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# Eikonal Approximation for Coupled Equations for Multichannel Scattering<sup>\*</sup>

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It is well known that the Glauber approximation for scattering amplitudes is obtained by applying the eikonal approximation to the Fourier transform of the transition operator. The eikonal approximation can also be applied to the coupled equations of scattering obtained by the expansion of the state function in terms of a suitable set of functions. The scattering amplitude can thus be obtained by solving the set of eikonal coupled equations. The latter approach is analyzed for a special class of channel-coupling potentials. The first-order approximation to the derived eikonal coupled equations is the eikonal Born approximation. Numerical illustrations in this approximation are given for the 1s-2s and 1s-2p excitations of hydrogen atoms by electron and positron impact. The results are compared with those obtained in the Glauber eikonal approximation and with experimental measurements.

#### I. INTRODUCTION

Recently there has been renewed interest in applying the eikonal approximation to atomic and molecular collisions.<sup>1</sup> There are two basically different ways in which the eikonal approximation has been applied to the determination of the collision amplitude for a multichannel many-body system.

The collision amplitude  $\mathcal{T}_{\beta b, \alpha a}$  for a transition  $\alpha a + \beta b$  may be written as

$$\mathcal{T}_{\beta b, \alpha a} = \langle \psi_b^{(\beta)} | V_\beta | \Upsilon_{a\alpha}^{(+)} \rangle ,$$

with

$$\Upsilon_{\alpha a}^{(+)} = \psi_a^{(\alpha)} + G(E+i\eta) V_\alpha \psi_a^{(\alpha)} , \qquad (1.2)$$

$$\psi_{a}^{(\alpha)}(\vec{\mathbf{r}}',\vec{\mathbf{R}}_{\alpha}) = \chi_{a}^{(\alpha)}(\vec{\mathbf{r}}')(2\pi)^{-3/2}e^{i\vec{\mathbf{k}}_{\alpha a}\cdot\vec{\mathbf{R}}_{\alpha}}$$
, (1.3a)

$$\psi_{b}^{(\beta)*}(\vec{\mathbf{r}},\vec{\mathbf{R}}_{\beta}) = \chi_{b}^{(\beta)*}(\vec{\mathbf{r}})(2\pi)^{-3/2}e^{-i\vec{k}_{\beta b}\cdot\vec{\mathbf{R}}_{\beta}} , \qquad (1.3b)$$

$$E = k_{\beta b}^{2} / 2\mu_{\beta} + \epsilon_{b}^{(\beta)} = k_{\alpha a}^{2} / 2\mu_{\alpha} + \epsilon_{a}^{(\alpha)}, \qquad (1.4)$$

where  $\chi_a^{(\alpha)}(\vec{\mathbf{r}}')$  and  $\chi_b^{(\beta)}(\vec{\mathbf{r}})$  are the products of the asymptotic eigenfunctions with eigenvalues  $\epsilon_a^{(\alpha)}$  and  $\epsilon_b^{(\beta)}$ , respectively;  $V_{\alpha}$  and  $V_{\beta}$  are the interaction potentials in channels  $\alpha$  and  $\beta$ , respectively; and  $G(E) = (E - H)^{-1}$  is the Green's function of the system.

The collision amplitude  $T_{\beta b, \alpha a}$  may also be written in terms of transition operator  $T_{\beta \alpha}$ ,

$$\mathcal{T}_{\beta b, \alpha a} = \langle \psi_{b}^{(\beta)} | T_{\beta \alpha} | \psi_{a}^{(\alpha)} \rangle , \qquad (1.5)$$

with

(1.1)

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$$T_{\beta\alpha} = V_{\beta} + V_{\beta}G(E + i\eta)V_{\alpha} \quad . \tag{1.6}$$

Utilizing the asymptotic channel states given by Eqs. (1.3a) and (1.3b), we may rewrite Eq. (1.5) as

$$\boldsymbol{\tau}_{\beta b, \alpha a} = \langle \chi_{b}^{(\beta)}(\mathbf{\tilde{r}}) \mid \boldsymbol{\tau}_{\beta \alpha}(\mathbf{\tilde{r}}, \mathbf{\tilde{r}}') \mid \chi_{a}^{(\alpha)}(\mathbf{\tilde{r}}') \rangle , \qquad (1.7)$$

with

 $\tau_{\alpha\beta}(\vec{\mathbf{r}},\vec{\mathbf{r}}') = (2\pi)^{-3} \int d\vec{\mathbf{R}}_{\alpha} d\vec{\mathbf{R}}_{\beta} \exp(i\vec{\mathbf{k}}_{\alpha a} \cdot \vec{\mathbf{R}}_{\alpha} - i\vec{\mathbf{k}}_{\beta b} \cdot \vec{\mathbf{R}}_{\beta}) \\ \times \langle \vec{\mathbf{r}}\vec{\mathbf{R}}_{\beta} \mid T_{\beta\alpha} \mid \vec{\mathbf{r}}'\vec{\mathbf{R}}_{\alpha} \rangle , \quad (\mathbf{1.8})$ 

where  $\tau_{\alpha\beta}$  is the Fourier transform of the transition operator  $T_{\beta\alpha}$  in the coordinate representation.

