PHYSICAL REVIEW A VOLUME 26, NUMBER 6 DECEMBER 1982

Distorted eikonal cross sections: A time-dependent view

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(Received 5 May 1982)

For Hamiltonians with two potentials, differential cross sections are written as time-correlation functions of reference and distorted transition operators. Distorted eikonal differential cross sections are defined in terms of straight-line and reference classical trajectories. Both elastic and inelastic results are obtained. Expressions for the inelastic cross sections are presented in terms of time-ordered cosine and sine memory functions through the use of the Zwanzig-Feshbach projection-operator method.

I. INTRODUCTION

Eikonal theory[1–10] of binary scattering is usually presented from a time-independent viewpoint. Recently, an alternate time-dependent description[11] has been used to rederive elastic eikonal cross sections.[12] Using time-dependent[13–15] solutions of the Zwanzig-Feshbach[16,17] projection-operator method inelastic eikonal cross sections have been obtained[18] which differ from the standard time-independent treatment.[1,10] Straight-line trajectories appear as a common feature in these eikonal approximations. However, distortions from linearity occur during a collision and are expected to play an important role. Thus it is desirable to build some distortion into the trajectories. One way of doing so[11,13] is to introduce reference classical trajectories associated with a reference Hamiltonian. This necessitates a two-potential formulation for the appropriate cross sections in terms of distorted collision operators.[11] Such a time-dependent description is presented in this paper.

In Sec. II distorted inelastic cross sections are defined in terms of time-correlation functions. Eikonal approximations are defined in Sec. III while explicit results for elastic scattering are presented in Sec. IV. Explicit inelastic results are given in Sec. V in terms of cosine and sine memory functions.

II. TIME-CORRELATION FUNCTIONS

The generalized cross section[19,20]

$$\sigma_{\text{gen}}(1\vec{p}\,''\rightarrow n\hat{R})=\text{Tr}[\,|\,n;\hat{R}\,\rangle\langle\, n;\hat{R}\,|\,](-i\mathscr{T})[\,|\,1;\vec{p}\,''\rangle(\mu h^3/p'')\langle 1;\vec{p}\,''\,|\,] \tag{2.1}$$

is a convenient starting point for obtaining time-correlation-function expressions for the differential cross section. It involves a plane-wave density $|\,1;\vec{p}\,''\rangle(\mu h^3/p'')\langle 1;\vec{p}\,''\,|$ which is transformed into a spherical density $|\,n;\hat{R}\,\rangle\langle n;\hat{R}\,|$ by the transition superoperator $\mathscr{T}=\mathscr{V}\Omega_L^{(+)}$. Here μ is the reduced mass, $\vec{p}\,''$ is the incoming momentum and $\hat{R}$ is the observation direction. The transition superoperator is the product of the potential superoperator $\mathscr{V}$, $\hbar^{-1}$ times the commutator with the potential V, and the Møller superoperator

$$\Omega_L^{(+)}=\lim_{t\rightarrow-\infty}\exp(i\mathscr{L}t)\exp[-i(\mathscr{K}+\mathscr{L}_{\text{int}})t]\ . \tag{2.2}$$

Here, $\mathscr{L}$ is the full Liouville or von Neumann superoperator, $\hbar^{-1}$ times the commutator with the Hamiltonian $H=K+H_{\text{int}}+V$, $\mathscr{K}$ is the drift or kinetic superoperator, $\hbar^{-1}$ times the commutator with the kinetic energy K, and $\mathscr{L}_{\text{int}}$ is the internal-state Liouville superoperator, $\hbar^{-1}$ times the commutator with the internal-state Hamiltonian H_{int}. This exact density-operator description[19,20] is equivalent to the usual wave-function representation of the scattering event.

The potential energy is now assumed to be the sum of a reference potential V_0 and a second potential V_1. Associated with these potentials are the superoperators $\mathscr{V}_0$ and $\mathscr{V}_1$, respectively. The reference potential is assumed to operate on the translational motion only and, thus, commutes with the internal-state Hamiltonian while the potential V_1 is responsible for the collisional coupling between the translational and internal motions. With this choice for V the Møller superoperator becomes a product,[11] namely,

$$\Omega_L^{(+)}=\Omega_{L,D}^{(+)}\Omega_{L_0}^{(+)} , \tag{2.3}$$

of the reference Møller superoperator

$$\Omega_{L_0}^{(+)}=\lim_{t\to-\infty}\exp(i\mathscr{L}_0 t)\exp(-i\mathscr{K}t) , \tag{2.4}$$

where $\mathscr{L}_0 f=\hbar^{-1}[H_0,f]_-$, $H_0=K+V_0$ and a distorted Møller superoperator

$$\Omega_{L,D}^{(+)}=\lim_{t\to-\infty}\exp(i\mathscr{L}t)\exp[-i(\mathscr{L}_0+\mathscr{L}_{\rm int})t]\times\mathscr{P}_c(\mathscr{L}_0) . \tag{2.5}$$

