathbf{v}_B}{v} \cdot (\mathbf{q}_B - \mathbf{p}_B) + \frac{\mathbf{v}_T}{v} \cdot (\mathbf{q}_r - \mathbf{p}_T) \ . \tag{2.54b}$$

Because the spread in each momentum distribution A_B and A_T is sufficiently narrow, the reduced matrix $T'_{d\bar a}(\mathbf{Q}_{\bar a}, q\hat{\mathbf{r}})$ may be considered constant with respect to the variables q_B and q_T. We therefore can approximate $T'_{d\bar a}(\mathbf{Q}_{\bar a}, q\hat{\mathbf{r}})$ by

$$T'_{d\bar a} = T'_{d\bar a}(\mathbf{p}_B, \mathbf{p}_T, \langle \mathbf{Q}_{\bar a} \rangle_{\rm av}, \langle q \rangle_{\rm av} \hat{\mathbf{r}}) \ , \tag{2.55}$$

where

$$\langle \mathbf{Q}_{\bar a} \rangle_{\rm av} = \mathbf{p}_B + \mathbf{p}_T = 0 \ . \tag{2.56}$$

Using Eqs. (2.48) and (2.55) we integrate Eq. (2.43) to obtain

$$\phi'(t) = \sum_d g_{d1} g_{d2} \frac{\langle f_{d\bar a} \rangle_{\rm av}}{r} \phi'_1(t) \ , \tag{2.57}$$

where

$$\phi'_1(t) = \frac{1}{i\langle q \rangle_{\rm av}} \frac{\partial \phi'_2(t)}{\partial r} \ . \tag{2.58a}$$

Here

$$\phi'_2 = \exp[-i(\langle \epsilon_d \rangle_{\rm av} t - \langle q \rangle_{\rm av} r)] \times G_B \left[X, Y, \frac{Z}{w_B} \frac{r - vt}{w_B v / v_B}\right] \times G_T \left[X, Y, \frac{Z}{w_T} + \frac{r - vt}{w_T v / v_T}\right] \ . \tag{2.58b}$$

The scattering amplitude $\langle f_{d\bar a} \rangle_{\rm av}$ is defined as

$$\langle f_{d\bar a} \rangle_{\rm av} = -4\pi^2 \mu T'_{d\bar a} \ . \tag{2.59}$$

In deriving Eqs. (2.58) we have used the fact that the expression for P defined by Eq. (2.54b) can be obtained by differentiating the exponential terms in Eq. (2.54a) with respect to r and multiplying by $-i$.

For the rest of our discussion we assume further that the momentum distributions of the beam and target particles are so narrow that

$$\langle q \rangle_{\rm av} \gg \frac{\mathbf{v}_B}{v} \cdot \boldsymbol{\delta}_B + \frac{\mathbf{v}_T}{v} \cdot \boldsymbol{\delta}_T \ , \tag{2.60}$$

where $\boldsymbol{\delta}_B$ ($\boldsymbol{\delta}_T$) is the standard deviation in the momentum vector of the beam (target) particle calculated from the momentum distribution A_B (A_T). Under this assumption the second and third terms in Eq. (2.54b) can be neglected so that Eq. (2.43) can be integrated to yield

$$\phi'(t) = \sum_d g_{d1} g_{d2} \frac{\langle f_{d\bar a} \rangle_{\rm av}}{r} \phi'_2(t) \ . \tag{2.61}$$

We now provide a qualitative discussion justifying the expression for the exit-channel wave function $\phi'(t)$. First, we reexpress the entrance-channel wave packet in terms of c.m. and r.m. coordinates and obtain the transformed wave function $\phi_{\rm cr}(t)$, where

$$\phi_{\rm cr}(t) = G_B \left[X_e + \frac{\langle \epsilon_T \rangle_{\rm av}}{\langle \epsilon_{\bar a} \rangle_{\rm av}} x_e, Y_e + \frac{\langle \epsilon_T \rangle_{\rm av}}{\langle \epsilon_{\bar a} \rangle_{\rm av}} y_e, \frac{Z_e}{w_B} + \frac{z_e - v_e t}{w_B v_e / v_B}\right] \times G_T \left[X_e - \frac{\langle \epsilon_B \rangle_{\rm av}}{\langle \epsilon_{\bar a} \rangle_{\rm av}} x_e, Y_e - \frac{\langle \epsilon_B \rangle_{\rm av}}{\langle \epsilon_{\bar a} \rangle_{\rm av}} y_e, \frac{Z_e}{w_T} + \frac{z_e - v_e t}{w_T v_e / v_T}\right] \exp[-i(\langle \epsilon_{\bar a} \rangle_{\rm av} t - \langle p_e \rangle_{\rm av} z_e)] \ . \tag{2.62}$$

