$$K(SL \rightarrow SL'') = V_a \frac{A(SL \rightarrow SL'')}{A(SL)} \sum_{M_L} Q_{|M_L|} , \quad (3.34)$$

$$\sum_{F,M_F} \tau(\tfrac{1}{2}1JIFM_F) = \tfrac{1}{3}(2J+1)(2I+1) , \quad (3.42)$$

$$K_Z(^2P_J \rightarrow {}^2S) = \frac{V_a}{2(2I+1)} \left(\frac{(2J+1)(2I+1)\,Q_1}{3} + \mu(\tfrac{1}{2}1JI)(Q_0 - Q_1) \right) , \quad (3.43)$$

$$K(^2P_J \rightarrow {}^2S) = \tfrac{1}{6} V_a (2J+1)(2Q_1 + Q_0) . \quad (3.45)$$

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Glauber Cross Sections for Excitation of the $2\,^1S$ State of Helium by Electron Impact*

A. C. Yates and A. Tenney
Department of Chemistry, Indiana University, Bloomington, Indiana 47401
(Received 8 May 1972)

The Glauber amplitude for describing collisions of charged particles with two-electron atoms, resulting in transitions between spherically symmetrical states, is reduced to a readily computable form. Application is then made to the $2^1S \leftarrow 1^1S$ transition in helium, for which angular distributions are determined for 26.5-, 34-, 50-, and 83-eV incident electrons. Comparison with experiment shows that the Glauber theory is capable of accurately predicting the angular distributions for even our lowest-energy calculation. In particular the theory predicts the recently observed structure in the differential cross section. The energy dependence of the "apparent" generalized oscillator strength is also demonstrated for incident energies in the range 300–1100 eV.

A number of recent papers have dealt with the applicability and usefulness of the Glauber approximation[1] with respect to collisions of charged particles with atomic systems. In particular, a fairly complete study of the approximation as applied to the elastic and inelastic (bound-state excitation) scattering of electrons and protons by hydrogen,[2–5] has shown the Glauber theory to be quite accurate in the energy range where the first Born approximation is known to fail and close-coupling theories[6] with their modifications[7] are not feasible. Additional applications have been made to helium[5,8,9] and lithium,[10] and quite recently the theory has been applied to impact ionization of hydrogen[11] by electrons, and multiple scattering effects[12] in electron-molecule collisions.

Although Thomas and Gerjuoy[4] have been able to obtain closed form expressions for the scattering amplitudes for the excitation of certain energy levels of hydrogen by electrons or protons, it is unlikely that such will be the case for many-electron atomic systems even with the simplest approximate wave functions. Using a particular form for the atomic wave function, however, Franco[13] has been successful in reducing the $(3Z+2)$-dimensional integral occurring in the amplitude expression (for scattering of charged particles by a Z-electron atom) to a one-dimensional integral involving products of the generalized ${}_1F_2(a;\, b,\, c;\, x)$ hypergeometric functions. This expression is quite appealing in its scope, but apart from (e^-, H) and (p^+, H) collisions, its numerical tractability has yet to be demonstrated. Thus, the essential aim of the present article is to present a simplification of the Glauber amplitude for the two-electron atom, for certain excitations by charged particles. Specifically, the amplitude for excitation by electrons, of ground state helium ($1\,^1S$), to the first metastable state ($2\,^1S$) is put in a readily computable form and evaluated. The differential cross sections for this process for selected energies in the 25–1100 eV range are presented and compared with experiment and other theoretical values.

