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# Large-angle inelastic electron-hydrogen scattering in the Glauber approximation*

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Large-angle inelastic scattering is considered using the Glauber approximation for the scattered wave function, but without the additional approximation of purely transverse linear momentum transfer. At large angles, the electron-proton interaction dominates and has Rutherford $q^{-4}$ behavior. Furthermore, with the direction of $\vec{q}$ unrestricted the Ly-$\alpha$ radiation is found to be, in general, elliptically polarized.

## I. INTRODUCTION

Previous authors[1,2] have discussed the advantanges of the Glauber[3] approximation for calculating total and differential electron-hydrogen cross sections for both elastic and inelastic scattering.

The Glauber scattering amplitude is one in which the exact scattered wave function $\Psi_{\vec{K}}^{+}$ is replaced by a phase-distorted plane wave, the distortion being calculated approximately according to

$$\Psi_{\vec{K}}^{+} \simeq \exp\left[i\left(\vec{K}\cdot\vec{R} - (\hbar v)^{-1}\int_{-\infty}^{z} V(\vec{R},\vec{r})\, dz\right)\right] u_i(\vec{r}) , \tag{1}$$

where $V(\vec{R},\vec{r})$ is the interaction potential between the incident particle and the target, $\vec{R}$ is the coordinate of the incident electron, $\vec{r}$ is the coordinate of the atomic electron, and $u_i(\vec{r})$ is the ground-state wave function. This approximation to $\Psi_{\vec{K}}^{+}$ resembles the eikonal approximation for an electron scattered by a static potential $V(\vec{R},\vec{r})$, in the approximation that the electron is scattered through small angles. It thus neglects, in zeroth order, large-angle elastic scattering and all inelastic scattering. Such processes can, of course, be calculated in first order using Eq. (1) as a zeroth-order approximation to $\Psi_{\vec{K}}^{+}$. This will be appropriate provided Eq. (1) is a good approximation to the exact wave function in the regions of space most heavily weighted in the matrix element

$$F(\vec{K}',\vec{K}) = (\Phi_{\vec{K}'}^{+} \,|\, V \,|\, \Psi_{\vec{K}}^{+}) , \tag{2}$$

where $\Phi_{\vec{K}'}^{+} = e^{i\vec{K}'\cdot\vec{R}} u_f(\vec{r})$. Note here that Eq. (2) places no restrictions on $\vec{K}'$ or $\vec{K}$, i.e., Eq. (2) can be used to calculate inelastic scattering amplitudes or large-angle elastic scattering.

Since Eq. (2) places no restrictions on the values that $\vec{K}'$ and $\vec{K}$ can have, the momentum transfer $\vec{q} = \vec{K} - \vec{K}'$ can be quite large, indeed it may be comparable to $\vec{K}$, and Eq. (2) will still be a good approximation provided that the scattering is dominated by the small-angle elastic contributions, which are well described in zeroth-order by Eq. (1), or by small-angle inelastic scattering in which the energy loss of the incident particle is small compared to its initial energy. This feature is common to both the Glauber approximation and the Born theory, where the zeroth-order approximation to $\Psi_{\vec{K}}^{+}$ incorporates no scattering at all.

The original formulation[3] of the Glauber theory also incorporated an additional approximation, namely, the assumption that $\vec{q}$ was perpendicular to $\vec{K}$. This approximation is only valid for small-angle elastic scattering and very-high-energy intermediate-angle inelastic scattering, considerably restricting the range of applicability of the theory. Indeed, the restricted Glauber approximation including this latter approximation does not apply to zero-degree inelastic scattering although the Born theory does. Substantial mathematical simplifications follow from this assumption; thus various prescriptions have been given for extending the Glauber amplitude to large angles, while keeping the mathematical simplicity of the restricted Glauber approximation. The simplest extension is to choose the axis of integration $\hat{z}$ in the phase factor so that $\vec{q}\cdot\hat{z} = 0$. Only this choice gives substantial overlap of the conventional Glauber approximation with the Born.[4] While this extension is quite reasonable in that it forces agreement with the Born at high energy and fixed momentum transfer but preserves the mathematical simplicity of the restricted approximation, it has its own unsatisfactory features. Firstly, the approximate wave function Eq. (1) requires that $\hat{z}$ lie along $\vec{K}$, thus $\vec{q}\perp\hat{z}$ is in general inconsistent with Eq. (1). However, more general eikonal approximations might be used to justify the condition $\vec{q}\perp\hat{z}$ but it is difficult to see how $\vec{q}\perp\hat{z}$ can be justified for zero-degree inelastic scattering, where $\vec{K}$, $\vec{q}$, and $\vec{K}'$ are collinear. Here the axis of integration is perpendicular to any reasonable trajectory of scattered particle. Secondly, and more important-ly, some unrealistic physical consequences concerning the polarization and distribution of decay radiation result from the symmetry of the Glauber transition amplitude, which does not seem to have a sound physical basis.

With the assumption that $\vec{q}\cdot\hat{z}=0$, we may integrate the amplitude Eq. (2) by parts to obtain[3]

$$F(i\to f,\vec{q})=(iK/2\pi)\langle u_f(\vec{r})\,|\,\Gamma(\vec{r})\,|\,u_i(\vec{r})\rangle, \tag{3}$$

where $\Gamma(\vec{r})$ is the Glauber transition operator,

$$\Gamma(\vec{r})=\int\left\{1-\exp\left(i(\hbar v)^{-1}\int_{-\infty}^{+\infty}V(\vec{b},\vec{r},z)\,dz\right)\right\}\times e^{i\vec{q}\cdot\vec{b}}\,d^2b\,, \tag{4}$$

and $\vec{b}$ is the projection of $\vec{R}$ on $\vec{q}$. The transition operator is invariant under two reflections: reflections in a plane perpendicular to $\vec{K}\times\vec{K}'$ and reflections in a plane perpendicular to $\hat{z}$. The first symmetry is a symmetry of the exact transition operator whereas the second is a consequence of assuming $\vec{q}\cdot\hat{z}=0$. This additional symmetry has significant physical consequences, in particular it implies that electron-excited Ly-$\alpha$ radiation detected in coincidence with the scattered electron is linearly polarized perpendicular to $\hat{z}$ and has no circular polarization. Section III B discusses this point in more detail.

