Calculation of proton-impact excitation of helium using the Glauber approximation

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Cross sections for the $1\,^1S \rightarrow n\,^1S$ ($n = 2,3,4$) excitations of atomic helium under proton impact are calculated with incident energy ranging from 25 to 1000 keV employing the Glauber approximation. A properly orthogonalized set of He wave functions are used. The generalized oscillator strengths for $1\,^1S \rightarrow 2\,^1S$ and $1\,^1S \rightarrow 3\,^1S$ excitations are also calculated with these wave functions, and the results are compared with the existing theoretical and experimental data. The full Glauber scattering amplitude is separated into single- and double-scattering parts. The single-scattering amplitude is evaluated from a closed-form expression. A numerical method is employed to calculate some integrals occuring in the double-scattering amplitude. At incident energies above 500 keV, the single-scattering contribution is found to dominate the Glauber result. The effect of the double-scattering term is appreciable at intermediate energies, where it substantially lowers the cross sections from the corresponding single-scattering result. The Glauber result at intermediate energies also underestimates most of the existing theoretical and experimental cross sections, which already show a wide variation among themselves in absolute values. However, the functional dependence of the Glauber cross sections on energy is similar to that depicted by other calculations and measurements. Furthermore, the average ratio of the Glauber cross sections for $3\,^1S$ and $4\,^1S$ excitations at high energies show reasonable agreement with those obtained from other theories, as also from the n^{-3} law of cross sections.

I. INTRODUCTION

Direct collisional excitation of atomic helium from its ground state under the incidence of ionic projectiles is a topic of much theoretical and experimental interest. For proton-impact excitation of ground-state He, a number of theoretical[1-11] as well as experimental[12-20] studies of the collision cross sections are available. The agreement between theory and experiment is more or less good for the optically allowed transitions.[3,19,20] But, for optically forbidden transitions,[3,11,19] the situation is far from satisfactory. Considering, for example, the ^1S excitations in p-He($1\,^1S$) collision, the available data[1-19] of cross sections, both theoretical and experimental, show a wide variation among themselves in respect of absolute values. Some new theoretical results may perhaps prove worthwhile in clarifying this situation. The present work is an attempt towards this direction.

Of the various approximate theoretical procedures available for calculating the ion-atom collision cross sections, the first Born approximation (FBA) is applicable at high incident energies of the projectile, but fails towards intermediate-energy regions. Furthermore, for optically forbidden transitions, the FBA method becomes unsuitable even at much higher energies than one would usually expect.[3,21] Some improvement may be obtained using the second Born approximation (SBA), but here the scattering amplitude involves an infinite summation over all the target eigenstates. Simplified forms of the SBA method have sometimes been successful in studying He excitations[6,11] at intermediate energies. The two-state distortion approximation[22] of Bates is another method and may often predict the qualitative features of the cross sections[7,11] down to much lower energies than the corresponding SBA method[11] can do. Some many-state calculations[3,5] have also been performed for ion-helium excitations, which are much more rigorous than the two-state ones, but involve lots of computational work. Besides these, a number of approximations have also been proposed, which include the second-order effects in atomic excitation processes. Thus the second-order diagonalization method[8] and the second-order potential method[9] have been applied with varied success. Among the notable exceptions, one can mention the Glauber approximation[23] which, in spite of its success in studying collisions involving atomic hydrogen targets at intermediate energies,[24] has found very few applications in ion-helium collisions.

The Glauber approximation[23] (GA) is one of the various eikonal-type methods which has been used by many workers in recent years to study composite atomic collision phenomena.[24] Extensive studies have been made on e-H and p-H collisions[25-28] for which the GA scattering amplitude is a five-dimensional integral. Such studies have revealed the superiority of the GA over the FBA method at intermediate regions of incident energy.[24] Great simplification in the Glauber calculation for hydrogen targets were later possible through the works of Thomas and Gerjuoy.[26] They expressed the ($1s$-ns)- and ($1s$-np)-scattering amplitudes in closed forms. However, application of the Glauber method to helium targets had to face a lot of complications at the beginning. This

was due to the fact that for He targets an eight-dimensional integral occurs in the expression for the GA scattering amplitude. Some numerical calculations were performed for e-He collisions after reducing the amplitude to three-dimensional[29,30] and two-dimensional[31,32] integrals. Finally, Franco[33] proposed a method for reduction of the amplitude integral to one-dimensional form and later applied it to study electron scattering from He targets.[34] However, an infinite integral over the impact-parameter variable is finally left in Franco's method[33] and the corresponding integrand involves a combination of hypergeometric functions. These functions diverge exponentially and make numerical computations in the method[33] very troublesome.[35] Thomas and Chan[35] later refined and simplified this method to some extent by separating the total Glauber amplitude for He targets into the so-called "single-scattering" and "double-scattering" parts. They also reduced the single-scattering terms into closed forms and expressed the double-scattering term in the form of a one-dimensional integral involving a modified version of the Lommel function. As long as the argument remains small, direct evaluation of the function is easy. But, for increasing argument values, calculations had to be done entirely in double precision.[35] However, for sufficiently large arguments Thomas and Chan[35] could employ an asymptotic series for the modified Lommel function. The method of Thomas and Chan[35] has since been applied by a number of workers[36] to study e-He collisions. Only in one calculation[37] has it been applied to investigate the 2^1P excitation of ground-state He by proton impact. The extreme scarcity of Glauber theoretical data on heavy-particle–neutral-helium collisions has led us to use the Glauber approximation for the present study.

Proton impact $1^1S \rightarrow n^1S$ ($n = 2, 3, 4$) excitations of ground-state He are investigated in the present work using the Glauber method. Instead of using a modified Lommel function for the evaluation of the double-scattering part of the total Glauber amplitude, we have employed an alternative numerical procedure[38] for the evaluation of the relevant integrals. This method[38] is applicable for a wide range of values of the argument of the modified Lommel function and can be handled with normal computer precision.