The eikonal approximation may be applied to the wave functions  $\psi_b^{(\beta)}$  and  $\Upsilon_{\alpha a}^{(+)}$  in the determination of the collision amplitude from Eq. (1.1). In this approximation, the state function  $\Upsilon_{\alpha a}^{(+)}$  given by Eq. (1.2) is expanded in terms of a suitable set of states and the eikonal approximation is then applied to the coefficient functions of the expansion.<sup>2,3</sup> Such an approach reduces Eq. (1.2) into a set of coupled equations for eikonal amplitudes. The collision amplitude  $\Upsilon_{\beta b,\alpha a}$  can then be determined in terms of the eikonal amplitudes by solving the coupled equations.

The eikonal approximation may also be applied to the Fourier transform of the transition operator given by Eq. (1.8) by treating the integrals of transformation as path integrals.<sup>4,5</sup> The collision amplitude can then be obtained by evaluating the matrix elements given by Eq. (1.7).

The two alternative approaches are equivalent for potential scattering, and they both lead to the well-known Molière expression<sup>6</sup>

$$\mathcal{T}_{\alpha a, \alpha a} = \frac{ik_{\alpha a}}{\mu_{\alpha}(2\pi)^2} \int b \, db \, J_0(k_{\alpha a} \, b\theta)(e^{i\Phi(b)} - 1), \quad (1.9)$$

where  $J_0$  is the Bessel function and  $\Phi(b)$  is the eikonal phase which in the straight-line approximation takes the form

$$\Phi(b) \cong -\left(\mu_{\alpha}/k_{\alpha a}\right) \int_{-\infty}^{\infty} V_{\alpha}(R) dz \quad . \tag{1.10}$$

For a multichannel many-body system, different simplification assumptions are usually made in carrying out the eikonal approximation. The two alternative approaches yield approximate formulas which are different in their range of validity and in their limitations.

The latter approach in which the eikonal approximation is carried out on the Fourier transform of  $T_{\beta\alpha}$  is an operator approach. For the case where the transition operator is local in R,

$$\langle \vec{\mathbf{r}} \, \vec{\mathbf{R}}_{\beta} \left| T_{\beta\alpha} \right| \vec{\mathbf{r}}' \vec{\mathbf{R}}_{\alpha} \rangle = T_{\beta\alpha} \langle \vec{\mathbf{r}}, \vec{\mathbf{r}}', \vec{\mathbf{R}}_{\alpha} \rangle \,\delta(\vec{\mathbf{R}}_{\alpha} - \vec{\mathbf{R}}_{\beta}) ,$$

$$(1.11)^{\circ}$$

we have from Eq. (1.8), with  $\vec{q} \equiv \vec{k}_{\alpha a} - \vec{k}_{\beta b}$ ,

$$\tau_{\beta\alpha}(\vec{\mathbf{r}},\vec{\mathbf{r}}') = (2\pi)^{-3} \int d\vec{\mathbf{R}}_{\alpha} e^{i\vec{\mathbf{t}}\cdot\vec{\mathbf{R}}_{\alpha}} T_{\beta\alpha}(\vec{\mathbf{r}},\vec{\mathbf{r}}',\vec{\mathbf{R}}_{\alpha}).$$
(1.12)

The well-known Glauber approximation is an eikonal approximation to Eq. (1.12) for the  $\alpha = \beta$  case<sup>4</sup>

$$\tau_{\alpha\alpha}(\mathbf{\ddot{r}},\mathbf{\ddot{r}}') \cong \delta(\mathbf{\ddot{r}}-\mathbf{\ddot{r}}') \frac{ik_{\alpha\alpha}}{\mu_{\alpha}(2\pi)^{3}} \times \int d^{2}b \, e^{i\mathbf{\ddot{r}}_{i} \cdot \mathbf{\ddot{r}}} [\exp(i\sum_{j}\Phi_{j})-1], \quad (1.13)$$

where  $\Phi_j$  is the eikonal phase due to pair interaction  $V_{ik}$  and the j sum sums over all the pair interactions which constitute  $V_{\alpha}$ .

The Glauber-type eikonal approximation has recently been applied to atomic collision systems such as  $(e^-, H)$ ,  $(p^*, H)$ ,  $(e^-, He)$ , etc., with surprisingly good results<sup>7-13</sup> in the intermediate energy range. The success has been attributed partly to the fact that the Glauber eikonal approximation provides the correct large-angle dependence of the differential cross section. This large-angle behavior appears to be related to the neglect of the momentum transfer in the incident direction which is one of the characteristic features of the Glauber approximation. The Glauber type of eikonal approximation has recently been generalized by Byron<sup>10</sup> to account for the effect of momentum transfer in the incident direction and channel coupling.

The purpose of the present paper is to investigate the former of the two approaches in which the eikonal approximation is carried out on the state function of the system. After presenting the multichannel eikonal approximation in Sec. II, we investigate its application to atomic collisions. Calculations are carried out for the 2s and 2p ( $e^{\pm}$ , H) excitations. The results are compared with those obtained in the Glauber eikonal as well as other approximations in Sec. III.

#### **II. MULTICHANNEL EIKONAL APPROXIMATION**

In this section, we consider the application of the eikonal approximation to multichannel collision problems at intermediately high energies,

$$E_{\alpha}(\mathbf{a.u.}) \equiv k_{\alpha a}^2/(2\mu_{\alpha}) \gg 1.$$

At these energies there are usually a very large number of channels open. It is clearly unrealistic to expect all the open channels to be treated explicitly. We shall therefore select only a number of channels which are strongly coupled with the particular channel (or channels) under consideration, and defer all the rest of the channels, both open and closed, into a generalized optical potential. Eikonal approximation is then applied to these sets of coupled open-channel equations for the determination of collision amplitude.