Since these various unsatisfactory features stem from choosing an axis of integration $\hat{z}$ perpendicular to $\vec{q}$, rather than any inherent unsuitability of the approximate wave function itself, it seems of interest to investigate Eq. (1) without the additional restriction $\vec{q}\cdot\vec{K}=0$ or the arbitrary reorientation of the original axis of integration. The unrestricted Glauber approximation will automatically agree with the Born for large $K$ but fixed $q$. Byron[5] has carried out such an investigation by evaluating the six-dimensional integral in Eq. (2) directly by Monte Carlo techniques. His numerical results show no marked improvement over the conventional approximation,[2,4] but it seems to us that the unrestricted approximation warrants further investigation, particularly since it may yield some circular polarization of decay radiation which the Born and the conventional approximation cannot.

We have therefore investigated the scattering amplitude Eq. (2) with the approximate wave function Eq. (1), but without the additional assumption $\vec{q}\cdot\hat{z}=0$. We find that the six-dimensional integral in Eq. (2) may be written in terms of a two-dimensional integral suitable for numerical integration. We do not carry out the numerical integrations here, rather we concentrate on the formal aspects of this modification to the Glauber approximation.

The circular polarization of electron-excited radiation is parametrized by the expectation value of $\vec{L}$ on the state function[6]

$$\Psi=\sum_m F_m u_m(\vec{r})\,, \tag{5}$$

where $F_m$ is the scattering amplitude for exciting the magnetic substate described by the wave function $u_m$. Now $(\Psi\,|\,\vec{L}\,|\,\Psi)$ must vanish if all the amplitudes in Eq. (5) are relatively real. Since the approximate wave function Eq. (1) is phase-distorted and since the distortion factor singles out the $z$ axis, we expect that this distortion will manifest itself by an $m$-dependent phase factor in Eq. (2), with a consequent nonzero value for $(\Psi\,|\,\vec{L}\,|\,\Psi)$. Since $(\Psi\,|\,\vec{L}\,|\,\Psi)$ relates to the circular polarization of the collision-excited light, this general prediction of our modified Glauber approximation can be experimentally studied. The experimental significance of $(\Psi\,|\,\vec{L}\,|\,\Psi)$ will be discussed more completely in Sec. III.

A second aspect of the Glauber theory, which we consider here, is large-angle inelastic scattering. Thomas and Gerjuoy[7] find that the large-angle (large $\vec{q}$) $1s\to 2s$ inelastic scattering cross section varies as $q^{-4}$, i.e., it varies as the Rutherford cross section. In contrast their $1s\to 2p$ cross section varies as $q^{-6}$ for large $q$. Both cross sections are considerably larger than the Born. Their enhancement was attributed by Tai *et al.*[2] to electron-proton interaction effects in Eq. (2), which are present in the Glauber approximation, but not in the Born.

This interpretation seems reasonable, but cannot be verified directly, since Eqs. (3) and (4) for the Glauber transition amplitude do not permit separate evaluation of the corresponding electron-proton and electron-electron interaction matrix elements $(\Phi_{\vec{K}'}\,|\,V_{ep}\,|\,\Psi_{\vec{K}})$ and $(\Phi_{\vec{K}'}\,|\,V_{ee}\,|\,\Psi_{\vec{K}})$ in Eq. (2), where $V_{ep}$ and $V_{ee}$ are the electron-proton and electron-electron interaction potentials and $V$ is the sum $V=V_{ep}+V_{ee}$. We find that with the assumption $q_z=0$ and with our order of performing the integration in Eq. (2) these separate integrals diverge and only the matrix element of the total interaction potential converges to give the result obtained by Thomas and Gerjuoy.

We find, however, that with $q_z\neq 0$ the separate integrals converge, and upon evaluating them for large-angle $1s$-$2p$ scattering to first order in inverse powers of $q^2$ that the only non-negligible term varies as $q^{-2}$ and arises from the electron-proton interaction, thus indicating that this term dominates the large-angle inelastic scattering. Hence we find the cross section for exciting the $2p$ states has $q^{-4}$ dependence as opposed to the $q^{-6}$ dependence of the conventional Glauber result.

The following is an outline of this paper. Section

II sketches the derivation of the double-integral expression for the scattering amplitude, which for $q_z = 0$ reduces to Eq. (28a) of Ref. 7. Section III sketches the method of approximately evaluating the integrals for large-angle scattering with arbitrary excitation and presents the results for large-angle scattering with $2p$ excitation. Section IV summarizes the principal results of this paper.

## II. DERIVATION OF INTEGRAL EXPRESSION

### A. General form

Our modified Glauber approximation to the scattering amplitude for an electron colliding with a hydrogen atom in initial state $i$ and exciting it to final state $f$ is[3]

$$F(i \to f, \vec{q}) = (-2m/4\pi\hbar^2) \int e^{i\vec{q}\cdot\vec{R}} V(\vec{R}, \vec{R}') \times \exp\left[(-i/\hbar v) \int_{-\infty}^{Z} V\,dz\right] u_f^* u_i \, d\vec{R}\, d\vec{r}, \quad (6)$$

with

$$V(\vec{R}, \vec{R}') = e^2(1/R' - 1/R), \quad (7)$$

where $m\vec{v} = \hbar\vec{K}$ is the incident electron's momentum, $\vec{R}$ and $\vec{r}$ are the coordinates (relative to the nucleus) of the incident and bound electrons, respectively, $\vec{R}' = \vec{R} - \vec{r}$, $\vec{q}$ is the momentum transfer $\vec{K} - \vec{K}'$, and $u_i$ and $u_f$ are the initial and final hydrogen bound states. Here $\hat{z}$ is parallel to $\vec{K}$.

In order to evaluate Eq. (6) for arbitrary hydrogenic states we replace $u_f^* u_i$ with the expression

$$C_{fi} \exp(-\mu r + i\vec{\gamma}\cdot\vec{r}). \quad (8)$$

Any product of the bound-state wave functions can be represented ($C_{fi}$ is the appropriate normalization constant) by a linear combination of terms generated by differentiating Eq. (8) with respect to $\mu$ and the components of $\vec{\gamma}$ after which $\vec{\gamma}$ is set equal to zero. Hence the scattering amplitude Eq. (6) can be written as

$$F(i \to f, \vec{q}) = (-2m/4\pi\hbar^2) C_{fi} D(\mu, \vec{\gamma}) \left\{ \int (e^{i\vec{q}\cdot\vec{R}} V(\vec{R}, \vec{R}') \exp\left[(-i/\hbar v) \int_{-\infty}^{Z} V\,dz\right] \exp(-\mu r + i\vec{\gamma}\cdot\vec{r})\, d\vec{R}\, d\vec{r} \right\}_{\gamma=0}, \quad (9)$$

where $D(\mu, \vec{\gamma})$ is the differential operator which generates the required wave functions when operating on Eq. (8). The conventional Glauber scattering amplitude can be obtained from Eq. (9) by setting $q_z = 0$.