Equation (2.5) involves the projection

$$\mathscr{P}_c(\mathscr{L}_0)A_{\rm op}=P_c(H_0)A_{\rm op}P_c(H_0) , \tag{2.6}$$

made onto the continuum of H_0. Here $A_{\rm op}$ is an operator. Making use of the Lippmann-Schwinger equation for the distorted Møller operator,

$$\Omega_{L,D}^{(+)}=\mathscr{P}_c(\mathscr{L}_0)-i\int_{-\infty}^{0}ds\,\exp[i(\mathscr{L}_0+\mathscr{L}_{\rm int})s]\mathscr{T}_D\exp[-i(\mathscr{L}_0+\mathscr{L}_{\rm int})s] , \tag{2.7}$$

the transition superoperator becomes

$$\mathscr{T}=(\mathscr{V}_0+\mathscr{V}_1)\Omega_{L,D}^{(+)}\Omega_{L_0}^{(+)}=\mathscr{T}_0+\mathscr{T}_D\Omega_{L_0}^{(+)}-i\int_{-\infty}^{0}ds\,\mathscr{V}_0\exp[i(\mathscr{L}_0+\mathscr{L}_{\rm int})s]\mathscr{T}_D\Omega_{L_0}^{(+)}\exp[-i(\mathscr{K}+\mathscr{L}_{\rm int})s] , \tag{2.8}$$

where $\mathscr{T}_D=\mathscr{V}_1\Omega_{L,D}^{(+)}$. To obtain the last form of Eq. (2.8) the intertwining relation

$$\exp(-i\mathscr{L}_0 s)\Omega_{L_0}^{(+)}=\Omega_{L_0}^{(+)}\exp(-i\mathscr{K}s) \tag{2.9}$$

has been used.

Since the generalized cross section is on the frequency shell of $\mathscr{K}$, it can be exactly written as the sum

$$\sigma_{\rm gen}(1\vec{p}''\to n\hat{R})=\sigma_{\rm gen}^{(0)}(\vec{p}''\to\hat{R})\delta_{n1}+\sigma_{\rm gen}^{(D)}(1\vec{p}''\to n\hat{R}) \tag{2.10}$$

of a reference generalized cross section

$$\sigma_{\rm gen}^{(0)}(\vec{p}''\to\hat{R})={\rm Tr}[\,|\hat{R}\rangle\langle\hat{R}|\,](-i\mathscr{T}_0)[\,|\vec{p}''\rangle(\mu h^3/p'')\langle\vec{p}''|\,] \tag{2.11}$$

and a distorted generalized cross section[21]

$$\sigma_{\rm gen}^{(D)}(1\vec{p}''\to n\hat{R})={\rm Tr}[\,|n;\hat{R}\rangle\langle n;\hat{R}|\,](-i\Omega_{L_0}^{(-)\dagger}\mathscr{T}_D\Omega_{L_0}^{(+)})[\,|1;\vec{p}''\rangle(\mu h^3/p'')\langle 1;\vec{p}''|\,] , \tag{2.12}$$

where the post-Møller superoperator is

$$\Omega_{L_0}^{(-)}=\lim_{t\to\infty}\exp(i\mathscr{L}_0 t)\exp(-i\mathscr{K}t) . \tag{2.13}$$

Equations (2.11) and (2.12) are the starting points for deriving the time-correlation expressions for the differential cross sections. The reference cross section is considered first.

A. Reference cross section

Following the procedure of Ref. 12, the generalized reference cross section becomes

$$\sigma_{\rm gen}^{(0)}(\vec{p}''\to\hat{R})=-(4\pi h^2\mu/p''){\rm Im}\int_0^\infty dp\,p^2\langle p\hat{R}\,|\,\Omega_0^{(+)}\,|\,\vec{p}''\rangle\langle\vec{p}''\,|\,t_0^\dagger\,|\,p\hat{R}\rangle \tag{2.14}$$

when the relation[22,23]

$$\Omega_{L_0}^{(+)}A_{\rm op}=\Omega_0^{(+)}A_{\rm op}\Omega_0^{(+)\dagger} \tag{2.15}$$

between the reference Møller superoperator and the reference Møller operator

$$\Omega_0^{(+)}=\lim_{t\to-\infty}\exp(iH_0t/\hbar)\exp(-iKt/\hbar)=1-(i/\hbar)\int_{-\infty}^{0}ds\,t_0(s) \tag{2.16}$$

is used. Here $t_0=V_0\Omega_0^{(+)}$ is the reference transition operator. The last form of Eq. (2.16) is the Lippman-Schwinger equation for the reference Møller operator in terms of the time-dependent reference transition operator

$$t_0(s)=\exp(i\mathscr{K}s)t_0=V_0(s)\Omega_0^{(+)}(s)\ . \tag{2.17}$$

This latter operator is the product of the time-dependent reference potential

$$V_0(s)=\exp(i\mathscr{K}s)V_0=V_0(\vec{r}_{op}+\vec{p}_{op}s/\mu) \tag{2.18}$$

and the time-dependent Møller operator

$$\Omega_0^{(+)}(s)=\exp(i\mathscr{K}s)\Omega_0^{(+)}=T\exp\left[(-i/\hbar)\int_{-\infty}^{s}ds_1V_0(s_1)\right], \tag{2.19}$$

where T is the Dyson chronological operator.[4,24]

Using Eq. (2.16) in Eq. (2.14) the generalized reference cross section becomes the difference

$$\sigma_{\rm gen}^{(0)}(\vec{p}''\to\hat{R})=\sigma^{(0)}(\vec{p}''\to\hat{R})-\sigma_{\rm tot}^{(0)}\delta^{(2)}(\hat{p}''-\hat{R})\ , \tag{2.20}$$

between the reference differential cross section

$$\sigma^{(0)}(\vec{p}''\to\hat{R})=(4\pi^2h\mu/p'')\mathrm{Re}\int_{-\infty}^{\infty}ds\int_0^{\infty}dp\,p^2\langle p\hat{R}\,|\,t_0(s)\,|\,\vec{p}''\rangle\langle\vec{p}''\,|\,t_0^\dagger\,|\,p\hat{R}\rangle \tag{2.21}$$

and the product of the reference total cross section

$$\sigma_{\rm tot}^{(0)}=-(4\pi h^2\mu/p'')\mathrm{Im}\langle\vec{p}''\,|\,t_0\,|\,\vec{p}''\rangle=\int d\hat{R}\,\sigma^{(0)}(\vec{p}''\to\hat{R})\ , \tag{2.22}$$

with a two-dimensional Dirac δ function in the forward direction. Equation (2.21) is the time-autocorrelation-function expression for the reference differential cross section. This process of relating the generalized cross section to the differential and total cross sections is now applied to the distorted expression, Eq. (2.12).