#### A. Coupled-Equation Theory

To select the desired channels, we make use of the projection-operator techniques and construct

$$P\Upsilon = \sum_{(\alpha,\alpha)}^{N_0} \chi_a^{(\alpha)} \Psi_{\alpha \alpha}(\vec{\mathbf{R}}_{\alpha}) , \qquad (2.1)$$

where P is a projection operator which selects the  $N_0$  desired open channels from  $\Upsilon$ , and  $\vec{R}_{\alpha}$  are the channel coordinates. We have by construction that

$$P = P^{\dagger} = P^2 \quad . \tag{2.2}$$

Let Q = 1 - P, it then follows from the idempotent property of P that PQ = 0. In terms of P and Q, the Schrödinger equation

$$(E-H)\Upsilon = 0 \tag{2.3}$$

can be rewritten in the Feshbach form<sup>14</sup>

$$(E-\mathcal{K})P\Upsilon = 0 \quad , \tag{2.4}$$

with

$$\Im \mathcal{C} = P\left(H + HQ \frac{1}{E - QHQ + i\eta} QH\right)P , \qquad (2.5)$$

where  $\eta - 0^*$  specifies the physical outgoing boundary.

Substitution of  $P\Upsilon$  into Eq. (2.4) yields, after forming matrix elements in  $\chi_a^{(\alpha)}$ ,

$$(E - K_{\alpha} - \epsilon_{a}^{(\alpha)} - \upsilon_{\alpha a}) \Psi_{\alpha a}(\vec{\mathbf{R}}_{\alpha})$$
$$= \sum_{(\beta b) \neq (\alpha a)}^{N_{0}} \upsilon_{\alpha a, \beta b} \Psi_{\beta b}(\vec{\mathbf{R}}_{\beta}), \quad (2.6)$$

with

$$\mathbf{U}_{\alpha a} = \langle \chi_a^{(\alpha)} | V_{\alpha} + HQ \frac{1}{E - QHQ + i\eta} QH | \chi_a^{(\alpha)} \rangle, \quad (2.7)$$

$$\mathcal{U}_{\alpha a,\beta b} = \langle \chi_b^{(\alpha)} | H + HQ \frac{1}{E - QHQ + i\eta} QH | \chi_b^{(\alpha)} \rangle , \quad (2.8)$$

$$V_{\alpha} = H - K_{\alpha} - H_{\alpha} \quad , \tag{2.9}$$

where  $K_{\alpha}$  is the center-of-mass kinetic-energy operator for the relative motion of the colliding particles in channel  $\alpha$  and  $H_{\alpha}$  is the structure Hamiltonian for  $\alpha$  channel. We have

$$(H_{\alpha} - \epsilon_{a}^{(\alpha)}) \chi_{a}^{(\alpha)} = 0.$$
(2.10)

The coupled equations given by Eq. (2.6) can be rewritten in the Lippmann-Schwinger form given by Eq. (1.2):

$$\Psi_{\beta b}^{(+)} = \delta_{\beta b, \alpha a} \Psi_{c \alpha a}^{(+)} + G_{\beta b} \left( E + i\eta \right) \sum_{(\gamma c) \neq (\beta b)}^{N_0} \upsilon_{\beta b, \gamma c} \Psi_{\gamma c}^{(+)} , \qquad (2.11)$$

with

$$G_{\beta b}(E+i\eta) = (E+i\eta - K_{\beta} - \epsilon_{b}^{(\beta)} - U_{\beta b})^{-1}, \qquad (2.12)$$

where the coherent state  $\Psi_{c\alpha a}^{(+)}$  is defined by<sup>15</sup>

$$(E+i\eta-K_{\alpha}-\epsilon_{a}^{(\alpha)}-\upsilon_{\alpha a})\Psi_{c\,\alpha a}^{(*)}(R_{\alpha})$$
$$=i[\eta/(2\pi)^{3/2}]e^{i\vec{k}_{\alpha a}\cdot\vec{R}_{\alpha}}. \quad (2.13)$$

The scattering amplitude for the  $\alpha a + \beta b$  transition is

$$\mathcal{T}_{\beta b,\alpha a} = \delta_{\beta b,\alpha a} \mathcal{T}_{\alpha a}^{(p)} + \left(\Psi_{c\beta b}^{(-)}, \sum_{(\gamma c) \neq (\beta b)}^{N_0} \upsilon_{\beta b,\gamma c} \Psi_{\gamma c}^{(+)}\right),$$
(2.14)

where  $\mathcal{T}_{\alpha a}^{(p)}$  is the elastic scattering amplitude due to potential  $\mathcal{V}_{\alpha a}$ ,

$$\mathcal{T}_{\alpha a}^{(p)} = ((2\pi)^{-3/2} e^{i\vec{k}} \alpha a^{*\vec{n}} \alpha}, \ \mathcal{U}_{\alpha a} \Psi_{c\alpha a}^{(+)}) . \qquad (2.15)$$

We shall now reduce the transition amplitude  $\mathcal{T}_{\beta b,\alpha a}$ and the function  $\Psi_{\beta b}^{(+)}$  in the eikonal approximation.

#### B. Eikonal Description of Collision

The eikonal approximation will be valid if

$$\hbar/ka_0 \ll 1$$
, (2.16)

where k is the magnitude of the center-of-mass momentum. For energy region  $E_{\alpha} \gg 1$ , the eikonal criterion is always satisfied.