The c.m. coordinates $\mathbf{R}_e$, $[\mathbf{R}_e=(X_e,Y_e,Z_e)]$ of the beam and target particles are defined as

$$\mathbf{R}_e=\frac{\langle \epsilon_B\rangle_{av}\mathbf{r}_B+\langle \epsilon_T\rangle_{av}\mathbf{r}_T}{\langle \epsilon_{\bar{a}}\rangle_{av}}\ , \tag{2.63}$$

and their r.m. coordinates $\mathbf{r}_e$ $[\mathbf{r}_e=(x_e,y_e,z_e)]$ are defined as

$$\mathbf{r}_e=\mathbf{r}_B-\mathbf{r}_T\ . \tag{2.64}$$

Here

$$\langle p_e\rangle_{av}=|\mathbf{p}_e|\ , \tag{2.65a}$$

where the average momentum of the r.m. system is

$$\mathbf{p}_e=\frac{\langle \epsilon_B\rangle_{av}\langle \epsilon_T\rangle_{av}}{\langle \epsilon_{\bar{a}}\rangle_{av}}\mathbf{v}_e\ . \tag{2.65b}$$

The reaction process can be described, classically, as one in which a particle with mass equal to the reduced mass of the entrance-channel system propagates along the z axis, interacts with a potential, becomes a particle of mass equal to the reduced mass of the exit-channel system, and scatters radially from the interaction region. The quantum-mechanical analogue of this description is that a wave packet corresponding to the r.m. system of the entrance channel propagates along the z axis, interacts with a potential, and scatters in the exit channel as a spherical wave. The implication is that the exit-channel wave function should maintain essentially the same form as the entrance-channel wave packet, with the principle difference being that the variables in the exit-channel wave function should be expressed in spherical coordinates rather than in Cartesian coordinates. Therefore to obtain the exit-channel wave function we must modify Eq. (2.62) in the following way: Each expression z_e-v_et (which shows that the r.m. system, in the entrance channel, propagates "on the average," along the z axis) should be replaced by $r-vt$, where r is the radial spherical coordinate [Eq. (2.51c)], and v is the average speed of the r.m. system in the exit channel [Eq. (2.48)]. For all other occurrences of the quantity v_e, the quantity v should be substituted. In addition the exit-channel wave function should contain a factor $1/r$ which is characteristic of spherical waves and also another term, the scattering amplitude, which is required for tempering the amount of spherical wave propagating in various directions. In Eq. (2.62) all occurrences of either x_e or y_e should be replaced by zero, since in the exit channel the terms which would correspond to these are replaced by the spherical polar and azimuthal angles which appear as variables in the scattering amplitude. Other modifications to Eq. (2.62) include replacing the quantity $\langle p_e\rangle_{av}$ by the magnitude of the average momentum of the r.m. system in the exit channel, $\langle q\rangle_{av}$, and replacing the quantity $\langle \epsilon_{\bar{a}}\rangle_{av}$ by the total average energy in the exit channel $\langle \epsilon_d\rangle_{av}$. Applying all these modifications to Eq. (2.62), we obtain Eq. (2.61).

In deriving the exit-channel wave function, Eq. (2.61), from the entrance-channel wave packet we have made certain assumptions which we now summarize.

(1) The range of the interaction is small enough so that the time during which the beam and target particles interact may be approximated by Eq. (2.2).

(2) The energies $\epsilon_{\bar{a}}$, Eq. (2.11), and ϵ_d, Eq. (2.22), may be evaluated using Taylor-series expansions, as was done in Eqs. (2.45) and (2.46).

(3) The scattering matrix may be evaluated using average values of its arguments, as was done in Eq. (2.59).

(4) The wave packet describing the two exit-channel particles applies only in regions where the interaction between the exit-channel particles may be neglected and when $r \gg 1/\langle q\rangle_{av}$ [see Eq. (2.51)].

The derivation of the exit-channel wave function depends strongly on whether assumptions (2) and (3) are satisfied. Assumption (2) is satisfied if the time during which $\phi'(t)$ is to be valid is of short enough duration that wave-packet spreading in the entrance and exit channels may be neglected (this condition should be satisfied in most experiments). Assumption (3) is valid if the energy uncertainty of each particle in the entrance channel is much less than its average energy. However, if the scattering matrix should exhibit a sharp energy resonance in the region of absorption, so sharp that its energy spread is less than that of either entrance-channel particle, assumption (3) would then be invalid.

In the remainder of this paper we are assuming that the scattered wave packet can be considered separately from the transmitted part of the incident wave packet. Thus, we are not considering situations which allow for the interesting possibility of interference between the scattered and unscattered waves. This has been implicit in our previous discussion in that we have denoted the position coordinates of the transmitted part of the incident wave packet by a set of labels different from those of the scattered wave packet, i.e., $\mathbf{r}_B$ and $\mathbf{r}_T$ are the position coordinates in the incident wave packet, and $\mathbf{r}_1$ and $\mathbf{r}_2$ are the position coordinates in the scattered wave packet. Stated equivalently, we have been assuming that experimental conditions have been chosen so that the states to be observed, χ_d, are orthogonal to the incident wave packet, thereby eliminating the possibility of interference. Nonetheless, such interference should occur when one of the incident particles and one of the reaction products are the same kind of particle. In such a situation it would be possible, under the right experimental conditions, to observe effects resulting from interference between the scattered and the unscattered wave packets. Recently, anomalous effects in electron-potassium differential scattering measurements have been attributed to this phenomenon.[11]