The collision amplitude $F_{fi}(\vec{q})$, where the atom (two electrons in the field of a doubly positively charged core, e.g., He, alkaline earths, Hg, etc.) is excited from some initial state i to some final state f by an incident electron, is given according to the Glauber theory by

$$F_{fi}(\vec{q}) = \frac{ik_i}{2\pi} \int d\vec{b}\, e^{i\vec{q}\cdot\vec{b}} \langle \Psi_f(\vec{r}_1, \vec{r}_2) | 1 - \gamma(\vec{b}, \vec{r}_1) \times \gamma(\vec{b}, \vec{r}_2) | \Psi_i(\vec{r}_1, \vec{r}_2) \rangle , \quad (1)$$

where

$$\gamma(\vec{b}, \vec{r}_i) = (|\vec{b} - \vec{s}_i| / b)^{2i\eta} \quad (2)$$

and $\eta = 1/k_i$. Here Ψ_i and Ψ_f are the wave functions representing the target state before and after collision. $\vec{k}_i$ and $\vec{k}_f$ are, respectively, the incident

and final momenta of the scattering electron, and $\vec{q}=(\vec{k}_i-\vec{k}_f)$ is the momentum transfer (note that Hartree atomic units are used). The vector $\vec{b}$ is two-dimensional and lies in a plane perpendicular to the incident direction, as does $\vec{q}$; $\vec{r}_i=\vec{s}_i+\vec{Z}_i$. A complete description of the coordinate system has been given by Tai, Bassel, Gerjuoy and Franco.[2]

For transitions between spherically symmetrical states, Franco[8] has shown that Eq. (1) may be reduced to

$$F_{fi}(\vec{q})=4\pi^2 ik_i\int dr\,d\theta\,d\varphi\,dz_1dz_2r^5\sin^3\theta\cos\theta \times\sin\varphi\cos\varphi\,J_0(qr\cos\theta)\Psi_f^*A(\theta,\ \varphi)\Psi_i\,, \quad (3)$$

where the integration variables r, θ, φ have arisen owing to a transformation of b, s_1, and s_2 to spherical polar coordinates, and $A(\theta,\ \varphi)$ is a function of products of Gauss hypergeometric functions. With the possible exception of functional forms depending explicitly on interelectronic distances, virtually all approximate wave functions for the types of states under consideration may be put in the form

$$\Psi_i(\vec{r}_1,\ \vec{r}_2)=\sum_j a_j^{(i)}r_1^{n_j^{(i)}}r_2^{m_j^{(i)}}e^{-b_j^{(i)}r_1}e^{-c_j^{(i)}r_2}, \quad (4)$$

where $n_i^{(i)}$ and $m_i^{(i)}$ are integers. Substituting (4) into (3) and carrying out the z integrations gives

$$F_{fi}(\vec{q})=16\pi^2 ik_iP\int_0^{\pi/2}d\theta\int_0^{\pi/2}d\varphi\,A'(\theta,\ \varphi) \times\int_0^{\infty}dr\,r^7J_0(qr\cos\theta) \times K_1(\alpha r\sin\theta\sin\varphi)K_1(\beta r\sin\theta\cos\varphi)\,, \quad (5)$$

with

$$P=\sum_{j,k}a_j^{(i)}a_k^{(f)}\left(\frac{-d}{db_j^{(i)}}\right)^{n_j^{(i)}}\left(\frac{-d}{db_k^{(f)}}\right)^{n_k^{(f)}}\left(\frac{-d}{dc_j^{(i)}}\right)^{m_j^{(i)}} \times\left(\frac{-d}{dc_k^{(f)}}\right)^{m_k^{(f)}} \quad (6)$$

and

$$\alpha=b_j^{(i)}+b_k^{(f)}\,,\quad \beta=c_j^{(i)}+c_k^{(f)}\,. \quad (7)$$

Equation (5) gives the amplitude in the form evaluated by Franco for elastic collisions. This expression may, however, be reduced further by noting that the infinite integration can be done analytically, with the result (see Appendix)

$$F_{fi}(\vec{q})=16\pi^2 ik_iP\int_0^{\pi/2}d\theta\int_0^{\pi/2}d\varphi\,A'(\theta,\ \varphi) \times B(\theta,\ \varphi;\ q)\,, \quad (8)$$

where

$$B(\theta,\ \varphi;\ q)=1536\sqrt{\pi}\,\alpha'\beta'\sum_{l=0}^{3}\frac{(-3)_l\Gamma(l+5)\Gamma(l+3)}{(l!)^2\Gamma(l+\frac{9}{2})} \times\frac{\lambda^{2l}}{[(\alpha'+\beta')^2+\lambda^2]^{l+5}}\ {}_2F_1(l+5,\ \tfrac{3}{2},\ l+\tfrac{9}{2};\ Z)\,, \quad (9)$$

with

$$\alpha'=\alpha\sin\theta\sin\varphi\,,\quad \beta'=\beta\sin\theta\cos\varphi\,,$$

$$\lambda=q\cos\theta\,,\qquad Z=\frac{(\alpha'-\beta')^2+\lambda^2}{(\alpha'+\beta')^2+\lambda^2}\,.$$