B. Distorted cross section

Using relations of the form of Eq. (2.15) for the various Møller superoperators the generalized cross section becomes

$$\sigma_{\rm gen}^{(D)}(1\vec{p}''\to n\hat{R})=-(4\pi h^2\mu/p'')\mathrm{Im}\int_0^{\infty}dp\,p^2\langle n;p\hat{R}\,|\,\Omega_0^{(-)\dagger}\Omega_D^{(+)}\Omega_0^{(+)}\,|\,1;\vec{p}''\rangle\langle 1;\vec{p}''\,|\,\Omega_0^{(+)\dagger}t_D^\dagger\Omega_0^{(-)}\,|\,n;p\hat{R}\rangle\ , \tag{2.23}$$

where $t_D=V_1\Omega_D^{(+)}$ is the distorted transition operator and where

$$\Omega_D^{(+)}=\lim_{t\to-\infty}\exp(iHt/\hbar)\exp[-i(H_0+H_{\rm int})/\hbar]=P_c(H_0)-(i/\hbar)\int_{-\infty}^{0}ds\,t_D(s) \tag{2.24}$$

is the distorted Møller operator. Equation (2.24) involves the time-dependent distorted transition operator

$$t_D(s)=\exp[i(\mathscr{L}_0+\mathscr{L}_{\rm int})s]t_D=V_1(s)\Omega_D^{(+)}(s) \tag{2.25}$$

which is the product of the interaction-picture potential

$$V_1(s)=\exp[i(\mathscr{L}_0+\mathscr{L}_{\rm int})s]V_1 \tag{2.26}$$

and the time-dependent Møller operator

$$\Omega_D^{(+)}(s)=T\exp\left[(-i/\hbar)\int_{-\infty}^{s}ds_1V_1(s_1)\right]. \tag{2.27}$$

To obtain distorted eikonal cross sections it is convenient to introduce a further transformation of these distorted operators. In particular, using the relation

$$\Omega_0^{(+)}\Omega_0^{(+)\dagger}=P_c(H_0) \tag{2.28}$$

the time-dependent distorted transition operator becomes

$$\Omega_0^{(-)\dagger}t_D(s)\Omega_0^{(+)}=S_0\bar{t}_D(s)\ , \tag{2.29}$$

where the transformed transition operator

$$\bar{t}_D(s)=U_1(s)\bar{\Omega}_D^{(+)}(s) \tag{2.30}$$

involves the potential

$$U_1(s)=\Omega_0^{(+)\dagger}V_1(s)\Omega_0^{(+)}=\Omega_{L_0}^{(+)\dagger}V_1(s)=\exp[i(\mathscr{K}+\mathscr{L}_{\rm int})s]\Omega_{L_0}^{(+)\dagger}V_1 \tag{2.31}$$

and the distorted Møller operator

$$\bar{\Omega}_D^{(+)}(s)=T\exp\left[(-i/\hbar)\int_{-\infty}^{s}ds_1U_1(s_1)\right]\ . \tag{2.32}$$

Equation (2.29) also involves the reference scattering operator

$$S_0=\Omega_0^{(-)\dagger}\Omega_0^{(+)}=1-(i/\hbar)\int_{-\infty}^{\infty}ds\ t_0(s)\ . \tag{2.33}$$

Applying Eqs. (2.24), (2.29), and (2.33) to Eq. (2.23) leads to the sum

$$\sigma_{\rm gen}^{(D)}(1\vec{p}''\to n\hat{R})=\delta_{n1}\sigma^{(C)}(1\vec{p}''\to 1\hat{R})+\sigma^{(D)}(1\vec{p}''\to n\hat{R})-\sigma_{\rm tot}^{(D)}\delta^{(2)}(\hat{p}''-\hat{R})\ , \tag{2.34}$$

where

$$\sigma^{(D)}(1\vec{p}''\to n\hat{R})=(4\pi^2h\mu/p'')\mathrm{Re}\int_{-\infty}^{\infty}ds\int_0^{\infty}dp\,p^2\langle n;p\hat{R}\,|\,S_0\bar{t}_D(s)\,|\,1;\vec{p}''\rangle\langle 1;\vec{p}''\,|\,\bar{t}_D^{\dagger}S_0^{\dagger}\,|\,n;p\hat{R}\rangle \tag{2.35}$$

is the time-autocorrelation-function representation of the distorted differential cross section, and where

$$\sigma^{(C)}(1\vec{p}''\to 1\hat{R})=(8\pi^2h\mu/p'')\mathrm{Re}\int_{-\infty}^{\infty}ds\int_0^{\infty}dp\,p^2\langle p\hat{R}\,|\,t_0(s)\,|\,\vec{p}''\rangle\langle 1;\vec{p}''\,|\,\bar{t}_D^{\dagger}S_0^{\dagger}\,|\,1;p\hat{R}\rangle \tag{2.36}$$

is the time-correlation-function representation of the coupling differential cross section; it represents quantal interference between the reference and distorted motions. Also,

$$\sigma_{\rm tot}^{(D)}=-(4\pi h^2\mu/p'')\mathrm{Im}\langle 1;\vec{p}''\,|\,S_0\bar{t}_D\,|\,\vec{p}''\rangle=\int d\hat{R}\left[\sigma^{(C)}(1\vec{p}''\to 1\hat{R})+\sum_{n=1}^{N}\sigma^{(D)}(1\vec{p}''\to n\hat{R})\right] \tag{2.37}$$

is the total distorted cross section.

