

of Appendix 2 take on all values $0 < C_i < \infty$ [paper submitted to The Physical Review; see also B. Holmberg, *Nuovo cimento* **9**, 597 (1952)].

Further, an important paper by I. M. Gel'fand and B. M. Levitan [*Doklady Akad. Nauk. S.S.S.R.* n Ser. **77**, 557 (1951)] has come to our attention. By adapting their methods to the present case the problem of finding the potential corresponding to given $f(k)$ and constants C_i is reduced to the solution of linear integral equations. One introduces an auxiliary potential $V^{(1)}(\gamma)$ with corresponding solutions $\varphi^{(1)}(k, \gamma)$ and bound states at $E_i^{(1)}$. It's "spectral function" $\rho^{(1)}(E)$ is defined by

$$\frac{d\rho^{(1)}(E)}{dE} = \sum C_i^{(1)} \delta(E - E_i^{(1)}), \quad E < 0,$$

$$\frac{d\rho^{(1)}(E)}{dE} = \frac{1}{\pi} \frac{\sqrt{E}}{|\rho^{(1)}(\sqrt{E})|^2}, \quad E \geq 0.$$

To find the potential $V(r)$ corresponding to a given $\rho(E)$ one evaluates

$$G(r, s) = \int d[\rho(E) - \rho^{(1)}(E)] \varphi^{(1)}(\sqrt{E}, r) \varphi^{(1)}(\sqrt{E}, s)$$

and solves the integral equations

$$K(r, s) + G(r, s) + \int_0^r K(r, t)G(s, t)dt = 0$$

for positive r . Then

$$V(r) = V_1(r) + 2 \frac{dK(r, r)}{dr}.$$

It is a simple consequence of this theory that for a given phase shift, the position of the bound states is completely arbitrary.

A paper on applications of the Gel'fand Levitan theory to scattering problems is in preparation.

Excitation Cross Section for Helium Atoms*

SAUL ALTSHULER

Department of Physics, Iowa State College, Ames, Iowa

(Received February 28, 1952)

The excitation scattering of electrons from helium atoms is investigated in order to examine quantitatively the errors introduced by the fact that the description of the helium target is only approximately known. The cross section is calculated in Born approximation using formally equivalent matrix elements which weight the wave functions differently in space. Similar shapes for angular distribution and total cross section vs energy curves are obtained although absolute values differ.

SINCE exact wave functions for complex atoms are not available, there is an uncertainty introduced in scattering calculations which is distinct from those inherent in the Born approximation. The approximate wave functions, such as those of Slater, usually are well determined with respect to the energy of the state and are less well determined in regions other than those which contribute the most to the energy. For scattering problems such errors may be quite serious. A similar situation occurs in the calculation of optical transition probabilities, and investigations have been reported.¹ This difficulty has never been quantitatively examined for collision problems.

To make this study, we follow the suggestion, advanced by Bates, Fundaminsky, and Massey,² of employing two formally equivalent expressions for the differential cross section, both of which are within the Born approximation. These expressions are not necessarily the same in actual calculation since they weight the various regions of coordinate space differently.

The cross section for a momentum change dK for excitation of an atom from state p to state q is given

in Born approximation³ by

$$I(K)dK = \frac{8\pi dK}{k_p^2 K^3} \left| \sum_i^n \int e^{-i\mathbf{K} \cdot \mathbf{r}_i} \psi_p \psi_q^* d\tau_1 d\tau_2 \cdots d\tau_n \right|^2, \quad (1)$$

where the summation is made over the atomic electrons, and where $\mathbf{K} = \mathbf{k}_q - \mathbf{k}_p$, k_p = wave number of the incident electron, k_q = wave number of the scattered electron, $k_q^2 = k_p^2 - 2\Delta E$, and $\Delta E = E_q - E_p$, the internal energy change of the target; in all of these symbols Hartree units have been used.

The summation over the atomic electrons is made readily if product type wave functions are used. For the ground state of helium

$$\psi_p = \psi_0(N|r_1)\psi_0(N|r_2), \quad (N = 1.687)$$

while for an excited state—other than an S state—the Eckhart approximation² to the wave function is used, i.e.,

$$\psi_q = 2^{-1/2} \{ \psi_0(2|r_1)\psi_{nlm}(1|r_2) + \psi_0(2|r_2)\psi_{nlm}(1|r_1) \},$$

where $\psi_{nlm}(N|r)$ is the wave function of a single electron in the nlm state moving in a field of charge N .

* The research reported in this paper has been sponsored by the Geophysical Research Division of the Air Force Cambridge Research Center.

¹ D. R. Bates and A. Damgaard, *Trans. Roy. Soc. (London)* **A242**, 101 (1949); S. Chandrasekhar, *Astrophys. J.* **102**, 223 (1945).

² Bates, Fundaminsky, and Massey, *Trans. Roy. Soc. (London)* **A243**, 93 (1950).

