Excitation Cross Section for Helium Atoms. II*

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The excitation scattering of electrons from helium atoms is investigated for the case of transition to the first excited singlet metastable level in order to examine quantitatively the error 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. The shape of the total cross section-energy curve is the same although absolute values differ while the angular distributions are considerably different.

IN a recent paper[1] (referred to as Paper I) the excitation scattering of electrons from helium atoms was investigated in order to examine the uncertainty introduced by the fact that the wave functions of the helium target are necessarily inaccurate. In Paper I, the investigation was confined to transitions to P-states. The present work follows the analysis in Paper I but pertains to the transition to the first excited metastable state of the helium atom. That is, two formally equivalent expressions for the differential cross section in Born approximation are employed, and these expressions do not lead to the same results in actual calculations because of the approximate nature of the helium atomic wave functions. As in Paper I, Method I will refer to the standard matrix element for the excitation differential cross section while Method II refers to results derived from the alternative expression obtained by the transformation

$$\psi_q^*\psi_p=\frac{\psi_q^*(\nabla_1^2+\nabla_2^2)\psi_p-\psi_p(\nabla_1^2+\nabla_2^2)\psi_q^*}{2(E_q-E_p)}. \qquad (1)$$

Here ψ_q and ψ_p refer to exact wave functions for the final and initial helium states, respectively. Hartree units are employed everywhere.

The wave function for the $(1s\,2s)^1S$ level was originally suggested by Vinti[2] and already employed by Massey and Mohr[3] and is given by

$$\psi_q=B(\varphi_2-\gamma\psi_p),\quad \gamma=\int\psi_p^*\phi_2 d\tau_1 d\tau_2,$$

where ψ_p is the ground state of helium taken to be

$$\psi_p=\psi_{100}(N/r_1)\psi_{100}(N/r_2),\quad (N=1.687),$$

while

$$\phi_2=\frac{\psi_{100}(\alpha/r_1)\psi_{200}(\beta/r_2)+\psi_{100}(\alpha/r_2)\psi_{200}(\beta/r_1)}{\{2(1+b^2)\}^{\frac{1}{2}}},$$

with

$$b^2=(2x)^3(x-1)^2/(x+\tfrac{1}{2})^8;\quad x=\alpha/\beta;\quad B=(1-\gamma^2)^{-\frac{1}{2}}.$$

$\psi_{nlm}(Z/r)$ is the wave function of a single electron in the *nlm* state moving in a field of charge Z. The values of the screening parameters α and β were found[3] by the Ritz condition of minimum energy to be

$$\alpha=1.98,\quad \beta=1.20.$$

It is clear that ψ_q is properly normalized and orthogonal to the ground state.

The differential cross section for a momentum change of magnitude dK for excitation transition $1^1S\rightarrow 2^1S$ is then calculated by Method I and is given by

$$I(K)dK=\frac{8\pi dK}{k_p^2K^3}\left|\frac{36.879}{(13.447+K^2)^2}+\frac{(11.457)(2.547+2.887K^2)}{(5.2304+K^2)^3}-\frac{52.863}{(11.384+K^2)^2}\right|^2 \quad \text{(by Method I)}.$$

The matrix element for the excitation differential cross section by Method I is transformed by using Eq. (1), with the result (see appendix):

$$\sum_{i=1}^{2}\int e^{-iKz_i}\psi_p\psi_q^* d\tau_1 d\tau_2 =\frac{1}{(1-\gamma^2)^{\frac{1}{2}}\Delta E}\left[K^2\int\varphi_2 e^{-iKz_1}\psi_p d\tau_1 d\tau_2 +2iK\int\varphi_2 e^{-iKz_1}\frac{\partial}{\partial z_1}\psi_p d\tau_1 d\tau_2\right], \qquad (2)$$

in which $\Delta E=E_q-E_p$, the transition energy change, equals 0.75584. The final result of the cross section for

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[1] S. Altshuler, Phys. Rev. **87**, 992 (1952).

[2] J. P. Vinti, Phys. Rev. **37**, 449 (1931).

[3] H. S. W. Massey and C. B. O. Mohr, Proc. Roy. Soc. (London) **A140**, 613 (1933).