For the wave functions of the n^1S states of He, we use the orthogonal set given by Winter and Lin[39] (WL). To judge the accuracy of the WL wave functions as well as that of the FBA cross sections predicted by them, we also calculate in the present paper the generalized oscillator strengths (GOS) of the transitions concerned. The GOS values of the $1^1S \rightarrow 2^1S$ transition are compared with the existing theoretical[4,40] and experimental[41,42] data, whereas the GOS values of the $1^1S \rightarrow 3^1S$ transition are compared with the available theoretical data.[4,40] For the transition $1^1S \rightarrow 4^1S$ in He, the GOS values with WL wave functions have already been calculated and compared with other theoretical results in the work of Sur *et al.*[11]

II. WAVE FUNCTION

For the ground state of the He atom, we take the product form of wave function due to Green *et al.*[43]:

$$\Psi_i \equiv \Psi(1^1S\,|\,\vec{r}_1, \vec{r}_2) = N_i u_0(r_1) u_0(r_2)\,, \tag{1}$$

where

$$u_0(r) = e^{-\alpha r} + a e^{-\beta r}\,, \tag{2}$$

while the final-state wave functions of Winter and Lin[39] are given in the form

$$\Psi_f \equiv \Psi(n^1S\,|\,\vec{r}_1, \vec{r}_2) = N_f[u_n(r_1) g(r_2) + u_n(r_2) g(r_1)] \tag{3}$$

with

$$g(r) = e^{-2\gamma}\,, \quad u_n(r) = e^{-\gamma r} \sum_{\rho=1}^{n} (-)^{\rho-1} c_\rho r^{\rho-1}\,. \tag{4}$$

Here α, β, γ, a, and c_ρ are wave-function-parameters, and N_i and N_f are the normalization constants. Ψ_f is orthogonal to all the lower states.

A. Generalized oscillator strength

The generalized oscillator strength $A(q)$ for the transition of a helium atom from its ground state (i) to any excited state (f) with a momentum transfer $\vec{q}$ is defined as

$$A(q) = (8\epsilon_{fi}/q^2)\,|\langle \Psi_f | e^{i\vec{q}\cdot\vec{r}} | \Psi_i \rangle|^2\,, \tag{5}$$

where ϵ_{fi} ($= \epsilon_f - \epsilon_i$) is the excitation energy from the ground state and $\vec{r}$ is the position vector of any bound electron.

III. THEORY

For impact excitation of a helium atom from an initial state $\Psi_i(\vec{r}_1, \vec{r}_2)$ to a final state $\Psi_f(\vec{r}_1, \vec{r}_2)$ under the incidence of a structureless particle with charge Z_i and relative velocity $\vec{v}_i$, the scattering amplitude $F(\vec{q})$ in the center of mass (c.m.) system is given, according to the Glauber approximation, by

$$F(\vec{q}) = \frac{iK_i}{2\pi} \int \Psi_f^*(\vec{r}_1, \vec{r}_2)\,\Gamma(\vec{b}, \vec{r}_1, \vec{r}_2) \times \Psi_i(\vec{r}_1, \vec{r}_2) e^{i\vec{q}\cdot\vec{b}}\, d^2b\, d\vec{r}_1\, d\vec{r}_2\,, \tag{6}$$

where

$$\Gamma(\vec{b},\vec{r}_1,\vec{r}_2)=1-\prod_{j=1}^{2}\left(\frac{|\vec{b}-\vec{s}_j|}{b}\right)^{2i\eta}, \tag{7}$$

and $\eta=-Z_t/v_i$. Here $\vec{K}_i$ and $\vec{K}_f$ are, respectively, the incident and final momenta in the c.m. system and $\vec{q}(=\vec{K}_i-\vec{K}_f)$ is the momentum transfer vector. The vectors $\vec{b}$ and $\vec{s}_j$ represent the respective projections of the position vectors of the incident particle and the jth bound electron ($\vec{r}_j$) onto the plane perpendicular to the Glauber path integration (the $\vec{b}$ plane).

Introducing polar cordinates on the $\vec{b}$ plane and performing the corresponding azimuthal angle integration in Eq. (6), we obtain

$$F(\vec{q})=iK_i\int \Psi_f^*\Gamma(\vec{b},\vec{r}_1,\vec{r}_2)\times\Psi_i J_0(qb)b\,db\,d\vec{r}_1\,d\vec{r}_2. \tag{8}$$

The composite two-particle $\Gamma(\vec{b},\vec{r}_1,\vec{r}_2)$ can be written in terms of single particle $\Gamma(\vec{b},\vec{r}_j)$ as[35]

$$\Gamma(\vec{b},\vec{r}_1,\vec{r}_2)=\Gamma(\vec{b},\vec{r}_1)+\Gamma(\vec{b},\vec{r}_2)-\Gamma(\vec{b},\vec{r}_1)\Gamma(\vec{b},\vec{r}_2), \tag{9}$$

where

$$\Gamma(\vec{b},\vec{r}_j)=1-(|\vec{b}-\vec{s}_j|/b)^{2i\eta}. \tag{10}$$

On substitution from Eq. (9) in Eq. (8), we can express the Glauber scattering amplitude as

$$F(\vec{q})=F_1(\vec{q})+F_2(\vec{q}), \tag{11}$$

where

$$F_1(\vec{q})=iK_i\int_0^\infty db\,bJ_0(qb)\Gamma_1(\vec{b}), \tag{12}$$

$$F_2(\vec{q})=-iK_i\int_0^\infty db\,bJ_0(qb)\Gamma_2(\vec{b}), \tag{13}$$

with

$$\Gamma_1(\vec{b})=2\langle\Psi_f|\Gamma(\vec{b},\vec{r}_1)|\Psi_i\rangle, \tag{14}$$

$$\Gamma_2(\vec{b})=\langle\Psi_f|\Gamma(\vec{b},\vec{r}_1)\Gamma(\vec{b},\vec{r}_2)|\Psi_i\rangle. \tag{15}$$

Here $F_1(\vec{q})$ gives the single-scattering contribution to the total Glauber amplitude.[24,35] The target He atom may be considered to consist of two hydrogenic atoms, each being composed of an electron and a unit positive charge at the nucleus, and thereby taking part in scattering as a single target. The sum of such contributions is contained in $F_1(\vec{q})$. The remaining part $F_2(\vec{q})$ of the total amplitude may then be interpreted as the double-scattering amplitude.