III. THE WAVE PACKET ASSOCIATED WITH EACH EXIT-CHANNEL PARTICLE

From Eq. (2.42) we obtain the probability, $P'(t)$, for the two-particle system in the exit channel,

$$P'(t)=|\phi'(t)|^2=\frac{v_e}{v}\left|G_B\left[X,Y,\frac{Z}{w_B}+\frac{r-vt}{w_Bv/v_B}\right]\right|^2 \times\left|G_T\left[X,Y,\frac{Z}{w_T}+\frac{r-vt}{w_rT/v_T}\right]\right|^2\frac{\sigma(\hat{\mathbf{r}})}{r^2} \tag{3.1}$$

where $\sigma(\hat{\mathbf{r}})$, the differential cross section, is

$$\sigma(\hat{\mathbf{r}})=\frac{v}{v_e}\sum_d \langle f_{d\bar{a}}\rangle_{\rm av}^*\langle f_{d\bar{a}}\rangle_{\rm av} . \tag{3.2}$$

This result has been obtained by summing (or integrating, as appropriate) over the degrees of the freedom of the internal wave functions and making use of their orthonormality.

We now assume that the size of the wave packet associated with the beam particle is very much larger than that associated with the target particle. Specifically

$$w_B \gg w_T . \tag{3.3}$$

This assumption allows us to approximate the probability density of the target particle, $|G_T|^2$, by a delta function. We can therefore integrate over the c.m. coordinates of the exit-channel wave function [Eq. (3.1)] to obtain the probability density $P_r'(t)$ of the r.m. system in the exit channel.

$$P_r'(t)=\frac{v_e}{v}\left|G_B\left[0,0,\frac{r-vt}{w_r}\right]\right|^2\frac{\sigma(\hat{\mathbf{r}})}{r^2} , \tag{3.4}$$

where

$$w_r=vT . \tag{3.5}$$

The quantity w_r, the coherence length, represents the size of the r.m. system in the radial direction. The expression for the coherence length, Eq. (3.5), can be understood as follows. The wave packet of the beam particle interacts with that of the target particle for an amount of time T. During this time the wave packet for the r.m. system is being created at $r=0$. As it is being created it propagates radially outward with speed v. Consequently, after time T the wave packet grows to size w_r as given by Eq. (3.5).

Applying the same assumptions used in obtaining Eq. (3.4), we can, in a similar manner, derive an expression for the probability density of each exit-channel particle. The calculation involves, first, transforming from the c.m. and r.m. coordinates, used as arguments in the probability density of the two-particle system [Eq. (3.1)], to the coordinates of the individual particles. Using the fact that the wave packet of the target particle may be approximated by a delta function, we can integrate out the coordinates of one of the particles to obtain the probability density of the other particle. However, because the argument of the delta function is a nontrivial function of the particle's coordinates, we must consider, for each particle i ($i=1,2$), three distinct cases. Each case is distinguished according to whether the $|\boldsymbol{\beta}_i|<1$, $|\boldsymbol{\beta}_i|=1$, or $|\boldsymbol{\beta}_i|>1$, where

$$\boldsymbol{\beta}_i=\beta_i\hat{\mathbf{e}}_3=\frac{v_T}{v_i}\hat{\mathbf{e}}_3 , \tag{3.6}$$

and v_i, the speed of the ith exit-channel particle, is

$$v_i=\frac{\langle\epsilon_d\rangle_{\rm av}-\langle\epsilon_i\rangle_{\rm av}}{\langle\epsilon_d\rangle_{\rm av}}v . \tag{3.7}$$

The probability density $P_i'(t)$ of each exit-channel particle is given as follows.

Case 1: whenever $|\boldsymbol{\beta}_i|<1$,

$$P_i'(t)=\frac{v_e}{v_i}\sigma(\hat{\mathbf{r}}_{i+})\frac{|G_B(0,0,\mu_{i+})|^2}{v_{i+}^2}J_{i+} . \tag{3.8a}$$

Case 2: whenever $|\boldsymbol{\beta}_i|=1$,

$$P_i'(t)=\begin{cases}2\dfrac{v_e}{v_i}\sigma(\hat{\mathbf{r}}_{i0})\dfrac{|G_B(0,0,\mu_{i0})|^2}{r_{i0}^2}J_{i0}, & \beta_iZ_i<0\\ \infty, & Z_i=0\\ 0 & \text{otherwise.}\end{cases} \tag{3.8b}$$

Case 3: whenever $|\boldsymbol{\beta}_i|>1$,

$$P_i'(t)=\begin{cases}\dfrac{v_e}{v_i}\left[\sigma(\hat{\mathbf{r}}_{i+})\dfrac{|G_B(0,0,\mu_{i+})|^2}{r_{i+}^2}J_{i+}+\sigma(\hat{\mathbf{r}}_{i-})\dfrac{|G_B(0,0,\mu_{i-})|^2}{r_{i-}^2}J_{i-}\right], & \beta_iZ_i\le 0 \text{ and } |Z_i|\ge(\beta_i^2-1)\rho_i\\ 0 & \text{otherwise.}\end{cases} \tag{3.8c}$$