In summary, the full generalized cross section, Eq. (2.1), can be exactly expressed as the difference

$$\sigma_{\rm gen}(1\vec{p}''\to n\hat{R})=\sigma(1\vec{p}''\to n\hat{R})-\sigma_{\rm tot}\delta^{(2)}(\hat{p}''-\hat{R}) \tag{2.38}$$

between the differential cross section

$$\sigma(1\vec{p}''\to n\hat{R})=\delta_{n1}[\sigma^{(0)}(\vec{p}''\to\hat{R})+\sigma^{(C)}(1\vec{p}''\to 1\hat{R})]+\sigma^{(D)}(1\vec{p}''\to n\hat{R}) \tag{2.39}$$

and the product of the total cross section

$$\sigma_{\rm tot}=\sigma_{\rm tot}^{(0)}+\sigma_{\rm tot}^{(D)} \tag{2.40}$$

with the two-dimensional Dirac δ function in the forward direction.

III. EIKONAL APPROXIMATION

A. Reference cross section

The reference eikonal potential[11]

$$V_0^{\mathrm{EA}}(s)=V_0(\vec{r}_{\mathrm{op}}+\vec{P}s/\mu) \tag{3.1}$$

is obtained from Eq. (2.18) when the momentum operator $\vec{p}_{\mathrm{op}}$ is approximated by a momentum parameter, namely, $\vec{P}$. Thus the reference eikonal Møller operator is

$$\Omega_0^{\mathrm{EA}(+)}(s)=\exp\left[(-i/\hbar)\int_{-\infty}^{s} ds_1 V_0(\vec{r}_{\mathrm{op}}+\vec{P}s/\mu)\right] \tag{3.2}$$

while the time integral of the eikonal transition operator is

$$\begin{aligned}\int_{-\infty}^{\infty} ds\langle p\hat{R}\,|\,t_0^{\mathrm{EA}}(s)\,|\,\vec{p}''\rangle &=\delta((p\hat{R}-\vec{p}'')\cdot\vec{P})(iP/h)\int_0^{\infty} db\, bJ_0(\,|\,p\hat{R}-\vec{p}''\,|\,b/\hbar)\{\exp[-i(p''/P)\chi_0(b)]-1\}\\ &=\mu h\delta((p\hat{R}-\vec{p}'')\cdot\vec{P})\langle p\hat{R}\,|\,t_0^{\mathrm{EA}}(0)\,|\,\vec{p}''\rangle\ ,\end{aligned} \tag{3.3}$$

where, for central potentials,

$$\chi_0(b)=(\mu/p''\hbar)\int_{-\infty}^{\infty} dz\, V_0((b^2+z^2)^{1/2}) \tag{3.4}$$

is the Glauber phase and where $J_0(x)$ is the zeroth-order Bessel function. Choosing $\vec{P}$ to be $\frac{1}{2}(p\hat{R}+\vec{p}'')$ and using Eq. (3.3) in Eq. (2.21) gives the reference eikonal differential cross section, namely,

$$\sigma^{\mathrm{EA}(0)}(\vec{p}''\rightarrow\hat{R})=(p''/\hbar)^2\cos^2(\tfrac{1}{2}\theta)\left|\int_0^{\infty} db\, bJ_0(2p''b\sin(\tfrac{1}{2}\theta)/\hbar)\{\exp[-i\sec(\tfrac{1}{2}\theta)\chi_0(b)]-1\}\right|^2, \tag{3.5}$$

where θ is the scattering angle ($\hat{R}\cdot\hat{p}''=\cos\theta$). This cross section reduces to the Born differential cross section when the Glauber phase is small.

B. Distorted cross sections

The reference potential naturally contains a straight-line trajectory to which the eikonal approximation can be made. However, the distorted potential $U_1(s)$, Eq. (2.31), has motion generated by the reference Liouville superoperator, $\mathscr{L}_0$, which quantally does not have an associated single trajectory. To define a distorted eikonal approximation[11] it is convenient to replace the exact quantal potential with an approximate quantal potential[13]

$$U_1^{\mathrm{CTA}}(s)=\int d\vec{r}\,d\vec{p}\ \,|\,\vec{r},\vec{p}\,\rangle\!\rangle_O \exp(i\mathscr{L}_{\mathrm{int}}s)\,{}_S\langle\!\langle\,\vec{r}+\vec{p}s/\mu,\vec{p}\,|\,\Omega_{L_0,\mathrm{cl}}^{(+)\dagger}\,|\,V_1\,\rangle\!\rangle_O\ , \tag{3.6}$$

which has motion generated by the classical reference Liouville superoperator (Poisson bracket with H_0). Here, $|\,\vec{r},\vec{p}\,\rangle\!\rangle_O=h^{-3}\Delta(\vec{r},\vec{p})$ and $|\,\vec{r},\vec{p}\,\rangle\!\rangle_S=\Delta(\vec{r},\vec{p})$ are ideal observable and statistical state elements[25] of the Weyl correspondence[26] (Wigner equivalence representation[27]) where[28]

$$\Delta(\vec{r},\vec{p})=\int d\vec{R}\exp(-i\vec{R}\cdot\vec{p}/\hbar)\,|\,\vec{r}-\tfrac{1}{2}\vec{R}\rangle\langle\vec{r}+\tfrac{1}{2}\vec{R}\,|\ . \tag{3.7}$$