On substitution for Ψ_i and Ψ_f from Eqs. (1) and (3) in Eqs. (14) and (15), we have, respectively,

$$\Gamma_1(\vec{b})=2N_f^*N_i[A_1\Gamma_{11}(\vec{b})+A_2\Gamma_{12}(\vec{b})], \tag{16}$$

$$\Gamma_2(\vec{b})=2N_f^*N_i\Gamma_{11}(\vec{b})\Gamma_{12}(\vec{b}), \tag{17}$$

where

$$A_1=\int u_0(r)g(r)\,d\vec{r}=8\pi\left[\frac{1}{l_1^3}+\frac{a}{l_2^3}\right],$$

$$A_2=\int u_0(r)u_n(r)\,d\vec{r}=4\pi\sum_{p=1}^{n}(-)^{p-1}c_p(p+1)!\left[\frac{1}{l_3^{p+2}}+\frac{a}{l_4^{p+2}}\right],$$

and

$$\Gamma_{11}(\vec{b})=\int u_0(r)u_n(r)\Gamma(\vec{b},\vec{r})\,d\vec{r}, \tag{18}$$

$$\Gamma_{12}(\vec{b})=\int u_0(r)g(r)\Gamma(\vec{b},\vec{r})\,d\vec{r}, \tag{19}$$

where $l_1=\alpha+2, l_2=\beta+2, l_3=\alpha+\gamma, l_4=\beta+\gamma$.

Introducing the function

$$\Gamma_0(\lambda,\eta,b)=\int\frac{e^{-\lambda r}}{r}\Gamma(\vec{b},\vec{r})\,d\vec{r}, \tag{20}$$

we can write

$$\Gamma_{11}(\vec{b})=-\sum_{p=1}^{n}c_p\left[\left(\frac{\partial}{\partial l_3}\right)^p\Gamma_0(l_3,\eta,b)+a\left(\frac{\partial}{\partial l_4}\right)^p\Gamma_0(l_4,\eta,b)\right] \tag{21}$$

and

$$\Gamma_{12}(\vec{b})=-\left[\left(\frac{\partial}{\partial l_1}\right)\Gamma_0(l_1,\eta,b)+a\left(\frac{\partial}{\partial l_2}\right)\Gamma_0(l_2,\eta,b)\right]. \tag{22}$$

The expression (20) for Γ_0 can be reduced along the lines of Ref. 35 to the form

$$\Gamma_0(\lambda,\eta,b)=-16\pi\eta^2K_0(\lambda,\eta,b), \tag{23}$$

where

$$K_0(\lambda,\eta,b)=\lambda^{-2}(i\lambda b)^{-2i\eta}\mathfrak{L}_{2i\eta-1,0}(i\lambda b), \tag{24}$$

the function $\mathfrak{L}_{\mu,\nu}(iu)$ being a modified version of the Lommel function introduced by Thomas and Chan.[35]

Combining Eqs. (16), (21), (22), and (23) and substituting the resulting expression for $\Gamma_1(\vec{b})$ in Eq. (12), we obtain the single-scattering amplitude as

$$F_1(\vec{q})=32iK_iN_f^*N_i\pi\eta^2\times\sum_{j=1}^{2}\sum_{k=1}^{n+1}d_{jk}\left(\frac{\partial}{\partial\xi_{jk}}\right)^{t_k}I(\xi_{jk},\eta,q), \tag{25}$$

where

$$I(\lambda,\eta,q)=\int_0^\infty db\,bJ_0(qb)K_0(\lambda,\eta,b) \tag{26}$$

and $d_{11}=A_2, d_{21}=aA_2, t_1=1, \xi_{11}=l_1, \xi_{21}=l_2$; $d_{1k}=c_{k-1}A_1, d_{2k}=ad_{1k}, t_k=k-1, \xi_{1k}=l_3, \xi_{2k}=l_4$ for $k=2,3,\ldots,n+1$. The integral in Eq. (26) can be evaluated[35] to give

$$I(\lambda,\eta,q)=-\tfrac{1}{2}\Gamma(i\eta)\Gamma(1-i\eta)q^{2i\eta-2}\lambda^{-2i\eta-2}\times {}_2F_1(1-i\eta,1-i\eta;1;-\lambda^2/q^2)\,, \quad (27)$$

which, when substituted in Eq. (25), gives the final closed-form expression for the single-scattering amplitude.

The present method of reduction of the amplitude differs from that of Thomas and Chan[35] in an early breaking of the full function $\Gamma(\vec{b},\vec{r}_1,\vec{r}_2)$ in terms of the functions $\Gamma(\vec{b},\vec{r}_j)$ via Eq. (9). This results in the expression (25) for the single-scattering amplitude where each term in the double summation involves only one wave-function-dependent parameter (ξ_{jk}). The corresponding expression in Thomas and Chan,[35] on the other hand, would have involved a greater number of two-parameter terms.

A. Evaluation of $F_2(\vec{q})$

To evaluate $F_2(\vec{q})$, we combine Eqs. (17), (21), (22), and (23) and substitute the resulting expression for $\Gamma_2(\vec{b})$ in Eq. (13). Thus, we have

$$F_2(\vec{q})=-512iK_iN_f^*N_i\pi^2\eta^4\int_0^\infty db\,bJ_0(qb)\left[\sum_{j=1}^{4}\sum_{k=1}^{n}h_{jk}\left(\frac{\partial}{\partial\xi_j}\right)K_0(\xi_j,\eta,b)\left(\frac{\partial}{\partial\xi_j}\right)^k K_0(\xi_j,\eta,b)\right], \quad (28)$$

where $h_{1k}=c_k, h_{2k}=h_{3k}=ac_k, h_{4k}=a^2c_k, \xi_1=\xi_2=l_1$, $\xi_3=\xi_4=l_2, \zeta_1=\zeta_3=l_3$, and $\zeta_2=\zeta_4=l_4$.