Although the amplitude, as given by Eq. (8) is not nearly as simple as the corresponding first Born amplitude, it is readily computed by numerical quadrature as illustrated by the following calculations of the differential scattering cross sections:

$$d\sigma_{fi}(\vec{q})=(k_f/k_i)\,|F_{fi}(\vec{q})|^2 \quad (10)$$

for the 2^1S-1^1S transition in helium.

For the ground state of helium we use an approximate Hartree-Fock function, with the one-electron orbitals chosen to be of the form

$$\varphi(r)=\frac{N_{1S}}{\sqrt{\pi}}\,(e^{-\alpha r}+\eta e^{-\beta r})\,.$$

The parameters chosen are those given by the Hartree-Fock[14] fit of Löwdin[15]: $\alpha=1.455\,799$, $\beta=2\alpha$, $\eta=0.60$, and $N_{1S}=1.484\,23$. The wave function for the $(1s\ 2s)\ 2^1S$ level is chosen to be orthogonal to the ground state and of the form

$$\Psi_{2^1S}=N(\Psi'_{2^1S}-\gamma\Psi_{1^1S})\,,\quad \gamma=\langle\Psi_{1^1S}\,|\,\Psi'_{2^1S}\rangle$$

and N is a normalization constant. The function Ψ'_{2^1S} is of the Eckart form,[16] as determined by Altshuler.[17] The transition energy change for these functions is $\Delta E=0.7239$ a.u. as compared to the experimental value of $\Delta E=0.7576$ a.u. The effect of these energy differences on the calculated cross sections was found to be very slight, and the reported results are for the experimental value of this quantity.

Figures 1–4 give, respectively, the results of our calculations for incident electron energies 26.5, 34, 50, and 82 eV; as compared with experiment, with the first Born approximation, and in Fig. 4, with the high-energy approximation of Hidalgo and Geltman.[20] In Fig. 5 the energy dependence of the "apparent" generalized oscillator strength

$$f_n(q)=\frac{\Delta E}{2}\,\frac{k_0}{k_n}\,d\sigma_{n0}(q)q^2$$

is demonstrated for incident energies in the range 300–1100 eV.

The excitation of the 2^1S state of helium by electron impact has been considered in detail by Rice *et al.*[18] for the energy range of primary interest here (25–100 eV). Their analysis was directed towards determining the qualitative and quantitative

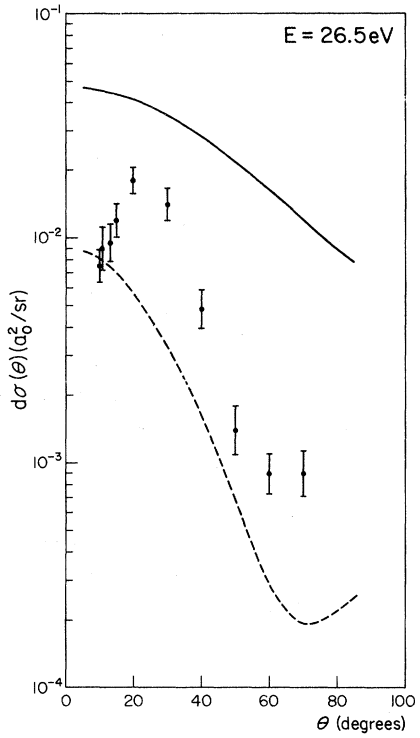

FIG. 1. Differential cross section vs scattering angle θ for incident electron energy $E = 26.5$ eV. Solid line, first Born approximation; dashed line, Glauber approximation; Φ, experimental results of Rice *et al.* (Ref. 18).