In these expressions

$$\mu_{i\pm}=\frac{r_{i\pm}-v_it}{v_iT} \tag{3.9a}$$

and

$$\mu_{i0}=\frac{r_{i0}-v_it}{v_iT} . \tag{3.9b}$$

The functions $J_\pm$ and J_0 are the Jacobians that result in transforming from c.m.-r.m. coordinates to the coordinates of the two exit-channel particles. Specifically,

$$J_{i\pm}=\frac{1}{|1-\boldsymbol{\beta}_i\cdot\hat{\mathbf{r}}_{i\pm}|} \tag{3.10a}$$

and

$$J_{i0}=\frac{1}{|1-\boldsymbol{\beta}_i\cdot\hat{\mathbf{r}}_{i0}|} . \tag{3.10b}$$

The vectors $\mathbf{r}_{i\pm}$ and $\mathbf{r}_{i0}$ connect the spatial coordinates of particle 2 to particle 1. The subscript i refers to whether the vector is expressed as a function of the coordinates of particle 1 or particle 2. The vectors $\hat{\mathbf{r}}_{i\pm}$ and $\hat{\mathbf{r}}_{i0}$ are unit vectors in directions of $\mathbf{r}_{i\pm}$ and $\mathbf{r}_{i0}$, respectively, while $r_{i\pm}=|\mathbf{r}_{i\pm}|$ and $r_{i0}=|\mathbf{r}_{i0}|$. Explicitly,

$$\mathbf{r}_{i\pm}=(-1)^{i+1}E_i(x_i,y_i,Z_i\pm\beta_i\beta_i) . \tag{3.11a}$$

$$\mathbf{r}_{i0}=(-1)^{i+1}E_i(x_i,y_i,\tfrac{1}{2}(Z_i-\rho_i^2/Z_i)) , \tag{3.11b}$$

where

$$B_i = [\rho_i^2(1-\beta_i^2)+Z_i^2]^{1/2} \ , \tag{3.12a}$$

$$E_i = \frac{\langle \epsilon_d \rangle_{\rm av}}{\langle \epsilon_d \rangle - \langle \epsilon_i \rangle_{\rm av}} \ , \tag{3.12b}$$

$$Z_i = z_i - v_T t \ , \tag{3.13}$$

and

$$\rho_i^2 = x_i^2 + y_i^2 \ . \tag{3.14}$$

Equations (3.8) apply only when

$$\langle q \rangle_{\rm av} r_{i\pm} \gg 1 \tag{3.15a}$$

or

$$\langle q \rangle_{\rm av} r_{i0} \gg 1 \ . \tag{3.15b}$$

This criterion is equivalent to that stated in Eq. (2.51c).

Equations (3.8) can be interpreted, physically, in a relatively straightforward manner. As the target particle propagates in the $+z$ direction, it appears to act as a source of two distinct spherical waves, each of which corresponds to the probability density of an exit-channel particle (see Fig. 1). The intensity of a particular spherical wave front, emitted from some location on the z axis, is controlled by that portion of the beam particle's probability density spatially coincident with that of the target particle. Furthermore, the intensity of a wave front propagating in various directions is modulated by the differential cross section. As a wave front propagates away from its source, its intensity is multiplied by a factor $1/r_{i\pm}^2$ or $1/r_{i0}^2$, which is characteristic of point sources. Finally, the Jacobian takes account of the motion of the target particle by effecting a clustering of wave fronts to the front of the target particle and a thinning out of wave fronts to the rear [see Fig. 1(a)].

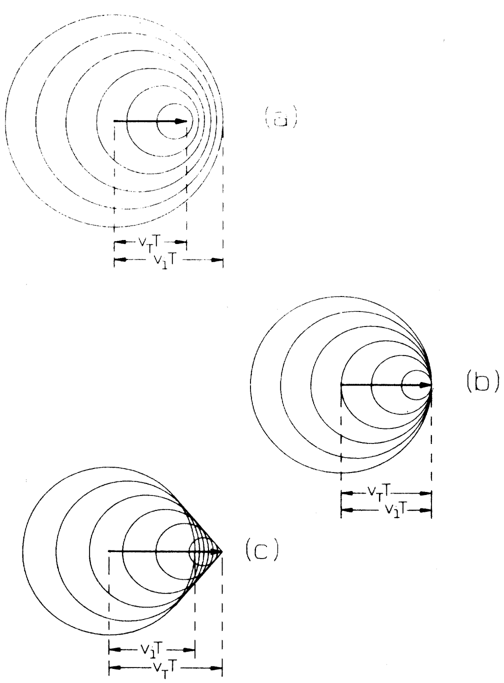

FIG. 1. Wave fronts associated with an exit-channel particle. Solid straight line represents the trajectory of the target particle whose speed is $|v_T|$. The spherical wave fronts associated with the exit-channel particle are traveling with speed v_i. Time T is the approximate time during which the beam and target particles interact. Depicted are the three cases: (a) $|v_T| < v_i$, (b) $|v_T| = v_i$, and (c) $|v_T| > v_i$.