Inserting the explicit form Eq. (7) for $V(\vec{R}, \vec{R}')$ and evaluating the integral in the phase factor of Eq. (9) gives the result

$$F(i \to f, \vec{q}) = (-K\eta/2\pi) C_{fi} D(\mu, \vec{\gamma}) \left\{ \int e^{i\vec{q}\cdot\vec{R}} (1/R' - 1/R) \exp[i\eta \ln(R' - Z') - i\eta \ln(R - Z)] \times \exp(-\mu r + i\vec{\gamma}\cdot\vec{r})\, d\vec{R}\, d\vec{r} \right\}_{\gamma=0}, \quad (10)$$

where $\eta = e^2/\hbar v$. If $\eta$ is given a small imaginary part $i\delta$, then using the definition of the gamma function[8] we may write

$$\exp[i\eta \ln(R' - Z')] = (R' - Z')^{i\eta} = [\Gamma(-i\eta)]^{-1} \int_0^\infty d\lambda\, \lambda^{-i\eta-1} \exp[-\lambda(R' - Z')]. \quad (11)$$

We emphasize here that the use of a limiting procedure in Eq. (11) is only a convenience. One could as well employ the representation

$$(R' - Z')^{i\eta} = [\Gamma(-i\eta)]^{-1} \int_0^\infty d\lambda\, \lambda^{-i\eta}(R' - Z') \times e^{-\lambda(R' - Z')}$$

which requires no limiting procedure. Since Eq. (11) has a well-defined meaning and gives simpler formulas we use it here. In fact the second representation may be obtained from the first by integrating by parts and then setting $\delta = 0$. When dealing with integrals that diverge at $\lambda = 0$ if $\delta = 0$, one may integrate by parts and then set $\delta = 0$. Substituting Eq. (11) into (10), taking the Fourier transform of the factors containing $R'$, and then integrating over $\vec{r}$ we obtain

$$F(i \to f, \vec{q}) = (-K\eta/2\pi) C_{fi} D(\mu, \vec{\gamma})(I' - I), \quad (12)$$

where the expression for $I'$, the integral of the $1/R'$ term in Eq. (10), is given by

$$I' = (-2/\pi)[\Gamma(-i\eta)]^{-1} (d/d\mu) \int_0^\infty d\lambda\, \lambda^{-i\eta-1} \int d\vec{R} \exp[i\vec{q}\cdot\vec{R} - i\eta \ln(R - Z)] \int d\vec{k} \exp(i\vec{k}\cdot\vec{R})[k^2 + 2i\lambda k_z]^{-1} \times [\mu^2 + (\vec{k} - \vec{\gamma})^2]^{-1}, \quad (13)$$

and the expression for $I$, the integral of the $1/R$ term in Eq. (10), is similar. The integral over $d\vec{k}$ in Eq. (13) is readily accomplished using Feynman integration. We obtain

$$I' = 2\pi[\Gamma(-i\eta)]^{-1}\frac{d}{d\mu}\int_0^\infty d\lambda\,\lambda^{-i\eta-1}\int_0^1 d\chi\,\Lambda^{-1}\frac{d}{d\Lambda} \times \int d\vec{R}\,(R^{-1})\exp(-\Lambda R + i\vec{q}'\cdot\vec{R})(R-Z)^{-i\eta}, \tag{14}$$

where $\Lambda$ and $\vec{q}'$ are defined by

$$\Lambda = [\lambda^2(1-\chi)^2 + 2i\lambda\chi(1-\chi)\gamma_z + \mu^2\chi + \gamma^2\chi(1-\chi)]^{1/2}, \tag{15a}$$

$$\vec{q}' = \vec{q} - i\lambda(1-\chi)\hat{z} + \chi\vec{\gamma}. \tag{15b}$$

Performing the $\vec{R}$ integration in Eq. (14) using parabolic coordinates[9] gives

$$I' = 2^{3-i\eta}\pi^2[\Gamma(-i\eta)]^{-1}\Gamma(1-i\eta)4\mu\left(\frac{d}{d\mu^2}\right)^2 \times \int_0^\infty d\lambda\,\lambda^{-i\eta-1}\int_0^1 d\chi\,\chi^{-1}(\Lambda^2+q'^2)^{i\eta-1} \times (\Lambda - iq_z')^{-i\eta}, \tag{16a}$$

and similarly

$$I = 2^{3-i\eta}\pi^2[\Gamma(-i\eta)]^{-1}\Gamma(1-i\eta)4\mu\left(\frac{d}{d\mu^2}\right)^2 \times \int_0^\infty d\lambda\,\lambda^{-i\eta}\int_0^1 d\chi\,\chi^{-1}(1-\chi)\Lambda^{-1} \times (\Lambda^2+q'^2)^{i\eta-1}(\Lambda - iq_z')^{-i\eta}. \tag{16b}$$

The result of substituting Eqs. (16a) and (16b) into (12) is the desired double-integral expression for $F(i\to f,\vec{q})$,

$$F(i\to f,\vec{q}) = \left[-2^{2-i\eta}\pi[\Gamma(-i\eta)]^{-1}\Gamma(1-i\eta)K\eta C_{fi}D(\mu,\vec{\gamma})4\mu\left(\frac{d}{d\mu^2}\right)^2\right] \times \left\{\int_0^\infty d\lambda\,\lambda^{-i\eta-1}\int_0^1 d\chi\,\chi^{-1}[\mathfrak{F}(1,0,0,0) - \mathfrak{F}(1,1,0,1)]\right\}, \tag{17a}$$

where

$$\mathfrak{F}(m,p,r,s) = \lambda^s(1-\chi)^s\Lambda^{-p}(\Lambda^2+q'^2)^{i\eta-m}(\Lambda-iq_z')^{-i\eta-r}. \tag{17b}$$