For the evaluation of the integral in Eq. (28), we are to calculate the function K_0 and its various derivatives. This may be done by using Eq. (24) for K_0, as expressed in terms of $\mathfrak{L}_{\mu,\nu}(iu)$ and making use of the recurrence relations[35] among $\mathfrak{L}_{\mu,\nu}(iu)$. However, calculation of the functions $\mathfrak{L}_{\mu,\nu}(iu)$ involves a lot of high precision numerical work. Thomas and Chan[35] have expressed $\mathfrak{L}_{\mu,\nu}(iu)$ as a combination of two hypergeometric series [Eq. (A6) of Ref. 35]. The expansion parameter in each of these series is $(\frac{1}{2}u)^2$. For small values of the argument u, $\mathfrak{L}_{\mu,\nu}(iu)$ can be calculated without difficulty. But as the value of u increases, the number of terms required for convergence of each of the two hypergeometric series becomes very large. Hence, for accurate numerical evaluation of $\mathfrak{L}_{\mu,\nu}(iu)$, the computations are to be performed entirely in double precision. For sufficiently large values of u, however, Thomas and Chan[35] have used an asymptotic expansion for $\mathfrak{L}_{\mu,\nu}(iu)$ in terms of $(\frac{1}{2}u)^{-2}$ [Eq. (A17) of Ref. 35].

An alternative numerical method for the evaluation of K_0 and its various derivatives have recently been proposed by Sur *et al.*[38] and has the advantage of requiring only normal precision during computation. To start with, we substitute the integral representation [Eq. (A7) of Ref. 35] of $\mathfrak{L}_{2i\eta-1,0}(iu)$:

$$\mathfrak{L}_{2i\eta-1,0}(iu)=-2^{2i\eta-1}(iu)^{2i\eta}\frac{\Gamma(i\eta)}{\Gamma(1-i\eta)}\times\int_0^\infty dt\,t^{-2i\eta+1}\frac{J_0(t)}{t^2+u^2} \quad (29)$$

in Eq. (24) and obtain

$$K_0(\lambda,\eta,b)=A(\eta)\lambda^{-2}\int_0^\infty dt\,t^{-2i\eta+1}\frac{J_0(t)}{t^2+u^2}\,, \quad (30)$$

where $u=\lambda b$ and $A(\eta)=-2^{2i\eta-1}\Gamma(i\eta)/\Gamma(1-i\eta)$. The integrand in Eq. (30) has a branch-point singularity at $t=0$, which makes it highly oscillatory in this limit. However, as long as $u>0$, the integrand is bounded as $t\to 0$. On the other hand, as $t\to\infty$, the function $J_0(t)$ gives rise to rapid oscillations of the integrand. These highly oscillatory natures of the integrand at both the limits of t make direct numerical evaluation of the integral in Eq. (30) extremely troublesome.

In order to avoid the above difficulties, Sur *et al.*[38] break up the range of integration in Eq. (30) into two parts, such that

$$K_0(\lambda,\eta,b)=A\lambda^{-2}[M_1(\eta,u)+M_2(\eta,u)]\,, \quad (31)$$

where

$$M_i(\eta,u)=\int_{a_i}^{b_i}dt\,t^{-2i\eta+1}\frac{J_0(t)}{t^2+u^2}, \quad i=1,2 \quad (32)$$

with $a_1=0, b_1=t_0; a_2=t_0, b_2\to\infty$. The function $J_0(t)$ in these two ranges can be represented, respectively, by[44]

$$J_0(t)=\sum_{k=0}^{6}a_k(t/t_0)^{2k}+O(10^{-8})\,, \quad t\le t_0; \quad (33)$$

and

$$J_0(t)=t^{-1/2}f(t)\cos\theta(t)\,, \quad t_0\le t<\infty\,, \quad (34)$$

where

$$f(t)=\sum_{k=0}^{6}b_k(t_0/t)^k+O(10^{-8})\,, \quad (34a)$$

$$\theta(t)=t+\sum_{k=0}^{6}d_k(t_0/t)^k+O(10^{-8}) \quad (34b)$$

with $t_0=3$ and a_k, b_k, and d_k being numerical constants.

On substitution for J_0 from Eq. (33) in Eq. (32), one obtains for M_1

$$M_1(\eta,u)=\sum_{k=0}^{6} a_k \int_0^{t_0} dt\, t^{-2i\eta+1}\frac{(t/t_0)^{2k}}{t^2+u^2}\,. \tag{35}$$

By a change of integration variable as $y=(t/t_0)^2$, M_1 becomes

$$M_1(\eta,u)=B(\eta)\sum_{k=0}^{6} a_k G_{k,1}(\eta,v)\,, \tag{36}$$

where

$$G_{p,m}(\eta,v)=\int_0^1 dy\,\frac{y^{p-i\eta}}{(y+v)^m} \tag{37}$$

with $B(\eta)=\frac{1}{2}t_0^{-2i\eta}$ and $v=(u/t_0)^2$. The integrals $G_{p,m}$ obey the recurrence relations (A2) through (A5) of the Appendix. Differentiation of M_1 can be performed via the relation (A5). The resulting functions $G_{p,m}$ can all be generated from such a single integral by making use of the relations (A2) through (A4). For efficient calculation, this integral is chosen to be the one with the largest value of each of the parameters p and m, and is evaluated numerically. The repeated use of the recurrence relations for the generation of other functions $G_{p,m}$ with lower values of p and m then do not cause any loss of precision. This has been ensured by actual computations.[38]

M_2 can be similarly written, after substitution for J_0 from Eq. (34) in Eq. (32) as

$$M_2(\eta,u)=\int_{t_0}^{\infty} dt\, t^{-2i\eta+1/2} f(t)\frac{\cos\theta(t)}{t^2+u^2}\,. \tag{38}$$