Equation (3.6) involves the phase-space function

$$\begin{aligned}{}_S\langle\!\langle\,\vec{r}+\vec{p}s/\mu,\vec{p}\,|\,\Omega_{L_0,\mathrm{cl}}^{(+)\dagger}\,|\,V_1\,\rangle\!\rangle_O &=\lim_{t\rightarrow-\infty}{}_S\langle\!\langle\,\vec{r}+\vec{p}s/\mu,\vec{p}\,|\,\exp(i\mathscr{K}t)\exp(-i\mathscr{L}_{0,\mathrm{cl}}t)\,|\,V_1\,\rangle\!\rangle_O\\ &=\lim_{t\rightarrow-\infty}{}_S\langle\!\langle\,\vec{r}+\vec{p}(s+t)/\mu,\vec{p}\,|\,\exp(-i\mathscr{L}_{0,\mathrm{cl}}t)\,|\,V_1\,\rangle\!\rangle_O\ .\end{aligned} \tag{3.8}$$

Upon writing $\vec{r}=\vec{b}+z\hat{p}$, $\vec{b}\cdot\vec{p}=0$ and then defining $t'=t+s+\mu z/p$ this phase-space function becomes

$$_S\langle\!\langle \vec{r}+\vec{p}s/\mu,\vec{p}\mid \Omega_{L_0,\mathrm{cl}}^{(+)\dagger}\mid V_1\rangle\!\rangle_O=\lim_{t'\to-\infty} {}_S\langle\!\langle \vec{b}+\vec{p}t'/\mu,\vec{p}\mid \exp[i\mathscr{L}_{0,\mathrm{cl}}(s+\mu z/p-t')]\mid V_1\rangle\!\rangle_O$$
$$=V_1(\vec{R}_0(s+\mu z/p\mid \vec{b},\vec{p});\vec{X}_{\mathrm{op}})\ , \tag{3.9}$$

where $\vec{X}_{\mathrm{op}}$ is the position operator associated with the internal-state Hamiltonian. The position trajectory $\vec{R}_0(t\mid \vec{b},\vec{p})$ is a solution of Hamilton's equations of motion subject to the initial condition

$$\vec{R}_0(t\mid \vec{b},\vec{p}) \underset{t\to-\infty}{\sim} \vec{b}+\vec{p}t/\mu\ . \tag{3.10}$$

Inserting Eq. (3.9) into Eq. (3.6) gives the classical-trajectory quantum potential from which the distorted eikonal potential can be derived. That is, replacing $\vec{p}$ with $\vec{P}$, a momentum parameter, in the classical trajectory in Eq. (3.9) leads to the distorted eikonal potential

$$U_1^{\mathrm{EA}}(s)=(P/\mu)\int_{-\infty}^{\infty}dt\int d^{(2)}\vec{b}\ \mid \vec{b}+\vec{P}(t-s)/\mu\rangle\{\exp[i\mathscr{L}_{\mathrm{int}}(s-t)]W_1^{\mathrm{EA}}(t)\}\langle \vec{b}+\vec{P}(t-s)/\mu\mid\ , \tag{3.11}$$

where

$$W_1^{\mathrm{EA}}(t)=\exp(i\mathscr{L}_{\mathrm{int}}t)V_1(\vec{R}_0(t\mid \vec{b},\vec{P});\vec{X}_{\mathrm{op}})\ . \tag{3.12}$$

Thus the distorted eikonal Møller operator, Eq. (2.32), becomes

$$\bar{\Omega}_D^{\mathrm{EA}(+)}(s)=T\exp\left[(-i/\hbar)\int_{-\infty}^{s}ds_1 U_1^{\mathrm{EA}}(s_1)\right]$$
$$=(P/\mu)\int_{-\infty}^{\infty}dt\int d^{(2)}\vec{b}\ \mid \vec{b}+\vec{P}(t-s)/\mu\rangle\{\exp[i\mathscr{L}_{\mathrm{int}}(s-t)]G^{\mathrm{EA}}(t;-\infty)\}\langle \vec{b}+\vec{P}(t-s)/\mu\mid\ , \tag{3.13}$$

where

$$G^{\mathrm{EA}}(t;-\infty)=T\exp\left[(-i/\hbar)\int_{-\infty}^{t}ds_1 W_1^{\mathrm{EA}}(s_1)\right] \tag{3.14}$$

is the time-ordered group associated with the potential $W_1^{\mathrm{EA}}(t)$. The time integral of the distorted transition operator is then

$$\int_{-\infty}^{\infty}ds\langle n;p\hat{R}\mid S_0^{\mathrm{EA}}\bar{t}_D^{\mathrm{EA}}(s)\mid 1;\vec{p}\,''\rangle$$
$$=(P/\mu h^3)\int_{-\infty}^{\infty}ds\int_{-\infty}^{\infty}dt\int d^{(2)}\vec{b}\langle n\mid W_1^{\mathrm{EA}}(t)G^{\mathrm{EA}}(t;-\infty)\mid 1\rangle$$
$$\times\exp\{-i(p\hat{R}-\vec{p}\,'')\cdot[\vec{b}+\vec{P}(t-s)/\mu]/\hbar+i\omega_{n1}(s-t)+(p''/P)\chi_0(b)\}$$
$$=\mu h\delta((p\hat{R}-\vec{p}\,'')\cdot\vec{P}+\mu\hbar\omega_{n1})\langle n;p\hat{R}\mid S_0^{\mathrm{EA}}\bar{t}_D^{\mathrm{EA}}(0)\mid 1;\vec{p}\,''\rangle\ , \tag{3.15}$$