validity of first-order plane-wave theories, a similar treatment having been given previously for the 2^1P excitation in helium. Contrary to their findings for the 2^1P excitation, they found that for even qualitative agreement at small angles, some allowance must be made for polarization of the target. Even so, their best approximation to the scattering amplitudes, which includes exchange and charge polarization (in the form of a two-parameter adiabatic polarization potential) gives differential cross sections which, when compared with experiment, are to be considered in quite poor agreement for the energy range 25–100 eV. These results show the need for more accurate representation of polarizing effects (important particularly for small-angle scattering) and distortion and exchange interactions (which become increasingly more significant for large angle scatterings).

With the exception of exchange interactions all of the above effects are to some extent included in the single Glauber amplitude [Eq. (1)]. Byron[5] and more recently Bransden and Coleman[25] have demonstrated the relationship between the Glauber approximation and the close-coupling and usual impact-parameter methods; and as Byron suggests, eikonal approximations are to be viewed "as close-coupling methods in which all channels are included at the expense of making certain approximations in each channel." Thus, core interactions enter into the theory in a very natural way. Birman and Rosendorff[3] have presented a revealing derivation which shows that if, prior to making the Glauber small-angle approximation one closes the summation over all states (appearing in the Lippmann-Schwinger equation) by replacing the intermediate propagation energies by the incident particle energy, then Eq. (1) is derived. It is this approximation which leads to divergence of the Glauber amplitude in the inelastically nonphysical limit of q approaching zero. This, of course, is reminiscent of similar difficulties in approximate second Born calculations.[26]

Figures 1 and 2 show our calculations for incident electron energies of 26.5 and 34 eV, respectively, as compared with the corresponding first Born approximation, and the experimental results of Rice *et al.* The Born approximation is seen to considerably overestimate the magnitude of the differential cross section (except for the very forward direction at 34 eV) and fails to give even qualitatively the shape of the angular distribution

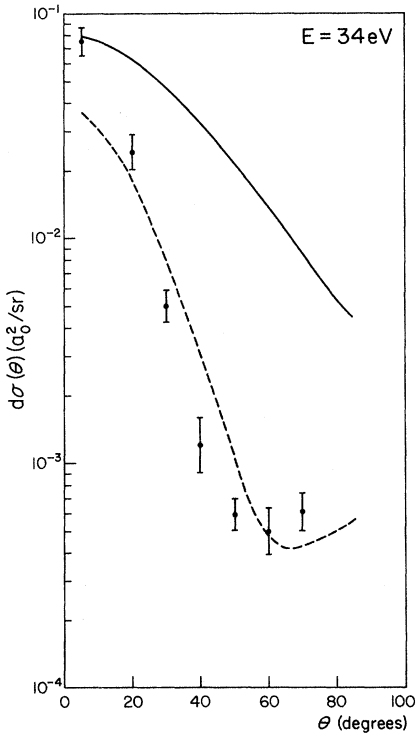

FIG. 2. Differential cross section vs scattering angle θ for incident electron energy $E = 34$ eV. Solid line, first Born approximation; dashed line, Glauber approximation; Φ, experimental results of Rice *et al.* (Ref. 18).