³ N. F. Mott and H. S. W. Massey, *Theory of Atomic Collisions* (Clarendon Press, Oxford, England, 1949), second edition, pp. 226 ff.

With these assumptions,

$$\sum_i^n \int e^{-iKz} \psi_p \psi_q^* d\tau_1 \cdots d\tau_n = \sqrt{2} \int e^{-iKz} \psi_0(N|r) \psi_{nlm}^*(1|r) d\mathbf{r}.$$

Choosing the final states with their polar axis along the momentum transfer vector \mathbf{K} establishes the selection rule $\Delta m=0$ for the process. Therefore, the differential cross section becomes

$$I(K)dK = \frac{16\pi dK}{k_p^2 K^3} \left| \int e^{-iKz} \psi_0(N|r) \psi_{ni}(1|r) d\mathbf{r} \right|^2. \quad (2)$$

By making use of the equations satisfied by exact helium atom wave functions, ψ_q and ψ_p , the product $\psi_q^* \psi_p$ appearing in (1) is replaced by

$$\psi_q^* \psi_p = \frac{\psi_q^* (\nabla_1^2 + \nabla_2^2) \psi_p - \psi_p (\nabla_1^2 + \nabla_2^2) \psi_q^*}{2(E_q - E_p)},$$

and by a straightforward analysis, using the Eckhart wave functions, an alternative expression for the differential cross section can be shown to be

$$I(K)dK = \frac{4\pi dK}{(\Delta E)^2 K k_p^2} \left| \int e^{-iKz} \left\{ \psi_{ni}^*(1|r) \frac{\partial}{\partial z} \psi_0(N|r) - \psi_0(N|r) \frac{\partial}{\partial z} \psi_{ni}^*(1|r) \right\} d\mathbf{r} \right|^2. \quad (3)$$

Equation (2) and Eq. (3) have been applied to two cases, namely, the transition 1^1S to 2^1P and 1^1S to 3^1P . All results using Eq. (2) will be designated as method I; those using Eq. (3) will be designated as method II. Method I is the one conventionally used and many applications appear in reference 2.⁴

For the transition 1^1S to 2^1P , the differential cross section per unit solid angle, $I(\theta)$, in units of πa_0^2 , after transforming from momentum to angular variables, is

$$2\pi I(\theta) = 1.176 \times 10^4 \frac{k_q}{k_p} \frac{1}{K^2(p^2 + K^2)^6} \text{ by method I,} \quad (4)$$

$$2\pi I(\theta) = 2.532 \times 10^2 \frac{k_q [8.069 - 0.687K^2]^2}{k_p K^2(p^2 + K^2)^6} \text{ by method II,} \quad (5)$$

where $p^2=4.783$. For this transition $\Delta E=0.779$ in Hartree units.

⁴ Application of method I in the present investigation reveals a slight discrepancy between cross sections reported here and those reported by Mott and Massey in reference 2 for the 1^1S to 2^1P transition.

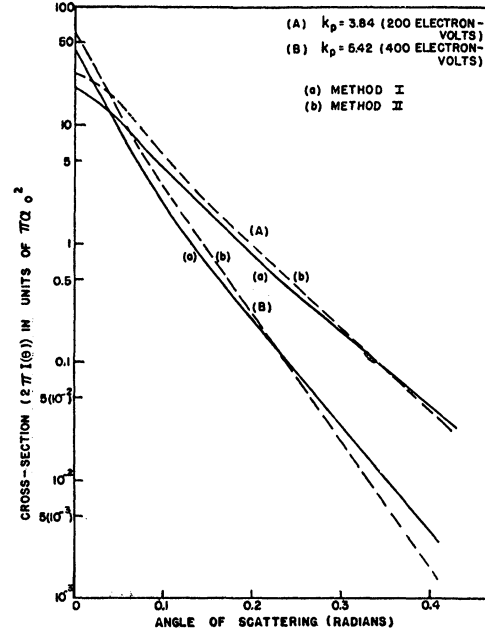


FIG. 1. Angular distributions for excitation scattering of electrons by helium atoms (1^1S to 2^1P transition).

The corresponding total cross sections,

$$\int_0^\pi 2\pi I(\theta) \sin\theta d\theta,$$

are

$$Q_I(k_p) = \frac{1.176 \times 10^2}{k_p^2} \left[\frac{1}{X^5} \left\{ 2.091 + 0.5464X + 0.1523X^2 + 4.777 \times 10^{-2}X^3 + 1.997 \times 10^{-2}X^4 + 4.176 \times 10^{-3}X^5 \ln \frac{K^2}{X} \right\} \right]_{k_p - k_q}^{k_p + k_q} \text{ by method I,} \quad (6)$$

$$Q_{II}(k_p) = 1.402 Q_I + \frac{2.987}{k_p^2} \left[\frac{5K^2 - 89.18}{X^5} \right]_{k_p - k_q}^{k_p + k_q} \text{ by method II,} \quad (7)$$

where $X = p^2 + K^2$.

