

sions of heavy ions with heavy atoms must be worked out in detail before any final interpretation of the data can be made. This present Letter is directed at pointing out these uncertainties in the interpretation of the available data, and the need for such detailed calculations. Experiments which selectively emphasize the high-energy part of the spectrum would clearly make the identification of MO x rays more reliable.⁵ Such measurements are in progress at our laboratory.

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Calculation of Total Cross Sections for the Ionization of Atomic Hydrogen by Electron Impact Using the Glauber Approximation

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Total cross sections for the ionization of atomic hydrogen by electron impact are calculated using the Glauber approximation. These cross sections are compared with the results obtained by the Born approximation and with experimental results.

Calculations of atomic ionization by electron impact have found useful applications in analyzing the effects of radiation on a variety of materials. Most of these calculations¹ are based on the Born approximation for direct Coulomb ionization established by Bethe.² In this paper we apply the more rigorous Glauber approximation³ to the ionization of atomic hydrogen by electron impact to compute the total cross section as a function of the energy of the incident electron.

The Glauber approximation has been derived³⁻⁵ in a number of ways. Conceptually, it corresponds to a "rigorous" distorted-wave Born approximation which approximately includes multiple scattering and is approximately unitary. It is a member of the class of eikonal approximations where straight lines have been chosen as

trajectories. With an appropriate choice of the projectile trajectory, the Glauber approximation reduces to the Born approximation at high energies.

There have been a number of applications⁵ of the Glauber approximation to scattering processes in atomic physics involving transitions from bound atomic states to bound atomic states. In the case of atomic hydrogen, the mathematical technique introduced by Franco⁶ and refined by Thomas and Gerjuoy⁷ for bound-state transitions has been used by McGuire *et al.*⁸ to derive expressions for excitation to continuum states, i.e., ionization.

For ionization from the ground state of hydrogen by electron impact, this scattering amplitude⁸ is given by

$$f(q, \vec{k}) = \left(\frac{8}{k}\right)^{1/2} \frac{ik_0}{(1 - e^{-2\pi/k})^{1/2}} \sum_{l=0}^{\infty} \frac{(-2ik)^l}{(2l+1)!} \exp(-i\delta_l) \left[\prod_{j=1}^l (j^2 + k^{-2}) \right]^{1/2} \\ \times \sum_{m=-l}^l Y_{lm}^*(\hat{k}) \sum_{n=0}^{\infty} A_n(l, k) (-k)^n \frac{d^{n+l} I_{lm}}{d\lambda^{n+l}} \Big|_{\lambda=1} = \sum_{l=0}^{\infty} \sum_{m=-l}^l f_{lm}(q, k) Y_{lm}^*(\hat{k}); \quad (1)$$

$$I_{lm} = \int \int r^l (e^{-\lambda r}/r) Y_{lm}(\hat{r}) e^{i\vec{q}\cdot\vec{r}} [1 - (|\vec{b} - \vec{s}|/b)^{2i/k_0}] d^3r d^2b;$$

$$A_0(l, k) = 1, \quad A_1(l, k) = -1/k(l+1), \quad A_n(l, k) = [(2l+n+1)n]^{-1} [-(2/k)A_{n-1} - A_{n-2}], \quad \delta_i = \arg\Gamma(l+1-i/k).$$

Here \vec{q} is the momentum transfer, \vec{k}_0 and \vec{b} are the momentum and impact parameter of the incident electron, \vec{k} is the ionized electron's momentum, and \vec{s} is the impact parameter of the atomic electron. By use of the technique of Thomas and Gerjuoy⁷ the integral expression for the I_{lm} 's may be evaluated analytically, so that the total cross section may be expressed as

$$\sigma(k_0) = (1/4\pi^3 k_0^2) \int_{q_{\min}}^{q_{\max}} q dq \int_0^{k(q)} k^2 dk \sum_{i=0}^{\infty} \sum_{m=-l}^l |f_{lm}|^2 (\pi \alpha_0^2), \quad (2)$$

where it is useful to perform the integrations in the order shown for computational efficiency.⁹ The cross section is dominated by the $l=1$ partial wave. For the energy range considered here, i.e., $E_0 < 100$ eV, the partial-wave series is terminated after the $l=3$ partial wave. In this energy range the $l=3$ partial wave is never greater than 5%, down by a factor of 5 from the $l=2$ partial wave, so it is expected that the inclusion of a larger number of partial waves in the calculation should change the results by at most $\approx 2\%$. This is the largest numerical error.