Eq. (17a) expresses the scattering amplitude in terms of double integrals which can be evaluated numerically for $q_z \neq 0$. The differentiations implied in Eq. (17a) may be evaluated using the recurrence relations

$$\frac{d}{d\mu^2}\mathfrak{F}(m,p,r,s) = \chi[(-\tfrac{1}{2}p)\mathfrak{F}(m,p+2,r,s) + (i\eta-m)\mathfrak{F}(m+1,p,r,s) - 2^{-1}(i\eta+r)\mathfrak{F}(m,p+1,r+1,s)], \tag{18a}$$

$$\frac{d}{d\gamma_x}\mathfrak{F}(m,p,r,s) = \chi[-p\gamma_x(1-\chi)\mathfrak{F}(m,p+2,r,s) + 2(i\eta-m)(q_x+\gamma_x)\mathfrak{F}(m+1,p,r,s) - (i\eta+r)\gamma_x(1-\chi)\mathfrak{F}(m,p+1,r+1,s)], \tag{18b}$$

and

$$\frac{d}{d\gamma_z}\mathfrak{F}(m,p,r,s) = \chi\{(-i)p[\mathfrak{F}(m,p+2,r,s+1) - i\gamma_z(1-\chi)\mathfrak{F}(m,p+2,r,s)] + 2(i\eta-m)(q_z+\gamma_z)\mathfrak{F}(m+1,p,r,s) - i(i\eta+r) \times [\mathfrak{F}(m,p+1,r+1,s+1) - i\gamma_z(1-\chi)\mathfrak{F}(m,p+1,r+1,s) - \mathfrak{F}(m,p,r+1,s)]\}. \tag{18c}$$

Since the dependence of $\mathfrak{F}(m,p,r,s)$ on $\gamma_y$ is the same as on $\gamma_x$, Eq. (18b) also applies for $\gamma_y$. Equations (18a)–(18c) show that evaluating the derivatives in Eq. (17a) produces a number of integral terms of the form

$$I(g;h;m,p,r,s) = \int_0^\infty d\lambda\,\lambda^{-i\eta-1} \times \int_0^1 d\chi\,\chi^{g-1}(1-\chi)^h\mathfrak{F}(m,p,r,s), \tag{19}$$

where $g$ is the total number of differentiations in Eq. (17a) and the integers $h,m,p,r,s$ have the possible values $h\geq 0$, $m\geq 1$, $p\geq s\geq 0$, $r\geq 0$.

### B. Small-angle elastic scattering

For small-angle elastic ($1s\to 1s$) scattering, where the conventional Glauber approximation is valid, we can set $q_z=0$ and show that Eq. (17a) reduces to the algebraic expression of Thomas and Gerjuoy,[7] obtained from the conventional approximation.

Note that Eq. (8) represents $u_f^* u_i$ for $1s \to 1s$ scattering when

$$\mu = 2/a_0 , \tag{20a}$$

$$C_{fi} = (\pi a_0^3)^{-1} , \tag{20b}$$

$$\gamma = 0 , \tag{20c}$$

where $a_0$ is the Bohr radius. So with $D(\mu, \vec{\gamma}) = 1$, Eq. (17a) together with Eqs. (20a)–(20c) represents $F(1s \to 1s, \vec{q})$. With the use of Eqs. (15a) and (15b) in Eqs. (17a) and (17b) the double integral of Eq. (17a) becomes ($q_z = 0$)

$$I = \int_0^\infty d\lambda\, \lambda^{-i\eta-1} \int_0^1 d\chi\, \chi^{-1}[1 - \lambda(1-\chi)\Lambda^{-1}] \times [q^2 + \mu^2\chi]^{i\eta-1}[\Lambda - \lambda(1-\chi)]^{-i\eta} , \tag{21}$$

where

$$\Lambda = [\lambda^2(1-\chi)^2 + \mu^2\chi]^{1/2} .$$

The change of variables $t = \lambda(1-\chi)(\mu^2\chi)^{-1/2}$ permits $I$ to be factored so that

$$I = \mu^{-2i\eta} q^{2i\eta-2} \int_0^1 d\chi\, \chi^{-i\eta-1}(1-\chi)^{i\eta}(1 + \mu^2\chi/q^2)^{i\eta-1} \times \int_0^\infty dt\, t^{-i\eta-1}[1 - t(1+t^2)^{-1/2}]\,[(1+t^2)^{1/2} - t]^{-i\eta} . \tag{22a}$$

The integral over $\chi$ can be written as a hypergeometric function[10] so that

$$\mu^{-2i\eta} q^{2i\eta-2} \int_0^1 d\chi\, \chi^{-i\eta-1}(1-\chi)^{i\eta}(1 + \mu^2\chi/q^2)^{i\eta-1} = (-1)^{i\eta}\Gamma(-i\eta)\Gamma(1+i\eta) q^{-2}(-\mu^2/q^2)^{-i\eta} \times {}_2F_1(1 - i\eta, -i\eta; 1; -\mu^2/q^2) , \tag{22b}$$

while the change of variables $v = [(1+t^2)^{1/2} - t]^2$ transforms the integral over $t$ so that

$$\int_0^\infty dt\, t^{-i\eta-1}[1 - t(1+t^2)^{-1/2}][(1+t^2)^{1/2} - t]^{-i\eta} = 2^{i\eta} \int_0^1 dv (1-v)^{-i\eta-1} = -2^{i\eta}(i\eta)^{-1} . \tag{23}$$

Combining Eqs. (17a) and (17b) and Eqs. (20)–(23) we find

$$F(1s \to 1s, \vec{q}) = (-1)^{i\eta}(-i) 2^5 K q^{-6} a_0^{-4} \Gamma(1 - i\eta)\Gamma(1 + i\eta) \times \frac{d^2}{dx^2}[x^{-i\eta}\, {}_2F_1(1 - i\eta, -i\eta; 1; x)] , \tag{24}$$

with $x = -\mu^2/q^2$. This is equivalent to Eq. (28a) of Thomas and Gerjuoy.

In Eq. (22a) the electronic ($I'$) and the nuclear ($I$) contributions to the scattering amplitude of Eq. (12) correspond to the terms with 1 and $t(1+t^2)^{-1/2}$ in the first bracket of the $t$ integrand. For large $t$ the integrals representing $I'$ and $I$ both go as $t^{-1}$, thus the separate integrals diverge logarithmically but the total $I' - I$ converges. Hence $q_z \neq 0$ is a necessary condition for unambiguously evaluating the individual electron-electron and electron-proton contributions to the Glauber scattering amplitude. In Sec. III we evaluate the separate electronic and nuclear contributions to $1s \to 2p$ scattering at large angles where $\mu/q_z \ll 1$.