Case 3 is sufficiently different from the other two cases to merit further discussion. In this case $|\beta_i| > 1$, and consequently the target particle is traveling faster than the exit-channel wave packet which it appears to emit. This case is similar to what occurs when a charged particle travels through a medium with a speed greater than the phase velocity of electromagnetic radiation propagating through the medium: the charged particle emits a shock wave referred to as Čerenkov radiation.[12] Similarly, case 3 describes the situation in which the target particle acts as the source of a shock wave, the wave packet associated with the exit-channel particle. The direction of propagation of the shock front relative to that of the target particle is defined by the angle θ_c, where

$$\cos\theta_c = \frac{1}{\beta_i} \ . \tag{3.16}$$

This is the same relationship that applies to Čerenkov radiation. In this case, the expression for the wave packet [Eq. (3.8c)] comprises a sum of two terms. The reason for this can be understood as follows. If one compares Fig. 1(a) to Fig. 1(c), one observes in Fig. 1(c) that at each point two circles intersect. This shows that the probability density at this space-time point derives from spherical wavelets which have been emitted from two different locations, hence the two terms in Eq. (3.8c).

A close inspection of Eq. (3.10a) shows that for case 3 the Jacobian diverges along the shock front, a situation which is characteristic of shock waves. However, this also implies that the probability density of the exit-channel particle diverges there. This can be shown to occur because the wave packet associated with the target particle has been approximated by a delta function. If a more realistic wave packet is assumed for the target particle, i.e., one which is less pathological, it can be shown that the singularity along the shock front will be smeared into a region whose spatial extent is of the same order of size as that of the target particle's wave packet.

We now reexpress the probability density of each exit-channel particle [Eqs. (3.8)] in a form which explicitly exhibits the coordinates of the exit-channel particle.

Case 1: whenever $|\beta_i| < 1$,

$$P_i'(t) = \frac{v_e}{v_i}\frac{1-\beta_i^2}{B_i}\sigma(\hat{\mathbf{r}}_+)\frac{|G_B(0,0,\mu_{i+})|^2}{\beta_i Z_i + B_i} \ . \tag{3.17a}$$

Case 2: whenever $|\beta_i| = 1$,

$$P_i'(t) = \begin{cases} 2\dfrac{v_e}{v_i}\sigma(\hat{\mathbf{r}}_{i0})\dfrac{|G_B(0,0,\mu_{i0})|^2}{Z_i^2+\rho_i^2}, & \beta_i Z_i < 0 \\ \infty, \ Z_i = 0 & \\ 0 \ \text{otherwise.} & \end{cases} \tag{3.17b}$$

Case 3: whenever $|\beta_i| > 1$,

$$P_i'(t)=\begin{cases}\dfrac{v_e}{v_i}\dfrac{1-\beta_i^2}{B_i}\left[\sigma(\hat{\mathbf{r}}_+)\dfrac{|G_B(0,0,\mu_{i+})|^2}{\beta_iZ_i+B_i}+\sigma(\hat{\mathbf{r}}_-)\dfrac{|G_B(0,0,\mu_{i-})|^2}{\beta_iZ_i-B_i}\right], & \beta_iZ_i\le 0 \text{ and } |Z_i|\ge(\beta_i^2-1)^{1/2}\rho_i\\ 0 \text{ otherwise.}\end{cases} \quad (3.17c)$$

Here

$$\mu_{i0}=-\frac{1}{2}\left[\frac{z_i^2-(v_it)^2+\rho_i^2}{v_iTZ_i}\right] \quad (3.18a)$$

and

$$\mu_{i\pm}=\frac{\beta_iz_i\pm B_i-v_it}{v_iT(1-\beta_i^2)}\ . \quad (3.18b)$$

Expressed in terms of the coordinates of the exit-channel particle Eqs. (3.15a) and (3.15b) are

$$\langle q\rangle_{\rm av}E_i\frac{\beta_iZ_i\pm B_i}{1-\beta_i^2}\gg 1 \quad (3.19a)$$

and

$$\langle q\rangle_{\rm av}(-\tfrac{1}{2})E_i\frac{Z_i^2+\rho_i^2}{Z_i}\gg 1\ . \quad (3.19b)$$

We now derive the coherence time for each exit-channel particle. Qualitatively, we mean the coherence time to be the duration of time required for a wave packet to pass a given location. The coherence time may be estimated as the difference in time between the arrival of the first and last wave fronts at the particular location. For cases 1 and 2 this calculation is straightforward since these two wave fronts correspond to those wave fronts emitted when the beam and target particles begin and finish interacting. The approximate location along the z axis where these wave fronts are emitted can be determined as follows. The midpoints of the beam- and target-particle wave packets coincide at time $t=0$, and since the time required for the beam particle to pass over the target particle is approximately T [see Eq. (2.2)], the location of the target particle is given, approximately, as $z=-v_TT/2$ when the interaction begins and $z=v_TT/2$ when the interaction finishes. Thus, calculating coherence time T_{ci}, at location (x,y,z) for the ith particle we obtain the result that in cases 1 and 2

$$T_{ci}=\left|T+\frac{\left[\rho^2+\left[z-v_T\dfrac{T}{2}\right]^2\right]^{1/2}-\left[\rho^2+\left[z+v_T\dfrac{T}{2}\right]^2\right]^{1/2}}{v_i}\right|, \quad (3.20a)$$