The expression for the f_{lm} 's of Eq. (1) is not directly applicable to the evaluation of total cross sections since the infinite series

$$\sum_{n=0}^{\infty} A_n(l, k) (-k)^n \left. \frac{d^{n+1} I_{lm}}{d\lambda^{n+1}} \right|_{\lambda=1}$$

is divergent for $E_k \geq 13.6$ eV. The functional dependence on k of the coefficients $A_n(l, k)$ may be separated out, giving an infinite series

$$\sum_{n=0}^{\infty} C_n \left(l, \frac{d^{n+1} I_{lm}}{d\lambda^{n+1}} \right) (-k)^{2n} \Big|_{\lambda=1}, \quad (3)$$

where the coefficients C_n are given by an infinite convergent sum depending on l and the derivatives of the I_{lm} 's. Although the series of Eq. (3) is still divergent, the method of Padé approximants¹⁰ may be applied to give a rational approximation which is convergent for much larger values of k . Using this method convergent scattering amplitudes may be practically obtained for $E_k \leq 70$ eV. For values of k corresponding to $E_k \geq 70$ eV appearing in the cross section integral, which occurs only for $E_0 \geq 80$ eV, the Glauber amplitude is replaced by the Born amplitude. Very little error (less than 1%) is introduced into the calculation as a result of this replacement, because the predominant portion of the cross section, as a function of k , occurs at very much smaller values of E_k , i.e., $E_k \leq 25$ eV. Integrations accurate to within 1% were performed nu-

merically by Rhomberg's method on an IBM 370/158 computer. The calculation of a cross section in the Glauber approximation at each energy took approximately 50 sec as compared to approximately 1.5 sec for the Born approximation.

Glauber cross sections computed by the above procedure are presented in Fig. 1 as are the corresponding Born calculations. These are compared with the experimental data of Fite and Brackmann¹¹ and Boyd and Boksenberg.¹² Also

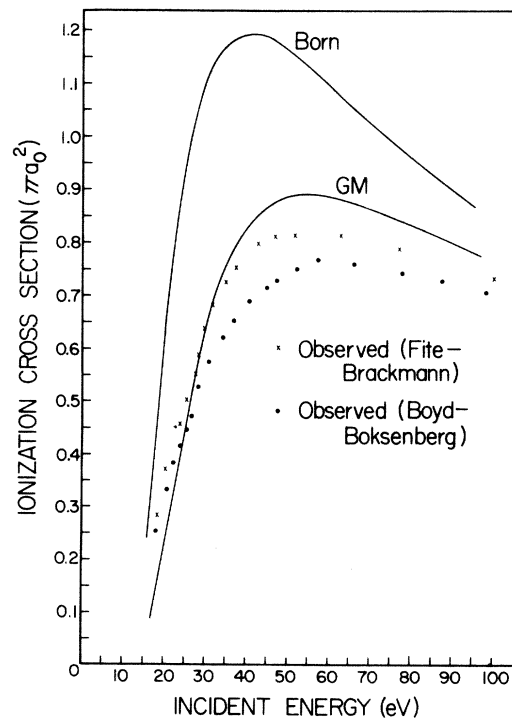


FIG. 1. Total cross section for the ionization of atomic hydrogen by electron impact versus projectile energy. The electrons are considered distinguishable. Data were extracted from Refs. 11 and 13. The Born calculations are described in Ref. 1 and "GM" represents our Glauber calculation.

TABLE I. Total cross sections (in units of πa_0^2) for the ionization of atomic hydrogen by electron impact as a function of the energy of the projectile.

E_0 (eV)	Glauber	Born	Glauber- exchange	Born- exchange
17.0	0.09	0.32	0.06	0.22
20.4	0.24	0.64	0.18	0.46
27.2	0.53	1.01	0.42	0.78
34.0	0.72	1.16	0.60	0.93
40.8	0.83	1.19	0.68	0.99
47.6	0.88	1.18	0.77	1.00
54.4	0.89	1.14	0.79	0.99
61.2	0.88	1.09	0.80	0.97
68.0	0.87	1.05	0.79	0.94
81.6	0.84	0.95	0.76	0.87
95.0	0.78	0.87	0.72	0.81

cross sections are presented in Fig. 2 in which exchange effects have been approximately included¹³ by limiting the maximum value k may take in the integration to

$$k_{\max} = \frac{1}{2}\sqrt{2}[k_0^2 - 1]^{1/2}. \tag{4}$$

The correct expression for the cross section would contain interference terms and would take the form

$$\sigma = \int d^3k (k_f/k_0) \int d\Omega_f [|f(\vec{k}, \vec{k}_f)|^2 - \frac{1}{2} \text{Re} f^*(\vec{k}, \vec{k}_f) f(\vec{k}_f, \vec{k})], \tag{5}$$

where \vec{k}_f is the final momentum of the "incident" electron. Geltman¹⁴ has made a comparison of the cross sections obtained by considering the electrons as indistinguishable [implying that each nonordered set of energies (E_k, E_f) is to be counted only once, thus introducing the limit given by Eq. (4)] and the cross sections given by Eq. (5), where in both cases the Born amplitude is used for $f(\vec{k}_f, \vec{k})$. Both results are roughly similar, with the cross section given by Eq. (5) being slightly the larger for $E_0 \leq 35$ eV and being the smaller of the two for larger energies. Although there is no rigorous reason to expect the Glauber cross sections to follow the trends just described for the Born cross sections, we have used Eq. (4) to estimate the effects of exchange since it is computationally impractical at present to include the interference term in Eq. (5). Numerical results are given in Table I.