## III. LARGE-ANGLE APPROXIMATION

For high-energy scattering at large angles, one can obtain an approximate scattering amplitude by expanding the integrand of Eq. (17a) in powers of $\mu/q$ and keeping the lowest-order terms. We have done this for $1s \to 2p$ scattering to determine the qualitative differences from conventional Glauber results.

In the Cartesian coordinates defined following Eqs. (42) an orthonormal basis for the $2p$ state is defined by

$$u(2p_x) = i\pi^{-1/2}(2a_0)^{-5/2} x \exp(-r/2a_0) , \tag{25a}$$

with similar expressions for $u(2p_y)$ and $u(2p_z)$. The normalized $1s$ wave function is

$$u(1s) = \pi^{-1/2}(a_0)^{-3/2} \exp(-r/a_0) . \tag{25b}$$

Comparing Eq. (8) with Eqs. (25a) and (25b) shows that the $1s \to 2p_x$ and $1s \to 2p_z$ scattering integrals can be generated by differentiating the integrand of Eq. (17a) with respect to $\gamma_x$ and $\gamma_z$ and setting $\vec{\gamma} = 0$. The result of these derivatives and those with respect to $\mu^2$ [cf. Eq. (17a)] is a number of integrals of the form of Eq. (19a) with the parameters $g = 3$, $h = 0$, $1 \leq m \leq 4$, $s \leq p \leq s+5$, $0 \leq s \leq 2$, and $0 \leq r \leq 3$.

Referring to Eqs. (15a) and (15b) one sees that the integrand of Eq. (17a) is degenerate with respect to $y$ when $\vec{\gamma} = 0$. Any $y$ dependence is introduced by differentiating with respect to $\gamma_y$ [cf. Eq. (18b)] which means the integrands have the same parity as the excited state. Since $u(2p_y)$ is odd, the integral over $d\vec{r}$ for $1s \to 2p_y$ excitation is zero.

### A. Rutherford term

In the high-energy limit $\mu^2/q^2 \ll 1$ and for $q_z \simeq q$, one may evaluate the integrals approximately by expanding the arguments in powers of $\mu/q$. Thus we write

$$(\Lambda^2 + q'^2)^{i\eta-m} = [q^2 - 2i\lambda q_z(1-\chi)]^{i\eta-m} + O(\mu^2/q^2) , \tag{26a}$$

$$(\Lambda - iq_z')^{-i\eta-r} = (-iq_z)^{-i\eta-r}\{1 - (i\eta + r)(-iq_z)^{-1} \times[\Lambda - \lambda(1-\chi)] + O(\mu^2/q_z^2)\}, \quad (26b)$$

to second order in $\mu/q$.

Substituting these approximations into Eq. (19) with the change of variable $t = \lambda(1-\chi)$ we have

$$I(3;0;m,p,r,s) = H(m,p,r,s) - (i\eta + r) \times H(m,p-1,r+1,s) + (i\eta+r)H(m,p,r+1,s+1), \quad (27)$$

where

$$H(m,p,r,s) = (-iq_z)^{-i\eta-r}\Gamma(3)\Gamma(1+i\eta)[\Gamma(4+i\eta)]^{-1} \times \int_0^\infty dt\, t^{-i\eta-1+s-p}(q^2 - 2iq_z t)^{i\eta-m} \times {}_2F_1(p/2, 3; 4+i\eta; -\mu^2/t^2). \quad (28)$$

Applying the analytic continuation formulas[11] and the change of variables $\lambda = \mu/t$ we find

$$H(m,p,r,s) = c(m,p,r,s;\epsilon)I(m,p,s;\epsilon), \quad (29a)$$

where

$$c(m,p,r,s;\epsilon) = \mu^{-i\eta+s-p}(-iq_z)^{-i\eta-r}(q^2)^{i\eta-m} \times\Gamma(3)\Gamma(1+i\eta)[\Gamma(4+i\eta)]^{-1}, \quad (29b)$$

$$I(m,p,s;\epsilon) = \int_0^\infty f(m,p,s;\epsilon;\lambda)d\lambda, \quad (29c)$$

$$f(m,p,s;\epsilon;\lambda) = \lambda^{m-1-s+p}(\lambda - i\epsilon)^{i\eta-m}(1+\lambda^2)^{-p/2} \times {}_2F_1(p/2, 1+i\eta; 4+i\eta; \lambda^2(1+\lambda^2)^{-1}), \quad (29d)$$

and

$$\epsilon = 2q_z\mu/q^2. \quad (29e)$$

For large angles $\epsilon \simeq \mu/q$ which is a small number for high energies. So to be consistent with the approximation in Eqs. (26a) and (26b), $H(m,p,r,s)$ should be approximated by the first two terms of a series in powers of $\epsilon$. The second-order McClaurin expansion of Eq. (29d) is

$$f(m,p,s;\epsilon;\lambda) = f(m,p,s;0;\lambda) - (i\eta - m)(i\epsilon) \times f(m,p,s+1;0;\lambda), \quad (30)$$

so Eq. (29c) implies

$$I(m,p,s;\epsilon) = I(m,p,s;0) - (i\eta - m)(i\epsilon)I(m,p,s+1;0). \quad (31)$$

Note that $f(m,p,s;0;\lambda)$ is singular at $\lambda = 0$ for $p \leq s$, but integration by parts produces integrals which can be evaluated to the lowest order in $\epsilon$. We found that terms with $p \leq s$ do not contribute to the scattering amplitude in first and second order.