This is conveniently put in the form

$$M_2(\eta,u)=\tfrac{1}{2}[F_+(\eta,u,1)+F_-(\eta,u,1)]\,, \tag{39}$$

where

$$F_\pm(\eta,u,s)=\int_{t_0}^{\infty} dt\, t^{-2i\eta+1/2} f\frac{e^{\pm i\theta}}{(t^2+u^2)^s}\,. \tag{40}$$

Derivatives of $F_\pm$ and hence of M_2 can be obtained using the recurrence relation (A6) of the Appendix. Direct numerical evaluation of Eq. (40) is still not possible because of the exponential phase terms in the integrand. One can, however, conveniently pass over to the complex $t(x-z)$ plane and rotate the path of integration on this plane parallel to the imaginary axis. This can be achieved by introducing the transformations $t=t_0\pm iz$ and choosing the contours of integration in the first and fourth quadrants, respectively, on the t plane. This results in the following expression for $F_\pm$:

$$F_\pm(\eta,u,s)=\pm\tfrac{1}{2}i\exp[\pm i(t_0+d_0)]\int_0^{\infty} dz\, e^{-z}N_\pm(z,s)\,, \tag{41}$$

where

$$N_\pm(z,s)=\frac{t^{-2i\eta+1/2}}{(t^2+u^2)^s} f\exp\left[\pm i\sum_{k=1}^{6} d_k\left(\frac{t_0}{t}\right)^k\right]. \tag{42}$$

The appearance of the exponential damping factor in the integral in Eq. (41) makes it easily integrable by the Gauss-Laguerre quadrature method. Thus one gets rid of the numerical trouble due to the infinite number of oscillations of $J_0(t)$ as $t\to\infty$.

After calculating M_1 and M_2 and their various derivatives by the above method, Eq. (31) can be used to obtain $K_0(\lambda,\eta,b)$ and its derivatives required for substitution in expression (28) for the double-scattering amplitude $F_2(\vec{q})$. This method is applicable for a wide range of values of $u=\lambda b$, except for very small values. At such small values, the direct series for $\mathfrak{L}_{\mu,\nu}(iu)$ [Eq. (A6) of Ref. 35] can be conveniently used to compute K_0 and its various derivatives by the help of Eq. (24).

The above method of calculation of K_0 and its derivatives has already been tested properly by Sur *et al.* in their work.[38] They used Eq. (24) to check their calculated values at certain limiting sets of values of the parameters λ,η, and b against those obtained from the method of Thomas and Chan[35] and found good agreement between the two results.[38]

The Glauber differential cross sections in the center of mass frame is given by

$$\sigma(q)=(K_f/K_i)\,|F_1(\vec{q})+F_2(\vec{q})|^2\,, \tag{43}$$

whence the total cross sections can be obtained as usual.

IV. RESULTS

A. GOS values

In Fig. 1, we have plotted against q^2 the present GOS values using the WL wave functions for the transitions $1^1S\to 2^1S$ and $1^1S\to 3^1S$ in He. The results are compared with the existing theoretical results of Kim and Inokuti[40] and of Van den Bos.[4] For the 2^1S excitation, we have also included in the same figure the experimental results of Vriens *et al.*[41] and of Silverman and Lassettre.[42] For both the 2^1S and 3^1S excitations, the present results are closer to the result of Kim and Inokuti[40] in comparison with that of Van den Bos.[4] Though fluctuations in experimental points are significant, the present 2^1S results have, on the average, satisfactory agreement with the experiments. This demonstrates the reliability of the WL wave functions. A similar inference has been drawn earlier by Sur *et al.*[11] from the calculation of the GOS values for the 4^1S excitation of He using the WL wave functions.

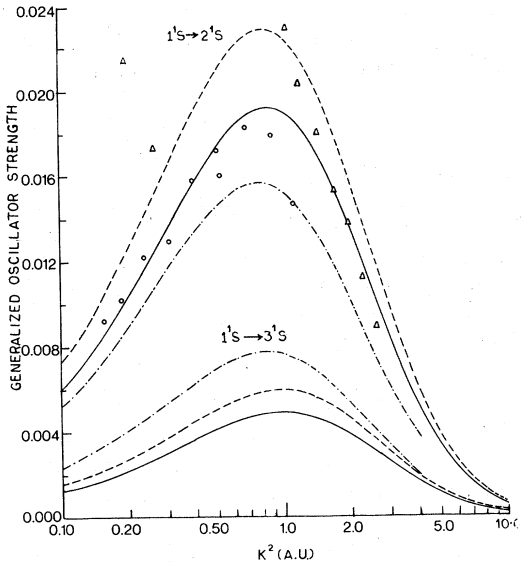

FIG. 1. Generalized oscillator strengths for the $2\,^1S$ and $3\,^1S$ excitations of helium. Theory, for $2\,^1S$ and $3\,^1S$: ———, present calculation; — — —, calculation of Kim and Inokuti (Ref. 40); — · — · —, calculation of Van den Bos (Ref. 4). Experiment, for $2\,^1S$: O, Vriens *et al.* (400, 300, and 225 eV of incident electron energy) (Ref. 41); △, Silverman and Lassettre (500 eV of incident electron energy) (Ref. 42).

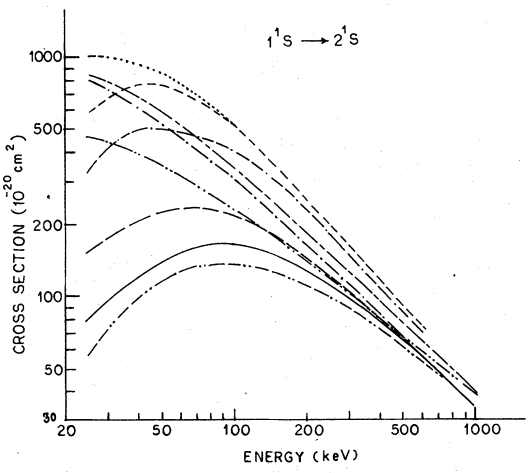

FIG. 2. Cross section for the $2\,^1S$ excitation of helium by proton impact. Theory: ———, present Glauber (full); — — —, present Glauber (single); — · — · —, present Born; — — — — —, Bell *et al.* (Ref. 1); · · ·, Baye and Heenen (Ref. 8); - - -, Flannery (Ref. 5); — — · — —, Begum *et al.* (Ref. 9); — · · — · · —, Roy and Mukherjee (Ref. 7); — — · · — — · ·, Joachain and Van der Poorten (Ref. 10).