where

$$\rho=x^2+y^2\ . \quad (3.20b)$$

For case 3 the situation is complicated by the fact that the target particle is traveling faster than the exit-channel particle so that the first and last wave fronts to arrive at a particular location may not be those emitted when the target particle is located at $z=-v_TT/2$ and $z=v_TT/2$. A careful analysis indicates that case 3 comprises four subcases, as depicted in Fig. 2. When the location at which the coherence time is to be determined is situated in region I or region IV, the first and last wave fronts to arrive at the location are emitted from $z=-v_TT/2$ and $z=v_TT/2$ (not necessarily respectively). When the location is situated in region II, the wave front arriving first is emitted from that point on the z axis defined by the intersection of the z axis with the gamma ray emanating from the location and crossing the shock front perpendicularly. The wave front arriving last is emitted from $z=-v_TT/2$. When the location is situated in region III, the first arriving wave front is emitted from the point on the z axis determined in the same manner as for region II; however, the last arriving wave front is emitted from $z=v_TT/2$. These four regions are defined by the following conditions placed on the z coordinate of the location at which the coherence time is to be determined.

Region I:

$$\operatorname{sgn}(v_T)z\ge\operatorname{sgn}(v_T)\left[\frac{\rho}{\beta_i(1-1/\beta_i^2)^{1/2}}+v_T\frac{T}{2}\right]. \quad (3.21a)$$

Region II:

$$\operatorname{sgn}(v_T)\left[\frac{\rho}{\beta_i(1-1/\beta_i^2)^{1/2}}+\frac{v_T}{2}\right]>\operatorname{sgn}(v_T)z\ge\left[\left[v_i\frac{T}{2}\right]^2+\frac{\rho^2}{\beta_i^2-1}\right]^{1/2}. \quad (3.21b)$$

Region III:

$$\left[\left[v_i\frac{T}{2}\right]^2+\frac{\rho^2}{\beta_i^2-1}\right]^{1/2}>\operatorname{sgn}(v_T)z\ge\operatorname{sgn}(v_T)\left[\frac{\rho}{\beta_i(1-1/\beta_i^2)^{1/2}}-v_T\frac{T}{2}\right]. \quad (3.21c)$$

Region IV:

$$\operatorname{sgn}(v_T)\left[\frac{\rho}{\beta_i(1-1/\beta_i^2)^{1/2}}-v_T\frac{T}{2}\right]>\operatorname{sgn}(v_T)z\ . \quad (3.21d)$$

Calculating the coherence time T_{ci} in each of these regions we obtain the following results.

In regions I and IV

$$T_{ci}=\left|T+\frac{[\rho^2+(z-v_T T/2)^2]^{1/2}-[\rho^2+(z+v_T T/2)^2]^{1/2}}{v_i}\right| . \tag{3.22a}$$

In region II

$$T_{ci}=\frac{[\rho^2+(z+v_T T/2)^2]^{1/2}-\rho(1-1/\beta_i^2)^{1/2}}{v_i}-\frac{z}{v_T}-\frac{T}{2} . \tag{3.22b}$$

In region III

$$T_{ci}=\frac{[\rho^2+(z-v_T T/2)^2]^{1/2}-\rho(1-1/\beta_i^2)^{1/2}}{v_i}-\frac{z}{v_T}+\frac{T}{2} . \tag{3.22c}$$

The coherence length, w_i, of the ith exit-channel particle, at a given location, can be defined as the product of its coherence time and average speed. Consequently,

$$w_i=v_i T_{ci} . \tag{3.23}$$

In order to show how these results can be applied in the calculation of the coherence time and coherence length we consider the following elementary example: the target particle is propagating in the $+z$ direction; the average speed of the exit-channel particle is equal to the average speed of the target particle, i.e., $v_i=|v_T|$ [see Fig. 1(b)]. We now calculate the coherence time and the coherence length at some location (z,ρ), where $\rho=0$ and $z>v_T T/2$. Since this example is one of the case 2 type, we may apply Eq. (3.20) and obtain the result that $T_{ci}=0$. This result may be understood, qualitatively, as follows: As the target particle is traveling with the same speed as the exit-channel particle, the wave fronts which are emitted during the interaction and which are propagating along the $+z$ direction are all superimposed on top of one another. Consequently, all these wave fronts pass a point on the z axis, outside of the interaction region, simultaneously. Therefore, the coherence time is zero, which implies the coherence length is also zero.

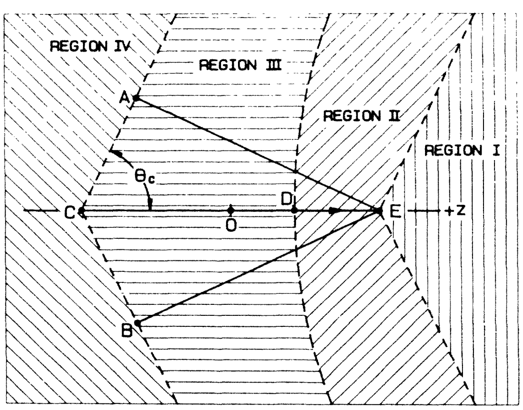

FIG. 2. Decomposition of space into four regions for determining the coherence time in case 3 ($v_T>v_i$). The pair of lines AEB represent the shock front associated with the exit-channel particle. The shock front is moving in the direction defined by the angle θ_c. Point C ($z=-v_T T/2$) represents the approximate location on the z axis where the beam and target particles begin interacting. Point E ($z=v_T T/2$) represents the approximate location where they stop interacting. The two rays represented by the dotted lines emanating from point E separate region I from region II. Dotted curve passing through point D ($z=v_i T/2$) separates region II from region III. This curve is the locus of all points for which wave fronts originating from points C and A arrive simultaneously. The two rays represented by the dotted lines emanating from point C separate region III from region IV. Point O indicates the origin of the z axis.