When $p > s$, the change of variables $x = \lambda^2(1+\lambda^2)^{-1}$ converts $I(m,p,s;0)$ to a form which appears in integral tables.[12] The result is

$$I(m,p,s;0) = [\Gamma(\tfrac{1}{2}p)]^{-1}\Gamma(\tfrac{1}{2}(i\eta+p-s))\Gamma(\tfrac{1}{2}(s-i\eta))\,{}_3F_2(\tfrac{1}{2}p, 1+i\eta, \tfrac{1}{2}(i\eta+p-s); 4+i\eta; \tfrac{1}{2}p; 1)$$
$$= \frac{\Gamma(\tfrac{1}{2}(i\eta+p-s))\Gamma(\tfrac{1}{2}(s-i\eta))\Gamma(\tfrac{1}{2}(6-i\eta-p+s))\Gamma(4+i\eta)}{2\Gamma(3)\Gamma(\tfrac{1}{2}p)\Gamma(\tfrac{1}{2}(8+i\eta-p+s))}. \quad (32)$$

Using Eqs. (27)–(31) we find that the electronic and nuclear contributions (where $\mu = \tfrac{3}{2}a_0$) to the $1s \to 2p_x$ and $1s \to 2p_z$ scattering amplitudes are

$$E(1s-2p_x,\vec{q}) = 2^2\mu^{-1}(2\pi)^{-1/2}(1-i\eta)^2(3+i\eta)^{-1}\Gamma(1+i\eta)\Gamma(-\tfrac{1}{2}i\eta)\Gamma(\tfrac{1}{2}(1-i\eta))\eta^3Kq_xq^{-6}(-i\epsilon)^{-i\eta-1}, \quad (33a)$$

$$E(1s-2p_z,\vec{q}) = i2^2\mu^{-2}(2\pi)^{-1/2}\Gamma(1+i\eta)\Gamma(\tfrac{1}{2}(1-i\eta))\Gamma(\tfrac{1}{2}(2-i\eta))K\eta^3q^{-4}(-i\epsilon)^{-i\eta-1}, \quad (33b)$$

$$N(1s-2p_x,\vec{q}) = i2^2\mu^{-3}(2\pi)^{-1/2}(1-i\eta)\Gamma(1+i\eta)\Gamma(\tfrac{1}{2}(1-i\eta))\Gamma(\tfrac{1}{2}(2-i\eta))K\eta^2q_xq^{-4}(-i\epsilon)^{-i\eta}, \quad (33c)$$

$$\begin{aligned}N(1s-2p_z,\vec{q}) = &-2\mu^{-4}(2\pi)^{-1/2}(3+i\eta)\Gamma(1+i\eta)\Gamma(\tfrac{1}{2}(2-i\eta))\Gamma(\tfrac{1}{2}(1-i\eta))K\eta^2q^{-2}(-i\epsilon)^{-i\eta}\\ &+2^{1-i\eta}\mu^{-4}(2\pi)^{-1/2}(1-i\eta)^2\Gamma(1+i\eta)\Gamma(\tfrac{1}{2}(1-i\eta))\Gamma(\tfrac{1}{2}(2-i\eta))K\eta^2q^{-2}(-i\epsilon)^{-i\eta+1}\\ &-i2^2\mu^{-2}(2\pi)^{-1/2}(1-i\eta)\Gamma(1+i\eta)\Gamma(\tfrac{1}{2}(1-i\eta))\Gamma(\tfrac{1}{2}(2-i\eta))K\eta^3q^{-4}(-i\epsilon)^{-i\eta-1}\\ &-2\mu^{-4}(2\pi)^{-1/2}(1-i\eta)\Gamma(1+i\eta)\Gamma(\tfrac{1}{2}(1-i\eta))\Gamma(\tfrac{1}{2}(2-i\eta))K\eta^2q^{-2}(-i\epsilon)^{-i\eta+1}\\ &+i2^2\mu^{-2}(2\pi)^{-1/2}\Gamma(1+i\eta)\Gamma(\tfrac{1}{2}(1-i\eta))\Gamma(\tfrac{1}{2}(2-i\eta))K\eta^3q^{-4}(-i\epsilon)^{-i\eta-1}.\end{aligned} \quad (33d)$$

The total scattering amplitude for $1s \to 2p_x$ or $1s \to 2p_z$ is the sum of the electronic and nuclear contributions from Eqs. (33a)–(33d). Since $\epsilon \simeq 2\mu/q$ when $q_z \simeq q$, the first term of $N(1s \to 2p_z, \vec{q})$ is proportional to $q^{-2}$, as is the Rutherford scattering amplitude, while for $q_x \simeq q$, all other terms of Eqs. (33a)–(33d) are at least proportional to $q^{-3}$. So to lowest order only the electron-proton interaction is important and only the $2p_z$ state is excited. In contrast, the proton contribution is identically zero in the first Born approximation, while the $2p_z$ excitation is identically zero (as a result of taking $q_z = 0$) in the restricted Glauber approximation.[2] Our asymptotic expansion assumes fixed $K$ but large $q$. For large $q$ but small fixed energy loss we have $q \sim 2k\sin(\theta/2)$, thus our expansion is in powers of $\sin(\theta/2)^{-1}$. Since the coefficients in the expansion depend upon $\eta \propto K^{-1}$ we cannot be certain that the expansion is also an expansion in inverse powers of $K$ for large $K$ but fixed $\theta$. We can show, however, for fixed $\theta$ but large $K$, that the electron-nucleus amplitude decreases at least as fast as $K^{-3}$, and the electron-electron terms as $K^{-5}$. The demonstration is quite tedious, but to support the conclusion that the electron-nucleus term dominates for large $K$ and fixed $\theta$ (which automatically ensures $\mu^2/q^2 \ll 1$) we sketch the proof for the electron-electron term. The arguments also apply to proton-hydrogen-atom scattering provided the incident proton velocity (not $K$) is large.

Our proof is conceptually very simple. We calculate an upper bound to the integrals $I(g;0;m,p,r,s)$ by replacing the argument of the double integral by its absolute value. Since $\eta$ occurs only in the phase factors in Eq. (17b) these upper bounds essentially depend only on $q$. The main effort consists of enumerating the relevant terms and the dominant power of $K$ in their coefficients obtained by applying the recurrence relations Eqs. (18a)–(18c) to Eqs. (17a) and (17b). These are tabulated in Table I. Only terms with $s=0$ or 1 appear. We first consider the bound for $s=1$.