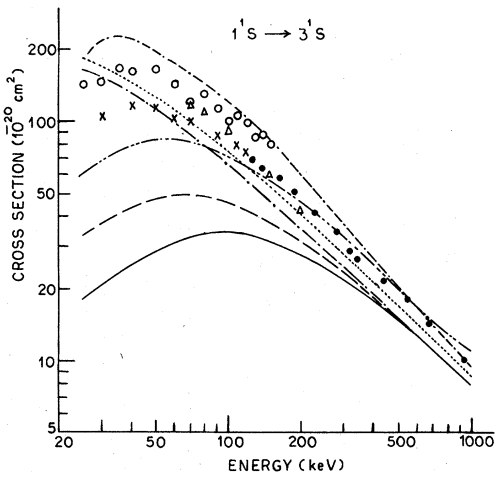

FIG. 3. Cross section for the $3\,^1S$ excitation of helium by proton impact. Theory: ———, Glauber (full); — — —, Glauber (single); — · — · —, Born; · · ·, Bell *et al.* (Ref. 1); — — · — —, Baye and Heenen (Ref. 8); — · · — · ·, Roy and Mukherjee (Ref. 7). Experiment: O, Van den Bos *et al.* (Ref. 16); ×, Dodd and Hughes (Ref. 12); △, Denis *et al.* (Ref. 15); ●, Scharmann and Schartner (Ref. 18).

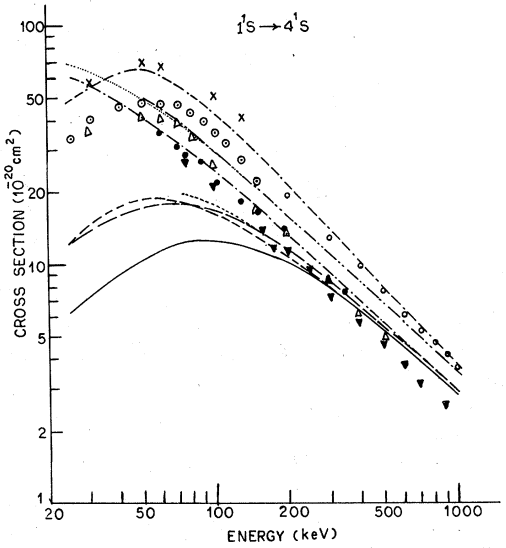

FIG. 4. Cross section for the $4\,^1S$ excitation of helium by proton impact. Theory: ———, Glauber (full); — — —, Glauber (single); — · — · — ·, Born; · · ·, Bell *et al.* (Ref. 1); - - -, Sur *et al.* (distortion approximation using WL wave function) (Ref. 11); ---, Sur *et al.* (second Born approximation using WL wave function) (Ref. 11); — · · — · · — · ·, Oldham (Ref. 2); · — — · — —, Baye and Heenen (Ref. 8). Experiment: ×, Dodd and Hughes (Ref. 12); ⊙, Van Bos *et al.* (Ref. 16) △, Denis *et al.* (Ref. 15); ●, Robinson and Gilbody (Ref. 14); ▽, Thomas and Bent (Ref. 13); o, Hasselkamp *et al.* (Ref. 19).

B. Excitation cross sections

For testing the present method of reduction of the Glauber scattering amplitude, we have applied it to calculate the differential cross sections for 2^1S excitation of He by electron impact using WL wave functions. A comparison with the graphical results of Yates and Tenney[32] shows that at 26.5 eV, the smallest incident energy considered by these authors, the large-angle cross sections agree within 5% with our results. The agreement is fairly good, especially when one considers the difference in wave functions used by Yates and Tenney[32] and by us. This also demonstrates the validity and usefulness of the present procedure.

Our proton-impact results for $1^1S \rightarrow n^1S$ ($n = 2$, 3, and 4) excitations of He are displayed graphically in Figs. 2–4. The single-scattering (F_1) and double-scattering (F_2) parts of the Glauber amplitude have been calculated separately and the corresponding single-scattering cross sections are included in these figures along with the total Glauber cross sections. In Figs. 2 and 3, we also include the FBA cross sections for proton impact 2^1S and 3^1S excitations of He using the WL wave functions.

1. $1\,^1S \rightarrow 2\,^1S$ transition

In Fig. 2, we compare the present Glauber cross sections with some of the existing theoretical calculations.[1,3-10] The FBA[4] and the four- and nine-state[3] results of Van den Bos, and also the SBA results of Holt *et al.*[6] are not included in Fig. 2. Whereas the coupled-state calculations[3] of Van den Bos agree well with that of Begum *et al.*,[9] the result of Holt *et al.*[6] shows an energy dependence similar to the present Born cross sections above 75 keV keeping consistently higher by almost 20% than the later result. No experimental data is available for this transition. The existing other theoretical cross section results for the 2^1S excitation show an appreciable amount of variation among themselves in absolute values, as may be seen from Fig. 2.

The present Glauber cross sections approach the corresponding FBA result using the WL wave functions in the high-energy region, the two results coinciding with each other above 500 keV. At such energies, single-scattering contributions dominate the cross sections. The effect of the double-scattering term (F_2) in the Glauber amplitude becomes appreciable at intermediate energies, where it substantially lowers the net Glauber cross sections from the corresponding single-scattering result. The total Glauber cross sections, although they underestimate most of the existing theoretical results, give values larger than the distorted-wave result of Joachain and Van der Poorten.[10] The last result also exhibits an energy dependence similar to the present results.