It will be seen that at low energies the Glauber results lie below both sets of experimental data,

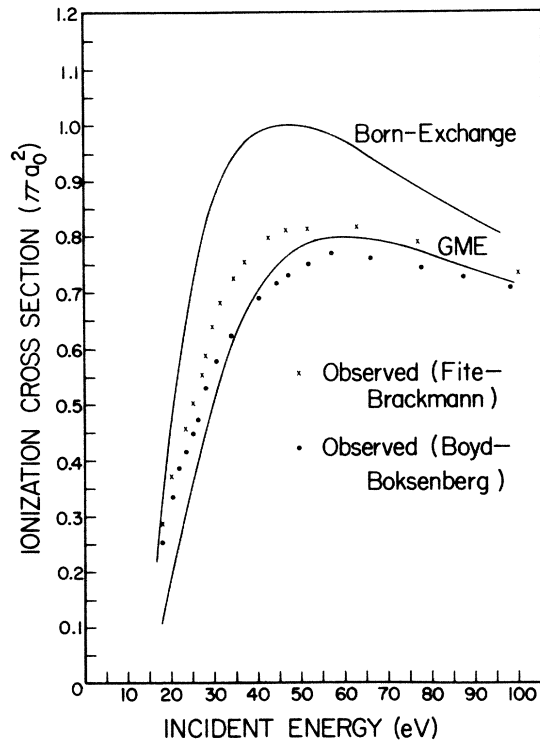


FIG. 2. Total cross section for the ionization of atomic hydrogen by electron impact versus projectile energy. Exchange effects are treated approximately (cf. text). Data are the same as in Fig. 1. The Born-exchange calculation is described in Ref. 13 and "GME" represents our Glauber calculation with exchange.

very much in analogy with the results of Tai *et al.*¹⁵ for excitation of atomic hydrogen by electron impact. In this low-energy range there is no rigorous justification for our results. In the range $30 \leq E_0 < 100$ eV the results presented here are superior to the corresponding Born calculations. Where the effects of particle indistinguishability have been included, Fig. 2, the Glauber results are seen to lie between the two sets of experimental data.

Since the Glauber approximation is more rigorous than the Born approximation, it is not surprising that the Glauber calculations lie closer to experiment than the Born results. Furthermore, it is encouraging that the Glauber method is also computationally practical.

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York, 1970). It is possible to show that our integral expression for the scattering amplitude, i.e., Eq. (14) of Ref. 8, is analytic in k within a strip between $\pm i\lambda$ running from 0 to ∞ along the real (i.e., physical) k axis. It is also possible to prove that there exists a sequence of Padé approximants which rigorously converges within this strip. Although we cannot prove that the sequence we use converges, it is convergent numerically. Until more definitive theorems for the convergence properties of Padé approximants are proved, or until an alternate method of evaluation of Eq. (14) of Ref. 8 is developed, our calculation is mathematically less rigorous than the corresponding Born calculation for $E_k \geq 13.6$ eV.

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ESR Observation of the Γ_6 Excited State of Er^{3+} in the Dilute Alloy PdEr

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We report the first ESR signal of an excited crystalline state (Γ_6) in a metal (PdEr). The intensity of the Γ_6 isotropic resonance compared to the $\Gamma_8^{(3)}$ resonances of the ground-state quartet allows the determination of the energy scaling parameter W of the crystalline field. A more precise value is deduced from the splitting of the transitions $1 \rightarrow 2$ and $3 \rightarrow 4$ of the $\Gamma_8^{(3)}$ ground state: $W = -0.163 \pm 0.015^\circ\text{K}$, in accordance with the work of Praddaude.

The effect of excited crystalline-field states on the relaxation rate of the ground-state multiplet has recently been observed in dilute alloys. Davidov *et al.*¹ measured the temperature dependence of the Er^{3+} ESR linewidth in AuEr and from this deduced a value of the energy separation Δ between the Γ_7 ground-state doublet and the first-excited $\Gamma_8^{(1)}$ quartet. In a previous paper Devine, Zingg, and Moret² measured the ESR in PdEr single crystals. The ground state of Er^{3+} was found to be a $\Gamma_8^{(3)}$ quartet. We have since observed a new resonance signal in PdEr , whose g value and temperature behavior indicate

that it is due to the first-excited Γ_6 doublet. The amplitude of the signal is related to the energy separation between the $\Gamma_8^{(3)}$ and Γ_6 levels, and allows a direct determination of the crystalline-field energy scaling parameter W .

The Er^{3+} free ion has a $J = \frac{15}{2}$ multiplet ground state which reduces in a cubic crystalline field to three Γ_8 quartets, one Γ_7 doublet, and one Γ_6 doublet. Devine, Zingg, and Moret² observed all possible transitions in the $\Gamma_8^{(3)}$ ground-state quartet and interpreted them with the effective-spin-Hamiltonian formalism³ ($\tilde{S} = \frac{3}{2}$). They found an x value as defined by Lea, Leask, and Wolf⁴