where $\omega_{n1}=\hbar^{-1}(E_n-E_1)$. Therefore the distorted eikonal differential cross section is

$$\sigma^{\mathrm{EA}(D)}(1\vec{p}\,''\to n\hat{R})=(2\pi h\mu)^2\int_0^{\infty}dp\,(p^2/p'')\delta((p\hat{R}-\vec{p}\,'')\cdot\vec{P}+\mu\hbar\omega_{n1})\mid\langle n;p\hat{R}\mid S_0^{\mathrm{EA}}\bar{t}_D^{\mathrm{EA}}(0)\mid 1;\vec{p}\,''\rangle\mid^2\ , \tag{3.16}$$

while the eikonal coupling differential cross section is

$$\sigma^{\mathrm{EA}(C)}(1\vec{p}\,''\to 1\hat{R})=-2(2\pi h\mu)^2\,\mathrm{Im}\int_0^{\infty}dp\,(p^2/p'')\delta((p\hat{R}-\vec{p}\,'')\cdot\vec{P})\langle p\hat{R}\mid t_0^{\mathrm{EA}}(0)\mid \vec{p}\,''\rangle$$
$$\times\langle 1;\vec{p}\,''\mid \bar{t}_D^{\mathrm{EA}\dagger}(0)S_0^{\mathrm{EA}\dagger}\mid 1;p\hat{R}\rangle\ . \tag{3.17}$$

Finally, the complete eikonal differential cross section is the sum

$$\sigma^{\mathrm{EA}}(1\vec{p}\,''\to n\hat{R})=\delta_{n1}[\sigma^{\mathrm{EA}(0)}(\vec{p}\,''\to\hat{R})+\sigma^{\mathrm{EA}(C)}(1\vec{p}\,''\to 1\hat{R})]+\sigma^{\mathrm{EA}(D)}(1\vec{p}\,''\to n\hat{R})\ . \tag{3.18}$$

IV. ELASTIC CROSS SECTIONS

For elastic cross sections the matrix element of the distorted transition operator becomes

$$\begin{aligned}\langle p\hat{R}\,|\,S_0^{\mathrm{EA}}\bar{t}_D^{\mathrm{EA}}(0)\,|\,\vec{\mathrm{p}}''\rangle &= (P/\mu h^3)\int_{-\infty}^{\infty} dt \int d^{(2)}\vec{\mathrm{b}}\, V_1(\vec{\mathrm{R}}_0(t\,|\,\vec{\mathrm{b}},\vec{\mathrm{P}}))\\ &\qquad \times \exp\Big[(-i/\hbar)[(p\hat{R}-\vec{\mathrm{p}}'')\cdot\vec{\mathrm{b}}+\hbar(p''/P)\chi_0(b)]\\ &\qquad\qquad + \int_{-\infty}^{t} ds\, V_1(\vec{\mathrm{R}}_0(s\,|\,\vec{\mathrm{b}},\vec{\mathrm{P}}))\Big]\\ &= i(P/2\pi\mu h^2)\int d^{(2)}\vec{\mathrm{b}}\exp[-i(p\hat{R}-\vec{\mathrm{p}}'')\cdot\vec{\mathrm{b}}/\hbar - i(p''/P)\chi_0(b)]\\ &\qquad \times\{\exp[-i\chi_1^D(\vec{\mathrm{b}})]-1\}\ , \end{aligned} \tag{4.1}$$

where the distorted Glauber phase is

$$\chi_1^D(\vec{\mathrm{b}}) = \hbar^{-1}\int_{-\infty}^{\infty} dt\, V_1(\vec{\mathrm{R}}_0(t\,|\,\vec{\mathrm{b}},\vec{\mathrm{P}}))\ . \tag{4.2}$$

To obtain Eq. (4.1) the δ function in Eq. (3.15) has been used to restrict the momentum transfer to the $\vec{\mathrm{b}}$ plane. Thus the elastic eikonal differential coupling cross section, Eq. (3.17), becomes

$$\begin{aligned}\sigma^{\mathrm{EA}(C)}(\vec{\mathrm{p}}''\to\hat{R}) &= -\pi^{-1}(p''/\hbar)^2\cos^2(\tfrac{1}{2}\theta)\\ &\quad\times \mathrm{Im}\int_0^{\infty} db\, bJ_0(2p''\sin(\tfrac{1}{2}\theta)b/\hbar)\{\exp[-i\sec(\tfrac{1}{2}\theta)\chi_0(b)]-1\}\\ &\quad\times\int d^{(2)}\vec{\mathrm{b}}'\exp[ip''(\hat{R}-\hat{p}'')\cdot\vec{\mathrm{b}}'/\hbar + i\sec(\tfrac{1}{2}\theta)\chi_0(b')]\{\exp[i\chi_1^D(\vec{\mathrm{b}}')]-1\} \end{aligned} \tag{4.3}$$

while the elastic distorted eikonal differential cross section is

$$\begin{aligned}\sigma^{\mathrm{EA}(D)}(\vec{\mathrm{p}}''\to\hat{R}) &= (p''/\hbar)^2\cos^2(\tfrac{1}{2}\theta)\,\Big|\,(2\pi)^{-1}\int d^{(2)}\vec{\mathrm{b}}\exp[-ip''(\hat{R}-\hat{p}'')\cdot\vec{\mathrm{b}}/\hbar - i\sec(\tfrac{1}{2}\theta)\chi_0(b)]\\ &\qquad\times\{\exp[-i\chi_1^D(\vec{\mathrm{b}})]-1\}\,\Big|^2\ . \end{aligned} \tag{4.4}$$

Again the momentum $\vec{\mathrm{P}}$ has been taken as $\frac{1}{2}(p\hat{R}+\vec{\mathrm{p}}'')$. The full elastic eikonal differential cross section is the sum of the eikonal reference differential cross section, Eq. (3.5), and Eqs. (4.3) and (4.4).