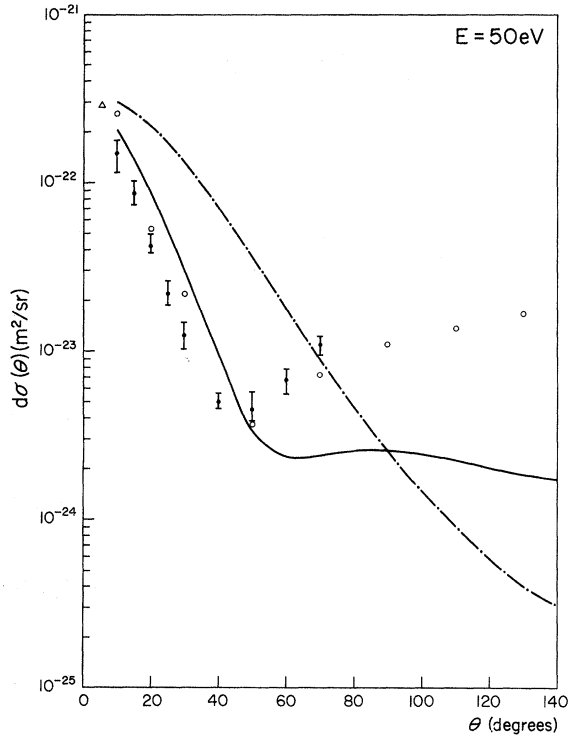

FIG. 3. Differential cross section vs scattering angle θ for $E = 50$ eV. Solid line, first Born approximation; dashed line, Glauber approximation; Φ, experimental results (at 55.5 eV) of Rice *et al.* (Ref. 18); ○, experimental results of Crooks and Rudd (Ref. 19).

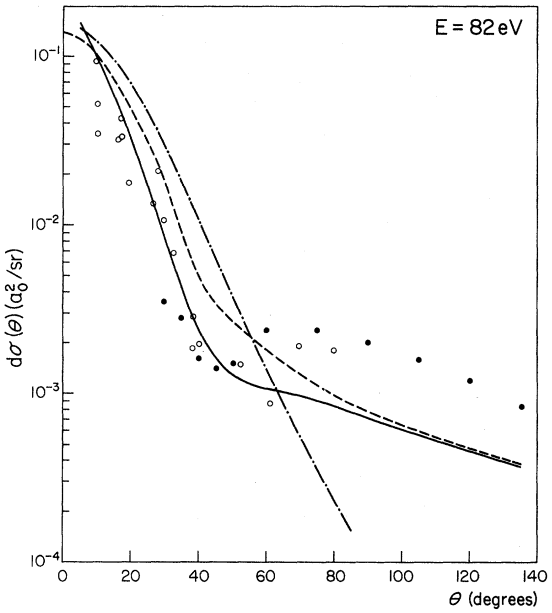

FIG. 4. Differential cross section vs scattering angle θ for $E = 82$ eV. Dot-dashed line, first Born approximation; solid line, Glauber approximation; dashed line, calculation of Hidalgo and Geltman (Ref. 20); ○, experimental, Rice *et al.* (Ref. 18); ●, experimental, Opal and Beaty (Ref. 21).

throughout the angular range. Rice *et al.* reach essentially identical conclusions with their first-order plane-wave polarization-exchange theories. Even for such relatively poor wave functions, the Glauber theory is strikingly successful at these energies. For 34 eV, the theory predicts results which are seen to be quantitative out to $\theta \approx 80°$; and, while the quantitative agreement is not as good for 26.5 eV, the shape of the cross section agrees quite well with experiment.

Comments similar to the above may be made regarding Figs. 3–4, where the calculations are extended to larger angles and to the energies 50 and 82 eV, respectively. In Fig. 3, we also plot the experimental results of Rice *et al.* (at 55.5 eV), Crooks and Rudd,[19] and Chamberlain *et al.*[27] The experimental results in Fig. 4 are those of Rice *et al.* and Opal and Beaty[21]; along with this the calculation of Hidalgo and Geltman[20] is given for comparison. The calculations of Hidalgo and Geltman differ from a first Born result in that allowance is made for the interaction of the incident electron with the nucleus. The effect of this is that some approximation to the distortion of the incident electron by the scatterer is included.