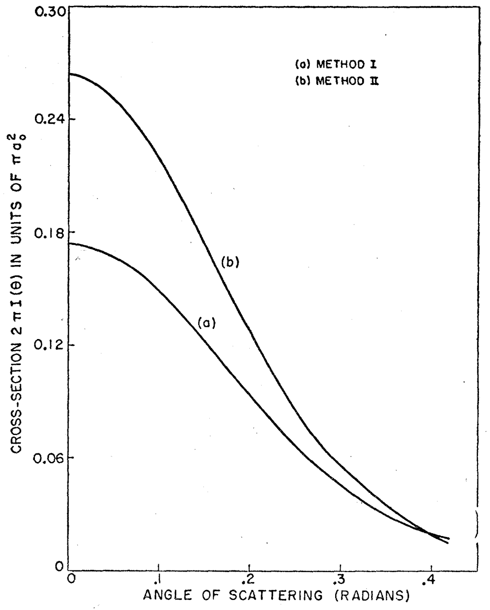

FIG. 1. Angular distributions for excitation scattering of electrons by helium atoms (1^1S to 2^1S transition) at an incident energy of 200 ev.

momentum change is given by

$$I(K)dK=\frac{8\pi dK}{k_p^2K^3}\left|3.7372\times10^2K^2\left[\frac{5.2159\times10^{-3}}{(13.4469+K^2)^2}+\frac{6.9338\times10^{-2}-9.876\times10^{-3}K^2}{(5.2304+K^2)^3}\right]\right|^2 \quad \text{(by Method II).}$$

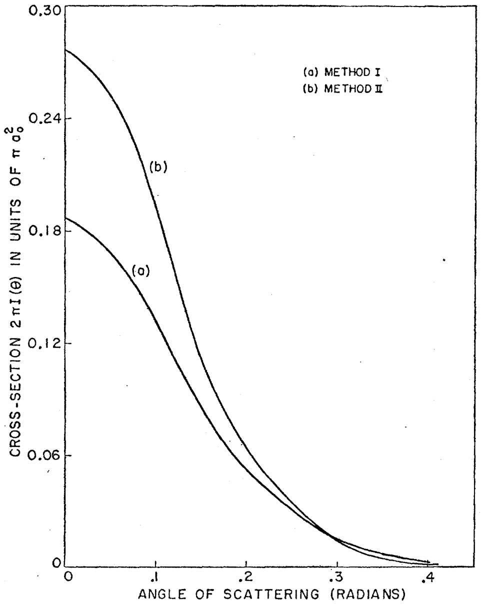

FIG. 2. Angular distributions for excitation scattering of electrons by helium atoms (1^1S to 2^1S transition) at an incident energy of 400 ev.

Comparative angular distributions of the differential cross section per unit solid angle, $I(\theta)$, in units of πa_0^2 (a_0=first Bohr radius) are portrayed in Figs. 1 and 2 for incident energies of 200 and 400 electron-volts, respectively. The total cross sections for both Methods I and II were obtained by numerical integration, and the results appear in Fig. 3.

DISCUSSION

Just as in the case of transitions to P-states (Paper I) we observe that the total cross section for either of the two methods may be normalized to measured values. However, such is not the case for the angular distributions in the case of the transition to the first excited metastable state. The disagreement in the shape of the angular distribution indicates that the Vinti function does not describe the metastable state as well as the Eckhart functions for the P-states (Paper I).

In order to discriminate between the results of either method it would be necessary to have accurate experimental data. Nevertheless, an argument may be advanced which favors the results of Method II. If we expand the exponential in Eq. (2) and exploit the symmetry of the wave functions, the matrix element may be rewritten

$$\sum_{i=1}^{2}\int e^{-iKz_i}\psi_p\psi_q{}^*d\tau_1d\tau_2$$

$$=2\int\psi_q{}^*\left\{-iKz_1+\left(\frac{-iKz_1}{2!}\right)^2+\cdots\right\}\psi_pd\tau_1d\tau_2. \quad (3)$$

It is then apparent that considerable contribution to the integral is made from regions of configuration space other than those which contribute most to the energy integral. The space weighting of the wave functions using Method II places more emphasis on the region closer to the origin since it involves derivatives of the wave functions, and thus more accurate results should be expected when employing Method II. Verification of this argument has been demonstrated in one pertinent case in photoabsorption calculations.[4] This work dealt with the calculation of the continuous absorption coefficient of the H^- ion, where it was shown that the matrix element of the momentum operator gives more reliable results than that of the dipole. In the case of small angle scattering the leading term in Eq. (3) (for transition to P-states) is precisely the dipole element, while the matrix element of the momentum operator corresponds to Method II.

APPENDIX

The alternative matrix element which is the basis of Method II, as given in Eq. (2), is established as follows:

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[4] S. Chandrasekhar, Astrophys. J. **102**, 223 (1945).

In the case of the transition considered in this note, $\psi_p\psi_q^*$ is symmetric. Therefore,

$$J \equiv \sum_{i=1}^{2} \int e^{-iKz_i}\psi_p(\bar{r}_1, \bar{r}_2)\psi_q^*(\bar{r}_1, \bar{r}_2)d\tau_1 d\tau_2 = 2\int e^{-iKz_1}\psi_p\psi_q^* d\tau_1 d\tau_2,$$

and, substituting from Eq. (1), we have

$$J = \frac{1}{\Delta E}\int e^{-iKz_1}\{\psi_q^*(\nabla_1^2+\nabla_2^2)\psi_p - \psi_p(\nabla_1^2+\nabla_2^2)\psi_q^*\}d\tau_1 d\tau_2$$

$$= \frac{1}{\Delta E}\left[\int e^{-iKz_1}\{\psi_q^*\nabla_1^2\psi_p - \psi_p\nabla_1^2\psi_q^*\}d\tau_1 d\tau_2 + \int e^{-iKz_1}\{\psi_q^*\nabla_2^2\psi_p - \psi_p\nabla_2^2\psi_q^*\}d\tau_1 d\tau_2\right].$$

The second term on the right vanishes identically because of the Hermitian property of ∇_2^2.