In the eikonal approximation, we have for the wave functions  $^{16}\,$ 

$$\Psi_{c\alpha a}^{(+)} = (2\pi)^{-3/2} A_{\alpha a}(\vec{\mathbf{R}}_{\alpha}) \exp[iS_{\alpha a}^{*}(\vec{\mathbf{R}}_{\alpha})], \qquad (2.17)$$

$$\Psi_{\gamma c}^{(+)} = (2\pi)^{-3/2} B_{\gamma c}(\vec{R}_{\gamma}) \exp[iS_{\gamma c}(\vec{R}_{\gamma})], \qquad (2.18)$$

and the Green's function

$$G_{\beta b}(E+i\eta) = C_{\beta b}(\vec{\mathbf{R}}_{\beta}, \vec{\mathbf{R}}_{\beta}') \exp[iS_{\beta b}(\vec{\mathbf{R}}_{\beta}, \vec{\mathbf{R}}_{\beta}')], \quad (2.19)$$

where the eikonals are defined by the path integrals

$$S_{\alpha a}(\vec{\mathbf{R}}_{\alpha}) = \int^{\vec{\mathbf{R}}_{\alpha}} \vec{\kappa}_{\alpha a}(\vec{\mathbf{R}}_{\alpha}') \, ds, \qquad (2.20)$$

$$S_{\beta b}(\vec{\mathbf{R}}_{\beta}, \vec{\mathbf{R}}_{\beta}') = \int_{\vec{\mathbf{R}}_{\beta}}^{\vec{\mathbf{R}}_{\beta}} \vec{\mathbf{k}}_{\beta b}(\vec{\mathbf{R}}_{\beta}'') ds , \qquad (2.21)$$

with the local momenta given by

$$\vec{\kappa}_{\alpha a} = \left[2\mu_{\alpha}(E - \epsilon \frac{(\alpha)}{a} - \upsilon_{\alpha a})\right]^{1/2} \quad . \tag{2.22}$$

In the energy region of our interest, the eikonal amplitudes in the coherent state  $\Psi_{caa}^{(+)}$  and the Green's function take the approximate forms

$$A_{\alpha a}(\vec{\mathbf{R}}_{\alpha}) \simeq \mathbf{1}, \qquad (2.23)$$

$$C_{\beta b}(\vec{\mathbf{R}}_{\beta}) \cong -(\mu_{\beta}/2\pi) |\vec{\mathbf{R}}_{\beta} - \vec{\mathbf{R}}_{\beta}'|^{-1}$$
 (2.24)

For the evaluation of the amplitude  $\mathcal{T}_{\beta b,\alpha a}$  in the eikonal approximation given by Eqs. (2.17)-(2.24), we shall make several further simplifications. We shall suppose that the eikonal amplitudes  $B_{\gamma c}(R_{\gamma})$ are slowly varying functions of the position and that the path integrals for the eikonals can be evaluated in the straight-line approximation for the classical trajectories. These are reasonable approximations in the  $E_{\alpha} \gg 1$  energy region.

The problem presented in Sec. IIA is a multichannel problem involving the possibility of rearrangement collisions. In addition, the diagonal and off-diagonal interactions are in general complex and nonlocal. To make this problem manageable, we shall make several restrictions. We shall restrict our consideration to cases where if rearrangement channels were contained in  $P\Upsilon$  [see Eq. (2.1)], the coordinates for the rearrangement channel  $R_{\beta}$  should be expressible asymptotically in terms of the scattering-channel coordinate  $R_{\alpha}$ to the order of  $O(R_{\alpha}^{-1})$ , i.e.,

$$R_{\beta} - R_{\alpha} + f(\hat{R}_{\alpha} \cdot \vec{\mathbf{r}}) + O(R_{\alpha}^{-1}) , \qquad (2.25)$$

where  $f(\hat{R}_{\alpha} \cdot \vec{r})$  is a function of the internal coordinates bounded in the  $R_{\alpha} \rightarrow \infty$  limit. This would permit  $P \Upsilon$  to satisfy the asymptotic boundary condition with a common radial coordinate.<sup>17</sup> We shall from now on drop the subscript for R.

The potentials  $\upsilon_{\alpha a}$  are in general nonlocal and complex. We may write

$$U_{\alpha a} = U_{\alpha a}^{(1)} + i U_{\alpha a}^{(2)}$$
 (2.26)

The local momenta given by Eq. (2.22)

$$\vec{\kappa}_{\alpha a} = \vec{\kappa}_{\alpha a}^{(1)} + i \vec{\kappa}_{\alpha a}^{(2)} \quad , \qquad (2.27)$$

with

$$\kappa_{\alpha a}^{(1)} = \mu_{\alpha}^{1/2} \left\{ \left[ (E - \epsilon_{a}^{(\alpha)} - \mathfrak{U}_{\alpha a}^{(1)})^{2} + (\mathfrak{U}_{\alpha a}^{(2)})^{2} \right]^{1/2} + (E - \epsilon_{a}^{(\alpha)} - \mathfrak{U}_{\alpha a}^{(2)})^{1/2} , \quad (2.28a) \right. \\ \left. \kappa_{\alpha a}^{(2)} = \mu_{\alpha}^{1/2} \left\{ \left[ (E - \epsilon_{a}^{(\alpha)} - \mathfrak{U}_{\alpha a}^{(1)})^{2} + (\mathfrak{U}_{\alpha a}^{(2)})^{2} \right]^{1/2} \right]^{1/2} \right\}$$

$$- (E - \epsilon_a^{(\alpha)} - \mathfrak{U}_{\alpha a}^{(2)}) \}^{1/2} . \quad (2.28b)$$