Figure 5, showing the "apparent" generalized oscillator strength, is intended as a summary of our higher energy calculations (300–1100 eV), giving the energy variation of the Glauber cross section. For comparison, various experimental

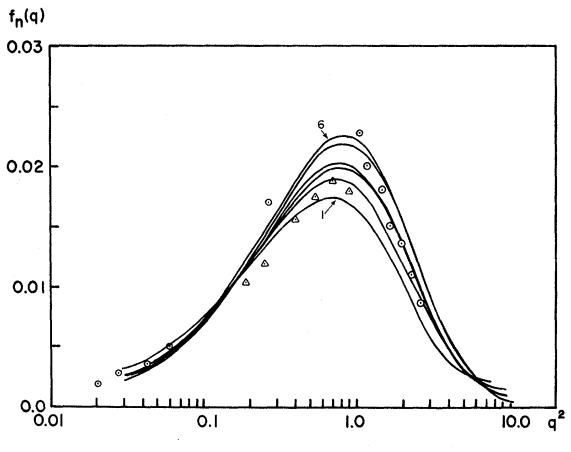

FIG. 5. "Apparent" generalized oscillator strength vs q^2. Curves 1–4, Glauber calculations for incident electron energies, $E = 300$, 500, 900 and 1100 eV, respectively; curve 5, first Born approximation; curve 6, calculation of Kim and Inokuti (Ref. 22). △, experimental results of Vriens *et al.* (Ref. 23) at 300, 400 eV; and ⊙, experimental results of Lasettre *et al.* (Ref. 24) at 500 eV.

results (see legend to Fig. 5) are included, together with a Born calculation using the wave functions discussed above, and the more accurate results of Kim and Inokuti.[22] In terms of the scattering angle, the maxima (for the energy-dependent calculations) vary from $\theta = 10°$ for 300 eV to $\theta = 6°$ at 1100 eV.

The deviation between experiment and our calculations are attributable, over-all, to a number of factors: approximate representation of polarization and distortion effects, neglect of exchange, relatively inaccurate wave functions, and of course the inherent small-angle nature of the Glauber approximation. Investigations to determine the effect of exchange and corrections to the theory are currently being explored.

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APPENDIX

The r integral in Eq. (5) is a special case of the more general integral

$$I(\rho,\ \nu,\ \mu) = \int_0^\infty dr\, r^\rho J_\nu(\alpha r) K_\mu(\beta r) K_\mu(\gamma r)\,. \qquad \text{(A1)}$$

Integrals of products of three Bessel functions, similar to the above have been treated by Bailey[28]; however, it appears that only the case $I(\nu+1,\ \nu,\ \mu)$ has been given in closed form.[28] We note that use of the integral transform[30]

$$K_\mu(\beta r) K_\mu(\gamma r) = \frac{1}{2}\int_0^\infty \frac{dt}{t}\, e^{-r^2 t - (\beta^2+\gamma^2)/4t} K_\mu(\beta\gamma/2t) \qquad \text{(A2)}$$

allows us to rewrite (A1) as

$$I(\rho,\ \nu,\ \mu) = \frac{1}{2}\int_0^\infty \frac{dt}{t}\, e^{-(\beta^2+\gamma^2)/4t} K_\mu(\beta\gamma/2t) \times \int_0^\infty dr\, r^\rho e^{-tr^2} J_\nu(\alpha r)\,, \qquad \text{(A3)}$$

where the order of integrations has been interchanged and the conditions $\mathrm{Re}(r) > 0$ and $\mathrm{Re}[\frac{1}{4}(\beta+\gamma)^2] > 0$ are required. Performing the r integration and replacing t by $1/t$ gives

$$I(\rho,\ \nu,\ \mu) = \frac{\alpha^\nu \Gamma(\frac{1}{2}\nu + \frac{1}{2}\rho + \frac{1}{2})}{2^{\nu+2}\Gamma(\nu+1)} \int_0^\infty dt\, t^{(\nu+\rho+1)/2 - 1} e^{-(\beta^2+\gamma^2)t/4} \times K_\mu(\tfrac{1}{2}\beta\gamma t)\, {}_1F_1(\tfrac{1}{2}\nu + \tfrac{1}{2}\rho + \tfrac{1}{2};\ \nu+1;\ -\tfrac{1}{4}\alpha^2 t)\,, \qquad \text{(A4)}$$

where ${}_1F_1(a;\ b;\ z)$ is the confluent hypergeometric function.