With the change of variables $t=\lambda(1-\chi)/(\mu\sqrt{\chi})$ we have for $I(3;0;m,p,r,s)$ in Eq. (19) the result

$$I(3;0;m,p,r,s)=\mu^{s-p-i\eta}\int_0^\infty dt\,t^{-i\eta-1+s}(t^2+1)^{-p/2}\int_0^1 d\chi\,(1-\chi)^{i\eta}\chi^{2-(p-s+i\eta)/2}(q^2+\mu^2\chi-2itq_z\mu\sqrt{\chi})^{i\eta-m}$$
$$\times\{[(t^2+1)^{1/2}-t]\mu\sqrt{\chi}-iq_z\}^{-i\eta-r}\,. \tag{34}$$

For $s=1$, the integral is bounded by

$$\mu^{s-p}\int_0^\infty dt\,(t^2+1)^{-p/2}\int_0^1 d\chi\,\chi^{5/2-p/2}[(q^2+\mu^2\chi)^2+4t^2q_z^2\mu^2\chi]^{-m/2}\{[(t^2+1)^{1/2}-t]^2\mu^2\chi+q_z\}^{-r/2}$$
$$\times\exp\left[-\eta\arctan\left(-\frac{2tq_z\mu\sqrt{\chi}}{q^2+\mu^2\chi}\right)\right]\exp\left[\eta\arctan\left(\frac{-q_z}{((t^2+1)^{1/2}-t)\mu\sqrt{\chi}}\right)\right]. \tag{35}$$

Since

$$q^4 \leq (q^2+\mu\chi)^2+4t^2q_z^2\mu^2\chi \tag{36a}$$

and

$$q_z^2 \leq [(t^2+1)^{1/2}-t]^2\mu^2\chi+q_z^2 \tag{36b}$$

Equation (35) is easily seen to be bounded by

$$e^{2\pi\eta}\mu^{s-p}q^{-2m}q_z^{-r}\int_0^\infty dt\,(t^2+1)^{-p/2}\quad\text{for } p\geq 2\,. \tag{37}$$

For the term with $p=1$ and $m=3$ it is necessary to integrate over $\chi$ before applying the bound (36a). The result is still a bound of the type (const) $q^{-2m}q_z^{-r}$. Combining the factor $K\eta^2$ from the coefficient of the integrals in Eq. (17a) with the factor of $\eta$ from the first column in Table I we see that all terms with $s=1$ go as $K\eta^3q^{-3}\propto K^{-5}$ for large $K$ and fixed $\theta$. For $s=0$ we must first integrate by parts according to our discussion of Eq. (11) and then apply the bounds. The integration by parts introduces a factor $(-i\eta)^{-1}$, but otherwise the bounds are similar to Eq. (37). We see that the

TABLE I. Terms in the electron-electron matrix element.

| Dominant coefficient | $m$ | $p$ | $r$ | $s$ |
|---|---|---|---|---|
| $\eta$ | 3 | 1 | 1 | 1 |
| | 2 | 3 | 1 | 1 |
| | 1 | 5 | 1 | 1 |
| | 2 | 3 | 1 | 1 |
| | 1 | 4 | 2 | 1 |
| | 2 | 2 | 2 | 1 |
| | 1 | 4 | 2 | 1 |
| | 2 | 2 | 2 | 1 |
| | 1 | 3 | 3 | 1 |
| $q_x, q_z$ | 4 | 0 | 0 | 0 |
| $\eta q_x, \eta q_z$ | 3 | 1 | 1 | 0 |
| | 2 | 3 | 1 | 0 |
| | 3 | 1 | 1 | 0 |
| | 2 | 2 | 2 | 0 |
| $\eta$ | 3 | 0 | 1 | 0 |
| | 2 | 1 | 2 | 0 |
| | 1 | 3 | 2 | 0 |
| | 2 | 1 | 2 | 0 |
| | 1 | 2 | 3 | 0 |

Table entries with $s=0$ all decrease as $K^{-5}$ or faster. Since the first term in our asymptotic expansion of the $p_z$ nuclear matrix element goes as $K\eta^2 q^{-2}$ we conclude that the nuclear Rutherford term dominates for large $K$ and fixed scattering angle. Note here that bounds of the form Eqs. (36a) and (36b) and (37) also apply to the individual terms in the expansions of Eqs. (26a) and (26b).

The presence of a Rutherford term multiplied by some power of $\eta$ in the excitation amplitude at large angles is expected on physical grounds since large-angle scattering at high energies requires considerable momentum transfer to the atom as a whole. For bound states most of the momentum is taken up by the nucleus, independent of whether the atom gets excited in the process. This transfer of momentum is most efficient if it is transferred directly to the nucleus, rather than to the bound electron and then to the nucleus. The direct transfer is described by the Rutherford formula, thus in our expression for the scattering amplitude we expect a term corresponding to the Rutherford amplitude $q^{-2}$. Thus, in agreement with Tai *et al.*,[2] we find that large-angle scattering is dominated by electron-nuclear effects, furthermore we trace these effects to the electron-nuclear term in Eq. (10).

We may understand the dominance of the electron-nuclear term by examining Eq. (10) in detail. The electron-nuclear interaction enters into both the potential $1/R' - 1/R$ and the phase factor. We expect large momentum transfer to correspond to close collisions with the nucleus, i.e., with small $R$. For small $R$ the phase term oscillates rapidly for fixed $\vec{r}$. The oscillation tends to decrease the contribution from small $R$, for both the $1/R'$ and $1/R$ terms. This decrease is partially compensated by the increase of $1/R$ in the electron-nucleus term, but there is no corresponding compensation for the $1/R'$ term at fixed $\vec{r}$.

### B. Polarization of radiation at large angles

Recently, experiments have been performed which detect the radiation emitted by a collision excited atom in coincidence with a scattered particle.[13,14] These experiments promise to give detailed information on the departure from the Born approximation. The polarization and angular distribution of the emitted radiation are of particular interest. We will discuss these types of measurements in terms of the "orientation" and "alignment" parameters commonly used, e.g., in optical-pumping work.[15] The relationship of these parameters to scattering amplitudes and to experiment will be briefly reviewed. Detailed discussion may be found in several works.[6,16,17] We will follow the development of Ref. 6.