This allows the eikonal to be written as  $S_{\alpha a} = S_{\alpha a}^{(1)} + i S_{\alpha a}^{(2)}$  with the path integrals for  $S_{\alpha a}^{(1)}$  and  $S_{\alpha a}^{(2)}$  expressed in terms of  $\vec{k}_{\alpha a}^{(1)}$  and  $\vec{k}_{\alpha a}^{(2)}$ , respectively. In the energy region of our interest, we have

$$\kappa_{\alpha a}^{(1)} = \left[ 2\mu (E - \epsilon_{\alpha}^{(a)} - U_{\alpha a}^{(1)}) \right]^{1/2} + \left\{ 2\mu \left[ E + (U_{\alpha a}^{(2)}/2E)^2 \right] \right\}^{1/2} + \cdots \qquad (2.29)$$

We shall assume that both the imaginary potential  $\upsilon_{\alpha\alpha}^{(2)}$  and the nonlocal part of  $\upsilon_{\alpha\alpha}^{(1)}$  are small in comparison with the local part of  $\upsilon_{\alpha\alpha}^{(1)}$ , and define the classical trajectory in terms of the local part of  $\upsilon_{\alpha\alpha}^{(1)}$ , if we desire to go beyond the straight-line approximation for the classical trajectories.

We shall further restrict our consideration to cases where the interaction can be written in the form  $^{18}\,$ 

$$\mathcal{U}_{\alpha a} = \mathcal{U}_{\alpha a} e^{i\lambda_{\alpha a}\varphi} \quad , \tag{2.30}$$

$$\upsilon_{\beta b,\alpha a} = \mathfrak{u}_{\beta b,\alpha a} e^{i\lambda_{\beta b,\alpha a}\varphi} , \qquad (2.31)$$

where  $\mathfrak{U}_{\alpha a}$  and  $\mathfrak{U}_{\beta b, \alpha a}$  are cylindrically symmetri-

cal and  $\varphi$  is the azimuthal angle with respect to the incident direction.

### C. Eikonal Coupled Equations

We now apply the eikonal approximation of Sec. II B to the determination of the scattering amplitude. To simplify our notations we shall denote the subscript  $\alpha a$  and  $\beta b$  simply by  $\alpha$  and  $\beta$ , respectively. We may think that the channel indices  $\alpha$  and  $\beta$  are being renumbered to include the description of internal states a and b.

In the eikonal approximation, we have

$$G_{\beta} \mathcal{U}_{\beta\gamma} \Psi_{\gamma}^{(\star)} = - \frac{\mu_{\beta}}{(2\pi)^{5/2}} \int d\vec{\mathbf{R}}' \frac{\mathcal{U}_{\beta\gamma} B_{\gamma}}{|\vec{\mathbf{R}} - \vec{\mathbf{R}}'|} \times \exp\{i[S_{\gamma}(\vec{\mathbf{R}}') + S_{\beta}(\vec{\mathbf{R}}, \vec{\mathbf{R}}')]\}, \quad (2.32)$$

where we have utilized Eqs. (2.18), (2.19), and (2.24). Equation (2.32) can be evaluated in the straight-line approximation to give<sup>3</sup>

$$G_{\beta} \mathcal{U}_{\beta\gamma} \Psi_{\gamma}^{(+)} \simeq - \frac{i e^{i S_{\beta}(\vec{R})}}{(2\pi)^{3/2}} \int_{-\infty}^{z} dz' \Lambda_{\beta\gamma} B_{\gamma}(z', b) , \qquad (2.33)$$

with

$$\Lambda_{\beta\gamma}(z', b) = v_{\gamma}^{-1} \mathfrak{U}_{\beta\gamma}(z', b) e^{-i\phi_{\beta\gamma}(z', b)}, \qquad (2.34)$$

$$\phi_{\beta\gamma}(z', b) \equiv S_{\beta}(\vec{\mathbf{R}}') - S_{\gamma}(\vec{\mathbf{R}}') \quad , \qquad (2.35)$$

where b is the impact parameter and  $v_{\gamma} = k_{\gamma}/\mu_{\gamma}$ . If  $\mathfrak{U}_{\beta\gamma}$  are nonlocal in position, the integrand in the z' integral in Eq. (2.33) would then be an integral itself. In this case, the z' integral as well as Eqs. (2.34) and (2.35) should be modified accordingly.

Substitution of Eq. (2, 33) back into Eq. (2, 11) gives

$$\Psi_{\beta}^{(+)} = \delta_{\beta\alpha} \Psi_{c\alpha}^{(+)} - \frac{i}{(2\pi)^{3/2}} e^{i S_{\beta}(\vec{R})} \sum_{\gamma \neq \beta} Q_{\beta\gamma}(z, b) , \qquad (2.36)$$

with

$$Q_{\beta\gamma}(z, b) = \int_{-\infty}^{z} dz' \Lambda_{\beta\gamma}(z', b) B_{\gamma}(z', b) . \qquad (2.37)$$

With the help of Eqs. (2.17), (2.18), and (2.23), Eq. (2.36) reduces to

$$B_{\beta}(z, b) = \delta_{\beta\alpha} - i \sum_{\gamma \neq \beta}^{N_0} Q_{\beta\gamma}(z, b) . \qquad (2.38)$$

Utilizing Eqs. (2.38) and (2.37) and differentiating the resultant with respect to z, we obtain the eikonal coupled equations

$$\frac{dQ_{\beta\beta'}}{dz} = \Lambda_{\beta\beta'} \,\delta_{\beta'\alpha} - i\Lambda_{\beta\beta'} \sum_{\gamma\neq\beta'}^{N_0} Q_{\beta'\gamma} \quad . \tag{2.39}$$