For the transition 1^1S to 3^1P , where $\Delta E=0.8474$, the final results are

$$2\pi I(\theta) = 1.507 \frac{k_q [52.55K^2 + 1.168 \cdot 10^2]^2}{k_p K^2(p^2 + K^2)^8} \text{ by method I,} \quad (8)$$

$$2\pi I(\theta) = 0.5245 \frac{k_q [-8.28K^4 + 87.62K^2 + 228.8]^2}{k_p K^2(p^2 + K^2)^8} \text{ by method II,} \quad (9)$$

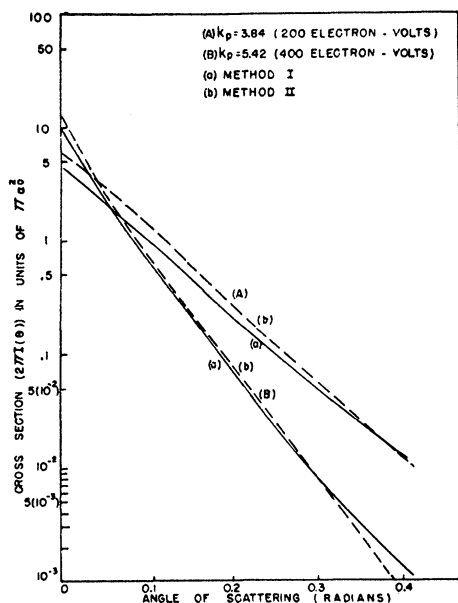


FIG. 2. Angular distributions for excitation scattering of electrons by helium atoms ($1S$ to 3^1P transition).

where $p^2 = 4.093$;

$$Q_I(k_p) = \frac{1.507}{k_p^2} \left[\frac{1}{X^7} \left\{ -1.012 \times 10^3 - 2.301 \times 10^2 K^2 \right. \right. \\ \left. \left. 67.93X + 19.92X^2 + 6.084X^3 + 1.982X^4 + 0.7265X^5 \right. \right. \\ \left. \left. + 0.3550X^6 + 8.675 \cdot 10^{-2} X^7 \ln \frac{K^2}{X} \right\} \right]_{k_p - k_q}^{k_p + k_q} \quad \text{by method I, (10)}$$

$$Q_{II}(k_p) = 1.335 Q_I - \frac{0.5245}{k_p^2} \left[\frac{1}{X^7} \left\{ 8.570K^6 - 1.241 \times 10^2 K^4 \right. \right. \\ \left. \left. - 1.303 \times 10^3 K^2 - 2.175 \times 10^3 \right\} \right]_{k_p - k_q}^{k_p + k_q} \quad \text{by method II, (11)}$$

where $X = p^2 + K^2$, as before.

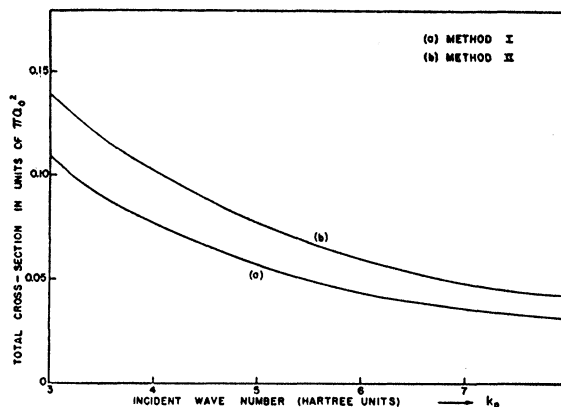


FIG. 3. Total excitation cross section for electron impact with helium atoms as a function of incident energy ($1S$ to 2^1P transition).

The angular distributions for the two transitions appear in Figs. 1 and 2, while the total cross sections are presented in Figs. 3 and 4. Particular significance is

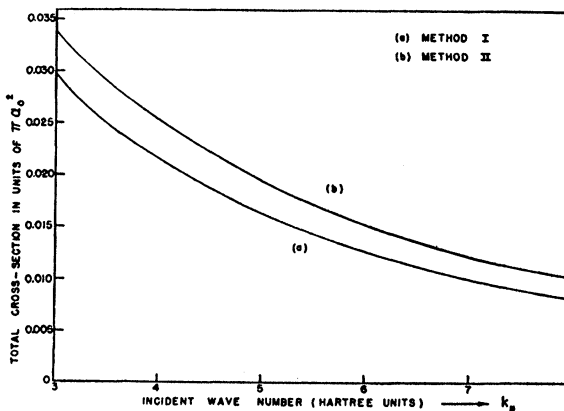


FIG. 4. Total excitation cross section for electron impact with helium atoms as a function of incident energy ($1S$ to 3^1P transition).

attached to the results since, except for magnitudes of the cross sections, the general behavior is quite similar for the two methods. Therefore, the results of either may be successfully normalized to measured cross sections.