V. INELASTIC CROSS SECTIONS

Using the definition of the internal-state group, Eq. (3.14), the inelastic matrix element of the distorted transition operator, Eq. (3.15), becomes

$$\begin{aligned}&\langle n;p\hat{R}\,|\,S_0^{\mathrm{EA}}\bar{t}_D^{\mathrm{EA}}(0)\,|\,1;\vec{\mathrm{p}}''\rangle\\ &\quad= (P/\mu h^3)\int d^{(2)}\vec{\mathrm{b}}\int_{-\infty}^{\infty} dt\langle n\,|\,W_1^{\mathrm{EA}}(t)G^{\mathrm{EA}}(t;-\infty)\,|\,1\rangle\exp\{-i[(p\hat{R}-\vec{\mathrm{p}}'')\cdot\vec{\mathrm{b}}/\hbar+(p''/P)\chi_0(b)]\}\\ &\quad= (iP/2\pi\mu h^2)\int d^{(2)}\vec{\mathrm{b}}\exp\{-i[(p\hat{R}-\vec{\mathrm{p}}'')\cdot\vec{\mathrm{b}}/\hbar+(p''/P)\chi_0(b)]\}\,[G_{n1}^{\mathrm{EA}}(\infty;-\infty)-\delta_{n1}]\ . \end{aligned} \tag{5.1}$$

It is of Glauber form due to the momentum-transfer δ function. Taking $\vec{\mathrm{P}}=\frac{1}{2}(p\hat{R}+\vec{\mathrm{p}}'')$ the distorted eikonal differential cross section becomes

$$\begin{aligned}\sigma^{\mathrm{EA}(D)}(1\vec{\mathrm{p}}''\to n\hat{R}) &= (P/h)^2\lambda_{n1}\,\Big|\int d^{(2)}\vec{\mathrm{b}}\exp\{-i[p''(\lambda_{n1}\hat{R}-\hat{p}'')\cdot\vec{\mathrm{b}}/\hbar+(p''/P)\chi_0(b)]\}\\ &\qquad\times[G_{n1}^{\mathrm{EA}}(\infty;-\infty)-\delta_{n1}]\Big|^2\ , \end{aligned} \tag{5.2}$$

where $\lambda_{n1}=(1-2\mu\hbar\omega_{n1}/p''^2)^{1/2}>0$. Because the momentum-transfer δ function in Eq. (3.16) has been evaluated the momentum parameter $\vec{\mathrm{P}}$ becomes $\frac{1}{2}p''(\lambda_{n1}\hat{R}+\hat{p}'')$ in Eq. (5.2). The coupling eikonal differential cross section, Eq. (3.17), follows in a similar manner.

This distorted eikonal differential cross section involves the group $G^{\mathrm{EA}}(\infty;-\infty)$, Eq. (3.14), which is responsible for the internal-state motion along the given reference classical trajectory $\vec{\mathrm{R}}_0(t\,|\,\vec{\mathrm{b}},\vec{\mathrm{P}})$. This group can be formally solved using the Zwanzig-Feshbach[16,17] projection-operator method. However, rather than using the standard energy-resolved solutions it is more convenient to use the explicitly time-dependent solutions[13–15]

$$G^{\mathrm{EA}}(t;-\infty)P=G_P^{\mathrm{EA}}(t;-\infty)M^{\mathrm{EAC}}(t;-\infty)P-iG_Q^{\mathrm{EA}}(t;-\infty)M^{\mathrm{EAS}}(t;-\infty)P\ . \tag{5.3}$$

Here the P space is taken to be the initial state of the target so that its projection operator can be written as $|1\rangle\langle 1|$. Therefore, only $G^{\mathrm{EA}}(t;-\infty)P$ need be calculated for the cross sections. The orthogonal internal-state projection to P is then $Q=1-P=\sum_{n=2}^{N}|n\rangle\langle n|$ (where H_{int} is assumed to admit N eigenstates).

Equation (5.3) involves the motion groups ($S=P,Q$)

$$G_S^{\mathrm{EA}}(t;-\infty)=ST\exp\left[-(i/\hbar)\int_{-\infty}^{t}ds\,SW_1(s)S\right]S \tag{5.4}$$

in the P and Q spaces, as well as the cosine memory operator

$$M^{\mathrm{EAC}}(t;-\infty)=T\cos\left[\int_{-\infty}^{t}ds\,B^{\mathrm{EA}}(-\infty;s)\right] \tag{5.5}$$

and the sine memory operator

$$M^{\mathrm{EAS}}(t;-\infty)=T\sin\left[\int_{-\infty}^{t}ds\,B^{\mathrm{EA}}(-\infty;s)\right]\ . \tag{5.6}$$

These memory operators have motion generated by the self-adjoint B operators; that is,

$$B^{\mathrm{EA}}(-\infty;s)=\hbar^{-1}G_P^{\mathrm{EA}}(-\infty;s)PW_1^{\mathrm{EA}}(s)QG_Q^{\mathrm{EA}}(s;-\infty)+\hbar^{-1}G_Q^{\mathrm{EA}}(-\infty;s)QW_1^{\mathrm{EA}}(s)PG_P^{\mathrm{EA}}(s;-\infty)\ . \tag{5.7}$$