For the special case where the potentials have cylindrical symmetry (i.e.,  $\lambda_{\alpha\alpha} \equiv \lambda_{\alpha} = 0$  and  $\lambda_{\alpha\beta} = 0$ ), it is not necessary to calculate each  $Q_{\beta\beta}$ , for the determination of  $\mathcal{T}_{\beta\alpha}$  [see Eq. (2.43)]. It is then convenient to define  $Q_{\beta}$ :

$$Q_{\beta} = \sum_{\beta' \neq \beta} Q_{\beta\beta'} \quad . \tag{2.40}$$

Equation (2.39), after summing over  $\beta'$ , can be written in the form

$$\frac{dQ_{\beta}}{dz} = \Lambda_{\beta\alpha} (1 - \delta_{\beta\alpha}) - i \sum_{\gamma \neq \beta} \Lambda_{\beta\gamma} Q_{\gamma} \quad . \tag{2.41}$$

These are the coupled equations derived in Ref. 3.

The transition amplitude  $\mathcal{T}_{\beta\alpha}$  can be expressed in terms of  $Q_{\beta\alpha}$ . Substitution of the eikonal wave functions in Eq. (2.14) yields

$$\mathcal{T}_{\beta\alpha} = \delta_{\beta\alpha} \mathcal{T}_{\alpha}^{(\beta)} + (2\pi)^{-3} \sum_{\gamma\neq\beta}^{N_0} \int d\mathbf{\vec{R}} B_{\gamma} \mathcal{U}_{\beta\gamma} e^{i(S_{\gamma}-S_{\beta})}.$$
(2.42)

Again expressing the volume element  $d\vec{R}$  in terms of the cylindrical polar coordinates, the path integral can be evaluated to give

$$\mathcal{T}_{\beta\alpha} = \delta_{\beta\alpha} \mathcal{T}_{\alpha}^{(p)} + (2\pi)^{-2} \sum_{\gamma \neq \beta}^{N_0} v_{\gamma}(-i)^{\lambda_{\beta\gamma}} \\ \times \int_0^\infty b db J_{\lambda_{\beta\gamma}} (k_\beta b \sin\theta) Q_{\beta\gamma}(b) e^{i \Phi_{\beta}(b)} ,$$
(2.43)

with

$$Q_{\beta\gamma}(b) = \lim Q_{\beta\gamma}(z, b) \quad \text{as } z \to \infty , \qquad (2.44)$$

$$\Phi_{\beta}(b) = k_{\beta} \int_{-\infty}^{\infty} dz \left[ 1 - (1 - 2\mu_{\beta} \mathfrak{U}_{\beta}/k_{\beta}^2)^{1/2} \right], \quad (2.45)$$

where the elastic scattering amplitude due to potential  $\mathcal{U}_{\beta}$  can in the eikonal approximation be written in the Molière form [see Eq. (1.9)]

$$\mathcal{T}_{\alpha}^{(p)} = -(-i)^{\lambda_{\alpha\alpha}+1} \frac{v_{\alpha}}{(2\pi)^2} \int b \, db \, J_{\lambda_{\alpha\alpha}}(k_{\alpha} b \, \sin\theta) \\ \times (e^{i\Phi_{\alpha}(b)} - 1) \, . \quad (2.46)$$

The total elastic scattering amplitude then takes the form

$$\mathcal{T}_{\alpha\alpha} = -(-i)^{\lambda_{\alpha\alpha}+1} \frac{v_{\alpha}}{(2\pi)^2} \int b \, db \, J_{\lambda_{\alpha\alpha}}(k_{\alpha}b\,\sin\theta) \\ \times \left\{ e^{i\Phi_{\alpha}(b)} \left[1 - i\Gamma_{\alpha}(b)\right] - 1 \right\}, \quad (2.47)$$

with

$$\Gamma_{\alpha}(b) = \sum_{\gamma \neq \alpha}^{N_{0}} (-)^{\lambda} \alpha \gamma^{-\lambda} \alpha \alpha} \frac{v_{\gamma} J_{\lambda \alpha \gamma}(k_{\alpha} b \sin \theta)}{v_{\alpha} J_{\lambda \alpha \alpha}(k_{\alpha} b \sin \theta)} Q_{\alpha \gamma}(b) ,$$
(2.48)

where  $i\Gamma_{\alpha}(b)$  accounts for dynamic coupling with all the open channels which are included in  $P\Upsilon$ given by Eq. (2.11).

## III. APPLICATION TO $(e^{\pm}, H)$ EXCITATION SCATTERING

In this section, we consider the application of the eikonal approximation to atomic scatterings. Applications of the eikonal approximation in the Molière form [see Eq. (1.9)] to atom-atom scatterings have been made for elastic and resonant electron-transfer processes with reasonable success even at energies where the classical description fails.<sup>19</sup> The modified Molière expression for complex-potential scattering [Eq. (2.46)] has been recently applied to the resonant electron-transfer and electron-detachment (H, H<sup>-</sup>) collisions<sup>20</sup> and to the elastic  $(e^-, He)$  scatterings.<sup>21</sup> We now consider the application of eikonal approximation to excitation scatterings using Eqs. (2, 39) and (2, 43). We take the 1s-2s and 1s-2p excitation of H atoms by electron and positron impact as our examples. Applications of the Glauber eikonal approximation [Eqs. (1.7) and (1.13)] to these excitations have recently been made.<sup>8,9</sup> This would provide a constructive comparison. In this paper, we report the results obtained in the eikonal Born approximation which is the first-order approximation to Eqs. (2, 39) and (2, 43). The results obtained in solving the 1s-2s-2p coupled eikonal equations will be reported in a subsequent paper.