IV. PHOTOIONIZATION

We apply the results of Sec. III to another elementary example, but one which is more physically based than that considered in the previous section. We consider the photoionization of the hydrogen atom at nonrelativistic energies. The hydrogen atom, the target particle, is at rest in the laboratory frame where it is to be ionized by a photon, the beam particle. The photon source is a uv gas discharge tube, the mean wavelength of whose photons is λ,[13]

$$\lambda=700\ \text{Å} . \tag{4.1}$$

The velocity of the photon is

$$\mathbf{v}_B=v\hat{\mathbf{e}}_3 , \tag{4.2}$$

where c is the speed of light. In the c.m. frame the velocity of the target particle is

$$\mathbf{v}_T=-\frac{\langle\epsilon_B\rangle_{\rm av}}{\langle\epsilon_B\rangle_{\rm av}+\langle\epsilon_r\rangle_{\rm av}}c\hat{\mathbf{e}}_3$$
$$=(-566\ \text{cm/s})\hat{\mathbf{e}}_3 , \tag{4.3}$$

where the rest energy of the hydrogen atom is

$$\langle\epsilon_T\rangle_{\rm av}\approx 938\ \text{MeV} , \tag{4.4}$$

and the energy of the photon is

$$\langle\epsilon_B\rangle_{\rm av}=\frac{hc}{\lambda}=17.7\ \text{eV} . \tag{4.5}$$

The speed of the r.m. system in the entrance channel is

$$v_e=|\mathbf{v}_B-\mathbf{v}_T|\approx c . \tag{4.6}$$

We can obtain an estimate of the photon wave-packet size, w_B, in its direction of propagation, using the following argument: the photon is produced from an excited state of an atom; the lifetime τ of the excited state represents the uncertainty in time during which the photon wave packet is created. Its size w_B can therefore be obtained from the relationship

$$w_B=v_B\tau . \tag{4.7}$$

The time, τ, is related to the energy spread, $\Delta\epsilon_B$, of the excited state by

$$\tau=\frac{\hbar}{\Delta\epsilon_B} . \tag{4.8}$$

From a classical argument[14]

$$\Delta\epsilon_B = K\frac{\langle \epsilon_B \rangle_{\rm av}}{\lambda\ (\text{Å})} , \tag{4.9}$$

where

$$K = \frac{mc^2}{\pi e^2} = 5.90\times 10^{-5}\ \text{Å} . \tag{4.10}$$

The quantities m and e are the mass and charge of the electron. Using Eqs. (4.1)–(4.9), we find that

$$w_B = 13.2\ \text{cm} . \tag{4.11}$$

Using Eqs. (2.38)–(2.40), we compute the average speed, v, of the r.m. system in the exit channel as

$$v = 1.20\times 10^8\ \text{cm/s} . \tag{4.12}$$

We then use Eqs. (3.7) and (4.12) to compute the speed of the ionized electron,

$$v_1 = 1.20\times 10^8\ \text{cm/s} , \tag{4.13}$$

and the speed of the proton,

$$v_2 = 6.50\times 10^4\ \text{cm/s} . \tag{4.14}$$

Thus

$$\beta_1 = 4.72\times 10^{-6} , \tag{4.15a}$$

and

$$\beta_2 = 8.71\times 10^{-3} . \tag{4.15b}$$

We now make the assumption that the wave-packet size associated with the photon, w_B, is very much larger than that associated with the hydrogen atom, w_T. In addition, since β_i, ($\beta_i = v_T/v_i$) is much less than 1, we can apply the results of Sec. III, neglecting terms of order β_i^2. Using Eqs. (3.17a), (3.18b), and (3.12)–(3.14), we obtain the probability density $P_i'(t)$ ($i=1$ for the electron, and $i=2$ for the proton) for each exit-channel particle is

$$P_i'(t) = \frac{v_e}{v_i}\sigma(\hat{\mathbf{r}}_+)\frac{|G_B(0,0,\mu_{i+})|^2}{(\rho_i^2+Z_i^2)^{1/2}[\beta_i Z_i + (\rho_i^2+Z_i^2)^{1/2}]} , \tag{4.16}$$

where

$$u_{i+} = \frac{\beta_i z_i + (\rho_i^2+Z_i^2)^{1/2} - v_i t}{v_i T} , \tag{4.17}$$

$$Z_i = z_i - v_T t , \tag{4.18}$$

and

$$T = \frac{w_B + w_T}{v_e} \approx \frac{w_B}{v_e} = 4.40\times 10^{-10}\ \text{s} . \tag{4.19}$$