The inelastic eikonal differential cross section is then the sum

$$\sigma^{\mathrm{EA}}(1\vec{\mathrm{p}}''\to n\hat{R})=\delta_{n1}[\sigma^{\mathrm{EA}(0)}(\vec{\mathrm{p}}''\to\hat{R})+\sigma^{\mathrm{EA}(C)}(1\vec{\mathrm{p}}''\to 1\hat{R})+\sigma^{\mathrm{EA}(D)}(1\vec{\mathrm{p}}''\to 1\hat{R})]+\sigma^{\mathrm{EA}(D)}(1\vec{\mathrm{p}}''\to n\hat{R})\ , \tag{5.8}$$

where the elastic eikonal differential cross section involves the eikonal reference differential cross section, Eq. (3.5), the eikonal coupling differential cross section

$$\begin{aligned}\sigma^{\mathrm{EA}(C)}(1\vec{\mathrm{p}}''\to 1\hat{R})=&-\pi^{-1}(p''/\hbar)^2\cos^2(\tfrac{1}{2}\theta)\\ &\times\mathrm{Im}\int_0^{\infty}db'\,b'J_0(2p''b'\sin(\tfrac{1}{2}\theta)/\hbar)\{\exp[-i\sec(\tfrac{1}{2}\theta)\chi_0(b')]-1\}\\ &\times\int d^{(2)}\vec{\mathrm{b}}\exp\{i[p''(\hat{R}-\hat{p}'')\cdot\vec{\mathrm{b}}/\hbar+\sec(\tfrac{1}{2}\theta)\chi_0(b)]\}\\ &\times[\langle 1|G_P^{\mathrm{EA}}(\infty;-\infty)M^{\mathrm{EAC}}(\infty;-\infty)|1\rangle^*-1]\ ,\end{aligned} \tag{5.9}$$

and the elastic distorted eikonal differential cross section

$$\begin{aligned}\sigma^{\mathrm{EA}(D)}(1\vec{\mathrm{p}}''\to 1\hat{R})=&\,(p''/\hbar)^2\cos^2(\tfrac{1}{2}\theta)\\ &\times\Big|(2\pi)^{-1}\int d^{(2)}\vec{\mathrm{b}}\exp\{-i[p''(\hat{R}-\hat{p}'')\cdot\vec{\mathrm{b}}/\hbar+\sec(\tfrac{1}{2}\theta)\chi_0(b)]\}\\ &\times[\langle 1|G_P^{\mathrm{EA}}(\infty;-\infty)M^{\mathrm{EAC}}(\infty;-\infty)|1\rangle-1]\Big|^2\ .\end{aligned} \tag{5.10}$$

Finally, the inelastic eikonal differential cross section is ($n\neq 1$)

$$\begin{aligned}\sigma^{\mathrm{EA}(D)}(1\vec{\mathrm{p}}''\to n\hat{R})=&\,(p''/2\hbar)^2\lambda_{n1}|\lambda_{n1}\hat{R}+\hat{p}''|^2\\ &\times\Big|(2\pi)^{-1}\int d^{(2)}\vec{\mathrm{b}}\exp\{-i[p''(\lambda_{n1}\hat{R}-\hat{p}'')\cdot\vec{\mathrm{b}}/\hbar+2\chi_0(b)/|\lambda_{n1}\hat{R}+\hat{p}''|]\}\\ &\times\langle n|G_Q^{\mathrm{EA}}(\infty;-\infty)M^{\mathrm{EAS}}(\infty;-\infty)|1\rangle\Big|^2\ .\end{aligned} \tag{5.11}$$

Equations (5.10) and (5.11) are equivalent to Eq. (5.2) since no approximations to the internal motion have, as yet, been made.

Two different types of approximation schemes can be applied to these distorted eikonal cross sections. In one, the standard time-independent approach,[1,10] the time scale for internal-state reorientations is assumed to be much larger than the duration of the collision. Thus the sudden approximation to Eq. (3.14) is used to describe the internal-state dynamics. That is, the motion generated by H_{int} is neglected so that the group becomes a simple exponential of the time integral of the potential $V_1(\vec{R}_0(t \mid \vec{b},\vec{P});\vec{X}_{op})$. This approximation is applied to Eq. (5.2). On the other hand, if the time scale for internal-state reorientations is of the order of, or less than, the duration of the collision, then the motion due to H_{int} cannot be neglected. In this case, an approximation scheme[18] based upon Eqs. (5.10) and (5.11) is more appropriate. That is, the memory operators are represented in the time-disordered approximation while a perturbation approximation is applied to the Q space group. Both approximations involve all orders of the potential V_1.

VI. DISCUSSION

Exact expressions for the differential cross section involving two potentials have been presented in terms of time-correlation functions. They were obtained directly from the generalized cross section[19,20] rather than from scattering amplitudes. Since both density operators and wave functions are equivalent descriptions of the scattering event, either one of them could have been used to derive these exact results. The density-operator description was used here since it emphasizes the observables, namely, the cross sections.

Distorted eikonal differential cross sections were obtained in terms of straight-line and reference classical trajectories. Inclusion of curved trajectories in eikonal theory, which is a high-energy semiclassical approximation, is expected to give a better representation of the collision event since the translational motion is treated in a more realistic fashion. It is to be noted that these distorted eikonal cross sections reduce to the standard straight-line eikonal cross section when the reference potential is taken to be zero.

ACKNOWLEDGMENTS

I would like to thank Dr. David Herbert, Professor John S. Dahler, and Professor Robert F. Snider for their help in completing this work.

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