For nonrelativistic electron-atom scattering in which the spin of the target atom is conserved, the exchange scattering contribution is negligible in comparison with the direct scattering contribution at  $E_{\alpha} \gg 1$ . The exchange contribution to the  $(e^{-}, H)$  excitation scattering has recently been cal-



FIG. 1. Angular dependence of the  $n=1 \rightarrow n=2$  differential excitation cross section of hydrogen atoms by electron impact at 50 eV. Experimental data (O) and ( $\Delta$ ) are those of Williams (Ref. 23) normalized at  $\theta = 20^{\circ}$  to the first-order Born and the Glauber eikonal values (Refs. 8 and 9), respectively. The 1s-2s-2p close-coupling results is evaluated at 54 eV (Ref. 24).

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FIG. 2. Angular dependence of the  $n=1 \rightarrow n=2$  differential excitation cross section of hydrogen atoms by electron impact at 100 eV. Experimental data (O and  $\Delta$ ) are those of Williams (Ref. 23) normalized at  $\theta = 21^{\circ}$  to the first-order Born and the Glauber eikonal values (Refs. 8 and 9), respectively.



FIG. 3. Angular dependence of the  $n=1 \rightarrow n=2$  differential excitation cross section of hydrogen atoms by electron impact at 200 eV. Experimental data (O) and ( $\Delta$ ) are those of Williams (Ref. 23) normalized at  $\theta = 21^{\circ}$  to the first-order Born and the Glauber eikonal values (Refs. 8 and 9), respectively.

culated in the eikonal approximation and found to be indeed negligible.<sup>22</sup> If we further neglect the coupling between the 2s and 2p final states, the 1s-2sand 1s-2p excitations may be treated in the twostate approximation.

We have from Eq. (2.43) the excitation amplitude

$$\begin{aligned} \hat{F}_{\beta\alpha} &= (-i)^{\lambda_{\beta\alpha}} \frac{v_{\alpha}}{(2\pi)^2} \\ &\times \int_0^\infty b \, db \, J_{\lambda_{\beta\alpha}}(k_{\beta}b\,\sin\theta) Q_{\beta\alpha}(b) e^{i\Phi_{\beta}(b)} , \quad (3.1) \end{aligned}$$

where the function  $Q_{\beta\alpha}(b)$  is the solution of the pair coupled equations obtained from Eq. (2.39):

$$\frac{dQ_{\beta\alpha}(z, b)}{dz} = \Lambda_{\beta\alpha} - i\Lambda_{\beta\alpha}Q_{\alpha\beta}(z, b), \qquad (3.2a)$$

$$\frac{dQ_{\alpha\beta}(z,b)}{dz} = -i\Lambda_{\alpha\beta}Q_{\beta\alpha}(z,b) .$$
 (3.2b)

If the back coupling is neglected,  $Q_{\beta\alpha}$  then takes the approximate form

$$Q_{\beta\alpha}(z, b) \cong \frac{1}{v_{\alpha}} \int_{-\infty}^{z} \mathfrak{U}_{\beta\alpha}(z', b) e^{-i\phi_{\beta\alpha}(z', b)} dz', \quad (3.3)$$



FIG. 4. Comparison of the angular dependence of the  $1_S \rightarrow 2_S$  and  $1_S \rightarrow 2_P$  differential excitation cross sections of hydrogen atoms by positron impact with that by electron impact at 50 eV in the first-order Born, eikonal Born, and Glauber eikonal (Refs. 8 and 9) approximations.



FIG. 5. Comparison of the angular dependence of the 1s-2s and 1s-2p differential excitation cross section of hydrogen atoms by positron impact with that by electron impact at 100 eV in the first-order Born, eikonal Born, and Glauber eikonal (Refs. 8 and 9) approximations.

where we have made use of Eq. (2.34).

In the straight-line approximation, the phase  $\phi_{\beta\alpha}(z', b)$  takes the form<sup>3</sup>

$$-\phi_{\beta\alpha}(z, b) \cong z(k_{\alpha} - k_{\beta}\cos\theta) + \delta\Phi_{\beta\alpha}(z, b) + \frac{1}{2} [\Phi_{\alpha}(b) - \Phi_{\beta}(b)], \quad (3.4)$$

with

$$\delta \Phi_{\beta\alpha}(z, b) = -\int_0^z (v_\alpha^{-1} \mathfrak{u}_\alpha - v_\beta^{-1} \mathfrak{u}_\beta) dz' \quad . \tag{3.5}$$

We then obtain the eikonal Born approximation

$$\mathcal{T}_{\beta\alpha}^{(B)} = (-i)^{\lambda_{\beta\alpha}} (2\pi)^{-2} \int_0^\infty b \, db \, J_{\lambda_{\beta\alpha}}(k_\beta b \sin\theta) Q_{\beta\alpha}^{(B)}(b) \\ \times \exp\{i[\Phi_\alpha(b) + \Phi_\beta(b)]/2\}, \qquad (3.6)$$

with

$$Q_{\beta\alpha}^{(B)}(b) = \int_{-\infty}^{\infty} \mathfrak{U}_{\beta\alpha}(z, b) \exp[i(k_{\alpha} - k_{\beta}\cos\theta)z + i\delta_{\beta\alpha}(z, b)]dz . \quad (3.7)$$

Equations (3.6) and (3.7) improve the usual distorted-wave Born approximation by providing a more careful analysis of the phase relations between the two states in the eikonal approximation.