Consequently (since the 2^1S state is real),

$$J = \frac{1}{\Delta E}\int e^{-iKz_1}\{\psi_q\nabla_1^2\psi_p - \psi_p\nabla_1^2\psi_q\}d\tau_1 d\tau_2.$$

Introducing

$$\psi_q = B(\varphi_2 - \gamma\psi_p),$$

we have

$$J = \frac{B}{\Delta E}\left[\int e^{-iKz_1}(\varphi_2 - \gamma\psi_p)\nabla_1^2\psi_p d\tau_1 d\tau_2 - \int e^{-iKz_1}\psi_p\nabla_1^2(\varphi_2 - \gamma\psi_p)d\tau_1 d\tau_2\right]$$

$$= \frac{B}{\Delta E}\left[\int e^{-iKz_1}(\varphi_2\nabla_1^2\psi_p - \psi_p\nabla_1^2\varphi_2)d\tau_1 d\tau_2\right].$$

We now employ the identity:

$$\int e^{-iKz_1}\psi_p\nabla_1^2\varphi_2 d\tau_1 d\tau_2 = \int \varphi_2\nabla_1^2(\psi_p e^{-iKz_1})d\tau_1 d\tau_2$$

$$= \int \varphi_2\{\psi_p\nabla_1^2 e^{-iKz_1} + e^{-iKz_1}\nabla_1^2\psi_p + 2\nabla\psi_p\cdot\nabla e^{-iKz_1}\}d\tau_1 d\tau_2.$$

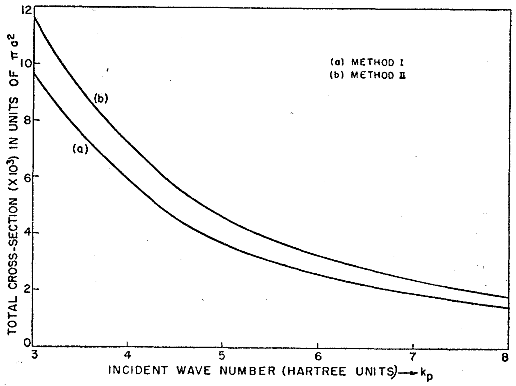

FIG. 3. Total excitation cross section for electron impact with helium atoms as a function of incident energy (1^1S to 2^1S transition).

Substituting, the expression for J becomes

$$J = \frac{B}{\Delta E}\left[\int\{-\varphi_2\psi_p\nabla_1^2 e^{-iKz_1} - 2\varphi_2\nabla_1\psi_p\cdot\nabla_1 e^{-iKz_1}\}d\tau_1 d\tau_2\right]$$

$$= \frac{B}{\Delta E}\left[K^2\int \varphi_2 e^{-iKz_1}\psi_p d\tau_1 d\tau_2 + 2iK\int \varphi_2 e^{-iKz_1}\frac{\partial}{\partial z_1}\psi_p d\tau_1 d\tau_2\right].$$

Note added in proof:—Errata in reference 1 are corrected as follows. The absolute value symbol in Eq. (3) should appear squared. The plus sign separating the two terms on the right in Eq. (7) should be changed to minus.

Equations (10) and (11) pertaining to the $^1S \rightarrow 3^1P$ transition should read

$$Q_I(k_p) = \frac{1.507}{k_p^2}\left[\frac{1}{X^7}\{-7.699\times 10^2 - \text{etc.}\cdots\}\right]_{k_p-k_q}^{k_p+k_q}, \quad (10)$$

$$Q_{II}(k_p) = 1.3515Q_I(k_p) - \frac{0.5245}{k_p^2} \times\left[\frac{1}{X^7}\{8.570K^6 - 1.241\times 10^2K^4 - 7.342\times 10^2K^2 - 9.380\times 10^2\}\right]_{k_p-k_q}^{k_p+k_q}. \quad (11)$$

The shape of Fig. 4 is not changed but the magnitudes are altered slightly. The following is a table of corrected values (units are the same as in reference 1).

k_p	3	4	5	6	7	8
$Q_I\times 10^3$	28.3	20.7	15.6	12.2	9.76	8.02
$Q_{II}\times 10^3$	35.6	26.4	20.1	15.7	12.7	10.4