The intensity of radiation is proportional to the squared matrix element

$$\sum_{m_0} |(\Psi|\hat{\epsilon}\cdot\vec{r}|\Psi_{m_0})|^2 , \tag{38}$$

where $\hat{\epsilon}$ is the polarization of the emitted light, $\Psi_{m_0}$ is a wave function of the state reached in the decay and $\Psi$ is given by

$$\Psi = \sum_m F_m \Psi_m . \tag{39}$$

Equation (38) has the structure of the expectation value of the operator

$$\sum_{m_0} \vec{r}'|\Psi_{m_0})(\Psi_{m_0}|\vec{r} , \tag{40}$$

which is a second-rank tensor. According to the Wigner-Eckart theorem the irreducible components of this tensor are proportional to the irreducible components of the tensors constructed from $(\hat{\epsilon}^\dagger\cdot\vec{L})(\vec{L}\cdot\hat{\epsilon})$ where $\vec{L}$ is the orbital-angular-momentum operator. Thus

$$I \propto \sum_{k,q} h^{[k]} Q_q^{[k]\dagger}(\hat{\epsilon}) g^{[k]} (\Psi|T_q^{[k]}|\Psi) , \tag{41}$$

where $h^{[k]}$ is a constant depending upon the angular momentum of the initial and final states, $Q_q^{[k]}(\hat{\epsilon})$ is an irreducible tensor depending only on the polarization and direction of emission of the observed photon, $g^{[k]}$ is a depolarization factor relating to the fine and hyperfine structure of the initial state, and $T_q^{[k]}$ is a tensor constructed from the elements of $\vec{L}$. Equation (41) is to be averaged over all directions of the scattered element in a noncoincidence experiment, but is not averaged when the electron and photon are detected in coincidence. Here we neglect the spin of the electron, which is also normally averaged over. Explicit equations for coefficients of $T_q^{[k]}$ in Eq. (41) may be found in Ref. 6. We concentrate on the values of $(\Psi|T_q^{[k]}|\Psi)$ as calculated with Eq. (39) using our asymptotic amplitudes for $F_m$, which are to be compared with similar quantities extracted from experiment, when such data becomes available.[14]

With $C = l(l+1)\sum_m |F_m|^2$ (where $l$ is the orbital-angular-momentum quantum number of the excited state) the alignment and orientation parameters of the excited states of hydrogen are defined[6] to be

$$O_{1-}^{\text{col}} = (\psi|L_y|\psi)/C , \tag{42a}$$

$$A_0^{\text{col}} = (\psi|3L_z^2 - L^2|\psi)/C , \tag{42b}$$

$$A_{1+}^{\text{col}} = (\psi|L_xL_z + L_zL_x|\psi)/C , \tag{42c}$$

$$A_{2+}^{\text{col}} = (\psi|L_x^2 - L_y^2|\psi)/C , \tag{42d}$$

where the coordinate system is chosen with $\hat{z}$ along $\vec{K}$, $\hat{y}$ along $\vec{K}\times\vec{K}'$ and $\hat{x}$ perpendicular to $\hat{z}$ and $\hat{y}$.

These quantities are the only nonvanishing components of tensors of rank 0, 1, and 2 constructed from the elements of $\vec{L}$. The other components vanish since they are not invariant to reflections in the scattering plane. The conventional Glauber transition operator is also invariant to reflections in a plane perpendicular to $\hat{z}$. Since $O_{1-}^{\text{col}}$ and $A_{1+}^{\text{col}}$ change sign under this operation, they vanish when $F_m$ is approximated by the conventional Glauber amplitudes. Our modified amplitudes do not have this additional symmetry so that our $O_{1-}^{\text{col}}$ and $A_{1+}^{\text{col}}$ may not be zero. Now $O_{1-}^{\text{col}}$ is the only axial vector quantity in Eq. (41), thus a measurement of this quantity must incorporate an axial vector. Such an axial vector is the axis of a circular polarizer. Since $O_{1-}^{\text{col}}$ is the only quantity which changes sign when the axial vector $L_y$ is reversed, the circular polarization, which is proportional to the difference of two signals with the direction of the axis of a circular polarizer reversed, is also proportional to $O_{1-}^{\text{col}}$.

When Ly-$\alpha$ light is observed perpendicular to the scattering plane in coincidence with the scattered particle, we find that the circular polarization $P_c$ relates to $O_{1-}^{\text{col}}$ explicitly by

$$P_c = (42/25)O_{1-}^{\text{col}},$$

in the approximation where hyperfine structure is neglected. In the absence of fine structure we have $P_c = 2O_{1-}^{\text{col}}$, thus the factor of 42/25 incorporates a slight depolarization due to fine structure.

Since excitation of the $2p_z$ state dominates for $\mu/q_z \ll 1$, to first approximation the alignment parameter $A_0^{\text{col}}$ of Eq. (42b) is unity which implies maximum linear polarization along the incident beam direction. This corresponds to the Born prediction since $\vec{q}$ is approximately parallel to the $z$ axis.

In second order, other amplitudes contribute. In contrast to the Born approximation and to the conventional Glauber approximation the $1s\to 2p_x$ amplitude differs in phase from the $1s\to 2p_z$ amplitude. In this case all the parameters of Eqs. (42a)–(42d) are nonzero including the orientation parameter $O_{1-}^{\text{col}}$ which relates to the circular polarization of the decay radiation (cf. Table II). The orientation is small but nonzero. Numerical calculations (now in progress) at smaller angles and lower energies are desirable to form an over-all picture of the polarization properties of the radiation in the Glauber approximation with $q_z \neq 0$.

TABLE II. Orientation parameter $O_{1-}^{\text{col}}$ as a function of scattering angle for $1s\to 2p$ electron-hydrogen excitation at 100 eV.

| Angle (deg) | $O_{1-}^{\text{col}}$ |
|---|---|
| 80 | 0.208 |
| 100 | 0.158 |
| 130 | 0.0919 |
| 160 | 0.0353 |
| 170 | 0.0176 |

## IV. SUMMARY

Our investigation of large-angle, inelastic electron-hydrogen scattering employing the Glauber scattered wave function (but not the assumption $q_z = 0$) in a modified Glauber amplitude shows that the integrals for the electron-electron and electron-proton interactions individually converge when $q_z \neq 0$ with the result that the electron-proton term dominates to give a $q^{-4}$ behavior to the inelastic differential cross section. We find, at large angles, that only the $2p_z$ state is excited (implying linear polarization of decay radiation) in first order in $\mu/q$ while in second order the radiation is elliptically polarized to a small extent.

We conclude that the Glauber approximation used here gives a satisfactory account of large-angle, Rutherford-like inelastic scattering, in that it traces such behavior to the electron-proton interaction. Furthermore, since our approximation, in general, predicts nonzero orientation, it shows that Byron's modified Glauber approach may describe a wider range of physical phenomena, i.e., circular polarization of radiation, than is possible when the assumption $q_z = 0$ is employed. Such phenomena relate more directly to the detailed assumptions of the theory, in particular, the symmetry aspects of the transition operator, than do scattering cross sections.

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