Calculation for the 1s-2s and 1s-2p excitation are carried out using Eqs. (3.6) and (3.7). In this calculation, we have taken  $\mathcal{V}_{\alpha}$  to be the 1s static potential,  $\mathcal{V}_{\beta}$  to be the 2s or 2p static potential, and  $\mathcal{V}_{\alpha\beta}$  to be the static 1s-2s of 1s-2p coupling potential. The quantity  $\lambda_{\beta\alpha}$  [see Eq. (2.33)] is 0 for the 1s-2s and 1s-2p<sub>0</sub> and 1 for 1s-2p<sub>±1</sub> coupling potentials. Comparisons of the eikonal Born results so obtained with other theoretical results as well as with available experimental measurements are presented in graphic forms.

In Figs. 1-3, the angular dependence of the n = 2 differential excitation cross section is compared with experimental observation<sup>23</sup> for three incident electron energies. For comparison we have included in these figures the results obtained in the first-order Born and the Glauber eikonal approximations. The absolute magnitude of the experimental cross section is determined by normalizing the data with the results obtained both in the Glauber eikonal and the first-order Born approximation at a scattering angle of  $20^{\circ}$  for  $E_{\alpha} = 50$  eV and  $21^{\circ}$  for  $E_{\alpha} = 100$  and 200 eV. Based on the normalization to the first-order Born approximation, it is seen that the eikonal Born approxima-



FIG. 6. Comparison of the angular dependence of the 1s-2s and 1s-2p differential excitation cross section of hydrogen atoms by positron impact with that by electron impact at 200 eV in the first-order Born, eikonal Born, and Glauber eikonal (Refs. 8 and 9) approximations.



FIG. 7. Details of the 1s - 2p differential excitation cross section of hydrogen atoms by positron and electron impact at 100 eV in the eikonal Born approximation.

tion provides a significant improvement over the first-order Born approximation. However, based on the normalization to the Glauber eikonal approximation, the eikonal Born approximation does not provide an over-all angular dependence as accurately as the Glauber eikonal approximation.<sup>8,9</sup> This is particularly true for scattering angles greater than those shown in these figures. Since the Glauber eikonal approximation yields total cross sections which are in closer agreement with experiment than does the first-order Born approximation at energy below 200 eV, the normalization to Glauber eikonal approximation seems to be preferable.<sup>24</sup> In Fig. 1, we have also included the results of Scott<sup>25</sup> at 54 eV obtained in the 1s-2s-2p close-coupling approximation supplemented by the values of the first-order Born approximation for the higher angular momentum states.

The failure of the eikonal Born approximation for large-scale scattering is expected in view of the straight-line approximation. The formulas derived in this paper are for small-angle scatterings. To extend the present treatment to largeangle scattering, one must follow the classical trajectory more closely. A variational technique based on the "principle of least action" for the

\*Research supported in part by the National Science Foundation Grant No. GP-20459, by the Atomic Energy calculation of the classical trajectory has been developed.  $^{16}\,$ 

In the Glauber eikonal approximation, the classical trajectories are also taken to lie along straight lines. The surprisingly good large-angle results of the Glauber eikonal approximation is a consequence of dropping the momentum transfer along the incident direction.<sup>26</sup> It can be shown that the longitudinal momentum transfer would give rise to a  $(k_{\alpha} - k_{\beta} \cos \theta) z$  term in the z integral along the straight-line trajectories similar to Eq. (3.7). The presence of such a term in the z integral has the effect of damping the scattering amplitude. This damping increases with increasing  $\theta$ . By neglecting the longitudinal momentum transfer, this damping is removed and consequently the scattering amplitude is increased, particularly at large angles. This increase then partially compensates the errors introduced by the straight-line approximation and yields results which are in better agreement with the observed large-angle behavior.

One of the interesting features of the eikonal Born approximation lies in its ability to distinguish the positron scattering from the electron scattering; a feature both the first-order Born and the Glauber eikonal approximations fail to have. In Figs. 4-6, the angular dependence of the 1s-2s and 1s-2p differential excitation cross section of H atoms by positron impact is compared with that by electron impact in the eikonal Born approximation. The results for positron impact are idential to that for electron impact in the first-order Born and the Glauber eikonal approximations. The 1s-2p results shown in these figures are the sum of the  $1s - 2p_0$  and  $1s - 2p_{\pm 1}$  results. The individual  $1s-2p_0$  and  $1s-2p_{\pm 1}$  contributions at 100 eV are shown in Fig. 7. The failure of the Glauber eikonal approximation to distinguish the positron scattering from the electron scattering is also a consequence of neglecting the momentum transfer along the incident direction. This would also be true for the eikonal Born approximation given by Eqs. (3.6) and (3.7) if the term  $(k_{\alpha} - k_{\beta}\cos\theta)z$  coming from the momentum transfer along the incident direction is dropped in Eq. (3.7), since then it can be shown that  $|\mathcal{T}_{\beta\alpha}^{(B)}|^2$  would not be dependent on the sign of the eikonal phases. Consequently, it is no longer capable of distinguishing the positron scattering from the electron scattering. In the work of Byron<sup>10</sup> the z component of momentum transfer was retained in the Monte Carlo calculation for the total cross section. A difference between the positron and electron scattering was found.

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