For the case $\rho = \nu + 2n + 1$, $n = 0,\ 1,\ 2,\ \ldots$, ${}_1F_1(a;\ b;\ z)$ reduces to an n-term polynomial in t, and

$$I(\nu+2n+1,\ \nu,\ \mu) = \frac{\alpha^\nu \Gamma(\nu+n+1)}{2^{\nu+2}\Gamma(\nu+1)} \sum_{k=0}^{n} \frac{(-n)_k (\frac{1}{4}\alpha^2)^k}{(\nu+1)_k\, k!} \times \int_0^\infty dt\, t^{\nu+n+k} e^{-(\alpha^2+\beta^2+\gamma^2)t/4} K_\mu(\tfrac{1}{2}\beta\gamma t)\,. \qquad \text{(A5)}$$

Subject to the restriction $\mathrm{Re}(\nu+n+k+1) > |\mathrm{Re}(\mu)|$, evaluation of the t-integral gives the result

$$I(\nu+2n+1,\ \nu,\ \mu) = 2^{2\mu+2n+\nu} \frac{\sqrt{\pi}\,\alpha^\nu \Gamma(\nu+n+1)(\beta\gamma)^\mu}{\Gamma(\nu+1)[(\beta+\gamma)^2+\alpha^2]^{\mu+\nu+n+1}} \sum_{k=0}^{n} \frac{(-n)_k \Gamma(\mu+\nu+n+k+1)\Gamma(\nu-\mu+n+k+1)}{(\nu+1)_k\, k!\, \Gamma(\nu+n+k+\frac{3}{2})} \times \left(\frac{\alpha^2}{(\beta+\gamma)^2+\alpha^2}\right)^k {}_2F_1\left(\mu+\nu+n+k+1,\ \mu+\tfrac{1}{2};\ \nu+n+k+\tfrac{3}{2};\ \frac{(\beta-\gamma)^2+\alpha^2}{(\beta+\gamma)^2+\alpha^2}\right). \qquad \text{(A6)}$$

There is little difficulty in showing that for $n = 0$, (A6) can be put in the form of the known result for $I(\nu+1,\ \nu,\ \mu)$.

The substitution of the combination $\nu = 0$, $n = 3$, and $\mu = 1$ in (A6) leads to the result given in Eqs. (8) and (9).

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Theory of Small-Energy-Transfer Collisions in Dominant Long-Ranged Forces: H^+-H_2 and e^--H_2 Vibrational Excitation

Burke Ritchie
Department of Chemistry, University of Alabama, University, Alabama 35486
(Received 1 February 1972)

In the two-state approximation analytic formulas are derived for the inelastic cross section in the limit in which the particle velocity is large relative to the energy defect. These formulas involve a mixing parameter and two eigenphase shifts. For scattering in a $C(X)/R^n$ potential, where X is an internal coordinate of the target, the integral cross section is presented in closed form, with parameters given by the elastic-superelastic potential-difference strength, the coupling strength, the velocity, and a cutoff for the singular potential, taken to be the target radius. Results are given for H^+-H_2, e^--H_2, and e^--N_2 vibrational excitation. The theory appears to be correct for the high-energy tail of the cross sections.

I. INTRODUCTION

It is desirable to obtain an analytic representation of the multichannel theory wherever possible to avoid the heavy labor of the numerical solution of the close-coupling equations. In addition, an analytic representation facilitates the study of the scattering as a function of laboratory parameters and is more easily generalizable to classes of problems; thus, it may be of more direct use to the experimentalist than a numerical representation. Also, the inversion of scattering data to determine the potential parameters is greatly facilitated. Olson and Smith[1] have pursued this approach in cases where well-defined curve crossings allow the use of the Landau-Zener inelastic probability in conjunction with the quantum-mechanical addition of amplitudes to yield analytic results for the cross section in which a maximum use is made of experimental data. It is the purpose of this paper to derive analytic formulas for the multichannel problem (using the two-state approximation as a convenient example) in which the criterion of validity for the method of solution used is that the particle velocity be large relative to the energy defect. It is found that diagonalization of the close-coupling equations for two open channels yields a constant mixing parameter and two eigenphase shifts. The