The low-energy cross section for photoionization is[15]

$$\sigma(\hat{\mathbf{r}}_+) = 64\pi\alpha a_0^2\left[\frac{\epsilon_0}{\langle\epsilon_B\rangle_{\rm av}}\right]^4 \frac{\exp[-4\gamma\cot^{-1}(\gamma)]}{1-\exp(-2\pi\gamma)]}\sin^2\theta , \tag{4.20}$$

where

$$\frac{1}{\gamma} = \left[\frac{\langle\epsilon_B\rangle_{\rm av}}{\epsilon_0} - 1\right]^{1/2} . \tag{4.21}$$

The quantity ϵ_0 is the ground-state energy of the hydrogen atom; α is the fine-structure constant; a_0 is the Bohr radius. The variable θ is the spherical polar angle describing the orientation of the vector $\hat{\rho}_{i+}$. With the aid of Eqs. (3.11) we can express $\sin^2(\theta)$ in terms of the coordinates of each exit-channel particle as follows:

$$\sin^2\theta \approx \frac{\rho_i^2}{(\rho_i^2+Z_i^2) + 2\beta_i Z_i(\rho_i^2+Z_i^2)^{1/2}} . \tag{4.22}$$

In Eq. (4.22) terms of order quadratic and higher in β have been neglected.

We now calculate the coherence times and coherence lengths associated with the ionized electron and proton wave packets. Using Eq. (3.20) and retaining terms of first order in β_i we obtain the following expression for the coherence time:

$$T_{ci} = T(1-\beta_i\cos\theta') . \tag{4.23}$$

The variable θ' is the spherical polar angular coordinate, measured with respect to the z axis, of the location at which the coherence time is to be determined. Using Eqs. (3.23) and (4.23) we obtain the coherence length of each exit-channel particle as

$$w_{ci} = v_i T(1-\beta_i\cos\theta') . \tag{4.24}$$

Using Eqs. (4.13), (4.14), (4.19), and (4.23), we calculate the coherence times of the ionized electron and proton wave packets to be

$$T_{c1} \approx T_{c2} \approx T = 4.40\times 10^{-10}\ \text{s} . \tag{4.25}$$

In addition, the coherence length of the proton wave packet is

$$w_{c2} = 2.90\times 10^{-5}\ \text{cm} , \tag{4.26}$$

and the coherence length of the electron wave packet is

$$w_{c1} = 5.30\times 10^{-2}\ \text{cm} . \tag{4.27}$$

In summary, we have derived explicit expressions for the wave packets of the ionized electron and proton and have shown that both wave packets assume, basically, the same shape as the ionizing photon wave packet. In addition, we have calculated the coherence times and coherence lengths associated with the ionized electron and proton wave packets. It is interesting to note that when the electron is bound to the proton its wave-packet size is about an angstrom, but after ionization its wave-packet size grows to almost 0.1 mm.[16]

V. CONCLUSIONS

Our interest in what factors were determining the size and structure of a wave packet motivated us to consider a general reaction process in which two particles in the entrance channel interact, thereby producing two arbitrary particles in the exit channel. Based on some rather broad assumptions about the nature of the interaction we were able to obtain, in the c.m. frame, the relationship between the wave function in the exit-channel system and wave functions of the two entrance-channel particles. Furthermore, under the assumption that the coherence length of one entrance-channel particle, the beam particle, was much greater than that of the other, the target particle, we derived an explicit expression for the wave function of each exit-channel particle in terms of the wave packet of the beam particle. We also showed that under this assumption there were three different cases which had to be considered, the first case in which the speed of the exit-channel particle was greater than that of the target particle, the second case in which they were equal, and the third case in which the speed of the exit-channel particle was less than that of the target particle. We found in all three cases that the target particle appeared to act as a source of a spherical wave packet which corresponded to the exit-channel particle. Also, it was found that these three cases could be interpreted, physically, in the same way as the corresponding situations in classical wave theory. Case 1 was corresponding to the situation in which the speed of the source was less than the speed of the wave which it was generating. Case 2 was corresponding to the situation in which the source and wave were traveling at the same speed. Case 3 was corresponding to the situation in which the speed of the source was greater than the speed of the wave so that the source was generating a shock wave. Finally, for each case we derived expressions for both the coherence time and coherence length of each exit-channel particle. We showed that, in general, these expressions were a complicated function of the coordinates at which the coherence time and coherence length were to be determined. However, when the speed of the target particle was much less than that of an exit-channel particle, we found that the expressions for the coherence time and coherence length assumed a simple spatial dependence [see Eqs. (4.23) and (4.24)].

The assumptions on which all of our results were based were quite general so that these results should apply in a variety of situations. The important assumptions may be summarized as follows:

(1) the range of the interaction between the particles in the entrance channel must be much less than the coherence length of one of the entrance-channel particles;

(2) the scattering cross section must not exhibit a sharp resonance in the region of energy where the reaction process occurs;

(3) the results are applied only in regions where interaction between the exit-channel particles may be neglected and when the distance separating them is large [see Eqs. (3.51)].

As a simple and semirealistic application of our formalism we considered the case of photoionization of the hydrogen atom at low energies. After making some assumptions about the source of the ionizing electromagnetic radiation, we were able to calculate the coherence length of both the ionized electron and proton. We found the coherence length of the electron to be approximately 0.1 mm, a result which may be surprising.

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