2. $1\,^1S \rightarrow 3\,^1S$ transition

Our results for the Glauber cross sections are displayed in Fig. 3 along with the available theoretical[1,7,8] and experimental[12,15-18] results. The discrepancies among various absolute measurements widely exceed the estimated error limits of the respective authors, especially in the intermediate-energy region. At such energies, different theoretical data show still greater spread among themselves. The calculation of Baye and Heenen[8] employing the second-order diagonalization method, however, shows somewhat good absolute agreement with experiments at all energies. The distortion calculation of Roy and Mukherjee[7] also does so in the high- and low-energy regions.

The Glauber and Born curves for 3^1S excitation cross sections exhibit features similar to those observed for 2^1S excitation. Again, the effect of the double-scattering term (F_2) on the total Glauber cross section is negligible at energies above 500 keV, where the two Glauber curves coincide also with the FBA curve. The FBA result apparently shows some better agreement with experiments in comparison with the Glauber results. However, the Born cross sections fail to predict the energy dependence of the observed data, which the Glauber results can give successfully.

3. $1\,^1S \rightarrow 4\,^1S$ transition

A good number of theoretical[2,4,8,11] as well as experimental[12-16,18,19] investigations have been made for this transition, although the situation concerning agreement between theory and experiment differs hardly from those of 2^1S and 3^1S cases. Some of the available cross-section results are shown in Fig. 4 along with the present Glauber results. We exclude from this figure the FBA calculation of Van den Bos[4] who used a set of improperly orthogonalized-wave functions in the calculation. The resulting cross sections largely overestimated the measured values even at the highest energies considered. A number of other previous Born calculations[1,2,11] using very accurate many-parameter wave functions can all show various degrees of absolute agreement with the experiments. But none of these calculations can exhibit the energy dependence of the data correctly throughout the energy regions considered. However, the functional dependence of the observed cross sections on energy are well predicted by the second-order diagonalization method[8] and the distortion method[11] down to an incident energy of

20 keV.

As regards the present Glauber calculations, the single-scattering cross sections, as earlier, contribute predominantly at high energies. The result compares closely with the distortion calculation of Sur *et al.*[11] with WL wave functions at intermediate energies and coincide with their corresponding SBA result above 150 keV. The total Glauber cross sections coincide with the distortion ones above 300 keV and can also give the energy dependence of the observed data down to much lower energies.

V. DISCUSSION

From a study of the differential cross sections (not presented here) corresponding to the various total cross-section results presented above, it has been observed that for intermediate proton energies, the relative contribution of the double-scattering term (F_2) in the Glauber amplitude is appreciable at all scattering angles and increases towards large angles. The overall effect of inclusion of F_2 on the total Glauber cross sections has always been to reduce the single-scattering result. However, this effect becomes negligible at high energies, where the single-scattering term (F_1) alone can predict the effective total Glauber cross sections.

As regards the absolute matching among various calculated and measured cross sections, the above results perhaps indicate that no rigorous comparison is possible. At intermediate energies, both theoretical and experimental data show wide variations in absolute values, an appreciable amount of which persists even at the highest energies considered. This is not quite unexpected for the theoretical data in view of the variety of He wave functions used in the different calculations. The cross sections are very sensitive to the choice of wave functions, especially for higher excitations. Even the high-energy Born cross sections have earlier[11] been found to vary by a factor of almost 2 due to inaccuracies like nonorthogonality in the wave functions. On the other hand, a variety of absolute calibration techniques have been used in different measurements. In any particular procedure, it was impossible to pay attention to all the criteria for valid and accurate data.[45]

Under such circumstances, the physically consistent feature of various data which can be compared meaningfully should be the functional dependence of the cross sections on energy. This was observed by Thomas[45] and later by Sur *et al.*[11] with regard to the $4\,^1S$ excitation of He by proton impact. In the present investigation also, except for the case of Born cross sections, we find reasonable agreement in energy dependence of the cross sections in different sets of data. Our Glauber results are in conformity with this agreement, as may be seen from Figs. 2–4.

A further consistency check is possible for calculations or measurements which make a systematic study of excited states with same total angular momentum but of varying principal quantum number n. The energy dependence of the excitation cross sections $\sigma(n)$ is found to be approximately similar in various data for such states. In a comparison of the cross-section ratios $\sigma(n)/\sigma(n+1)$ obtained by various experimental groups, the systematic errors in absolute calibration should cancel out and hence give similar values.[16,45] To verify this we compare the ratio of cross sections for $3\,^1S$ and $4\,^1S$ states as obtained from the data of Van den Bos *et al.*,[16] Dodd and Hughes,[12] Denis *et al.*,[15] and Scharman and Schartner,[18] as also from the calculations of Baye and Heenen[8] and ours. The average values of the ratios $\sigma(3\,^1S)/\sigma(4\,^1S)$ determined for all energies above 50 keV are shown in Table I. The agreement is found to be poor in case of experimentally measured cross sections. As observed by Thomas,[45] this is attributable to the poor detection sensitivity for measuring the $3\,^1S \rightarrow 2\,^1P$ line emission. The average cross-section ratios predicted by the theoretical calculations, on the other hand, show excellent agreement among themselves. Incidentally, the ratios at different energies above 50 keV in the calculation of Baye and Heenen[8] show a fluctuation exceeding ±10% about the average value shown in Table I. The present Born and Glauber cross sections, however, behave much more consistently, the fluctuations barely exceeding ±1%.

In view of the above agreement in average theoretical cross-section ratios, it may be interesting

TABLE I. Average ratio of cross sections $[\sigma(3\,^1S)/\sigma(4\,^1S)]$ at energies above 50 keV.

Theory				Experiment			
Baye and Heenen (Ref. 8)	Present Born	Present Glauber	n^{-3} law	Van den Bos *et al.* (Ref. 16)	Dodd and Hughes (Ref. 12)	Denis *et al.* (Ref. 15)	Scharman and Schartner (Ref. 18)
2.74	2.72	2.74	2.37	3.50	1.65	3.37	4.26

to consider in addition the asymptotic high-energy behavior of the cross sections. This was originally done by Bethe[46] and subsequently by others[11,47] with reference to the Born approximation. For collisional transitions of a single electron from the ground state to nl states, the Born cross sections are found to be proportional to n^{-3}, when the other features of the collision remains unchanged. The average theoretical cross-section ratios $\sigma(3\,^1S)/\sigma(4\,^1S)$ given in Table I are in reasonable agreement with the value (2.37) obtained from the n^{-3} law.

VI. CONCLUSION

For direct collisional excitation of ground-state He by incident protons, a reliable physical feature for comparison between theory and experiment is the functional dependence of cross sections on energy rather than the absolute values of the cross sections. Furthermore, for excited states of He having same total angular momentum but varying principal quantum number, the average ratio of cross sections at high energy predicted by different theoretical data can show reasonable agreement among themselves, as also with the n^{-3} law of cross sections. Due to possible inaccuracies in measuring the absolute $3\,^1S$ cross sections, this may not be apparent from the experimental cross-section ratios presented in Table I. However, as one may observe from the work of Thomas,[45] the cross-section ratio furnishes a good consistency check on measured data for still higher n states.

The present calculation for proton impact $2\,^1S$, $3\,^1S$, and $4\,^1S$ excitations of ground-state He using the Glauber approximation conforms to the above observations. Though the Glauber results at intermediate energies underestimate other absolute theoretical and observed cross sections to some extent, the energy dependence of the cross sections are predicted well from intermediate- to high-energy regions. The Glauber method is also able to give a good estimate of the cross-section ratio for $3\,^1S$ and $4\,^1S$ states in agreement with other theories.

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APPENDIX

A. Recurrence relations for $G_{p,m}(\eta,x)$

The integral $G_{p,m}(\eta,x)$ has been defined in Eq. (37) of text as

$$G_{p,m}(\eta,x)=\int_0^1 dy\,\frac{y^{p-i\eta}}{(y+x)^m}\,, \tag{A1}$$

where $p\geq 0$ and $m>0$. The integrand is bounded at the lower limit as long as $x>0$.

Considering the integral $G_{p-1,m-1}(\eta,x)$ on partial integration we have

$$G_{p-1,m-1}(\eta,x)=\frac{1}{p-i\eta}\left(\frac{y^{p-i\eta}}{(y+x)^{m-1}}\right)_{y=0}^{y=1}+\frac{m-1}{p-i\eta}\int_0^1 dy\,\frac{y^{p-i\eta}}{(y+x)^m}\,.$$

The first term on the right-hand side vanishes at the lower limit, while the integral in the second term can be identified as $G_{p,m}(\eta,x)$ whence we obtain

$$G_{p-1,m-1}(\eta,x)=\frac{1}{p-i\eta}\left(\frac{1}{(1+x)^{m-1}}+(m-1)G_{p,m}(\eta,x)\right), \tag{A2}$$

which is valid for $p\geq 1, m>1$. Again, multiplying the integral in Eq. (A1) by $x\,[=(y+x)-y]$ gives

$$xG_{p,m}(\eta,x)=\int_0^1 dy\,\frac{y^{p-i\eta}}{(y+x)^{m-1}}-\int_0^1 dy\,\frac{y^{p+1-i\eta}}{(y+x)^m}\,.$$

The two integrals on the right-hand side are identifiable as $G_{p,m-1}(\eta,x)$ and $G_{p+1,m}(\eta,x)$, respectively, whence on transposition we have

$$G_{p,m-1}(\eta,x)=G_{p+1,m}(\eta,x)+xG_{p,m}(\eta,x)\,. \tag{A3}$$

Alternatively, redefining the index p in Eq. (A3), it can be written as

$$G_{p-1,m}(\eta,x)=(1/x)[G_{p-1,m-1}(\eta,x)-G_{p,m}(\eta,x)]\,. \tag{A4}$$

Finally, we can perform repeated differentiations of $G_{p,m}(\eta,x)$ with respect to x as

$$\left(\frac{d}{dx}\right)^l G_{p,m}(\eta,x)=\int_0^1 dy\,y^{p-i\eta}\left[\left(\frac{d}{dx}\right)^l (y+x)^{-m}\right],$$

where we have changed the orders of integration and the repeated differentiations. It is straightforward to show that

$$(d/dx)^l(y+x)^{-m}=(-1)^l(m)_l(y+x)^{-m-l}\,.$$

Hence we can write

$$\left(\frac{d}{dx}\right)^l G_{p,m}(\eta,x)=(-1)^l(m)_l G_{p,m+l}(\eta,x). \qquad \text{(A5)}$$

For studying n^1S excitation the various $G_{p,m}$ integrals required are those for which $p=1,2,\ldots,6$ and $m=1,2,\ldots,n+1$. The numerical integration is performed only for $G_{7,m+2}(\eta,x)$, whence all others can be generated by repeated use of relations (A2) through (A4) in order.

B. Recurrence relation for $F_\pm(\eta,x,s)$

The integral $F_\pm(\eta,x,s)$ defined in Eq. (40) of text may be repeatedly differentiated with respect to x in the form

$$\left(\frac{1}{x}\frac{d}{dx}\right)^l F_\pm(\eta,x,s)=\int_{t_0}^{\infty} dt\, t^{-2i\eta+1/2} f(t) e^{\pm i\theta(t)} \times\left[\left(\frac{1}{x}\frac{d}{dx}\right)^l (t^2+x^2)^{-s}\right],$$

where we have changed, as earlier, the order of integration with the repeated differentiations. Now, since

$$\left(\frac{1}{x}\frac{d}{dx}\right)^l (t^2+x^2)^{-s}=(-2)^l(s)_l (t^2+x^2)^{-s-l},$$

we have

$$\left(\frac{1}{x}\frac{d}{dx}\right)^l F_\pm(\eta,x,s)=(-2)^l(s)_l F_\pm(\eta,x,s+l). \qquad \text{(A6)}$$

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