PHYSICAL REVIEW A VOLUME 16, NUMBER 5 NOVEMBER 1977

Elastic scattering of electrons by helium at intermediate energies*

T. T. Gien
Department of Physics, Memorial University of Newfoundland, St. John's, Newfoundland, Canada A1C 5S7
(Received 22 March 1977)

A modified Glauber amplitude proposed earlier by this author for electron-atom scatterings is applied to the analysis of elastic scattering of electrons by helium at various intermediate energies. The results are found to be in good agreement with experimental data acquired by various research groups with absolute measurements. Thus, the present work confirms reasonably clearly that the failure of the Glauber approximation for elastic scattering of electrons by helium stems mainly from the inadequacy of its second-order eikonal term. A comparison with results of other methods of approximation will also be made.

I. INTRODUCTION

In a recent paper,[1] it was shown that the straight-line approximation used in the derivation of the Glauber amplitude[2] affects mostly the second-order term of its eikonal expansion. As a result, a significant contribution from the second-order term of the expansion has been missing from this scattering amplitude. Therefore, if one does not take this approximation very seriously, the Glauber amplitude should be modified in such a way that this missing contribution could, to some extent, be recovered. The simplest way is obviously to replace this second-order eikonal term by its counterpart prior to eikonization, i.e., the second-order Born term.

In view of the fair success that the Glauber eikonal method has enjoyed[3] since it was first applied to study atomic and molecular collision processes by Franco in his pioneering work,[4] we believe that the Glauber amplitude could be retained as a good approximation for these collision processes at intermediate energies, provided that its defects are singled out and then adequately corrected. Our approximation as proposed is, indeed, chosen within this spirit. With the consideration of this modification, some very serious defects of the Glauber amplitude are rectified, while the characteristics of the eikonal method remaining in the rest of the amplitude still can be preserved. Besides, with this choice of amplitude for electron-atom scatterings, one can avoid an unnecessary cutoff of higher-order eikonal terms such as f_{G4}, f_{G5}, ... from the scattering amplitude. These terms are often found to be of significant magnitude and their contribution to the scattering amplitude as a whole is also not negligible, usually. The dropping of these terms from the scattering amplitude cannot, thereby, be very well justified.

Calculations have been performed with the Glauber amplitude so modified for elastic scattering of electrons at intermediate energies by a hydrogen atom in its ground state.[1,5] The results were found to be in good agreement with experimental data recently made available by absolute measurement.[6] Encouraged by these results, we wish, in this paper, to apply this so-called modified Glauber amplitude to the study of elastic scattering of electrons at intermediate energies by a helium atom in its ground state. In Sec. II, a brief review on the reduced forms for various amplitudes needed for our subsequent calculations will be made. Results of our calculations for e^--He elastic scattering at different intermediate energies (100, 200, 300, 400, and 500 eV) will be shown together with discussion in Sec. III. Comparison with existing data by different experimental groups as well as with results obtained in some other methods of approximation previously considered for this process (all recalculated by us) will also be made. Finally, some conclusions will be drawn from the results of this work.

II. FORMALISM

As was discussed in a previous paper,[1] the deficiency of the Glauber amplitude in electron-atom scattering may originate mainly from the second-order term of its eikonal expansion. In order to recover the loss of a significant contribution coming from this term, we proposed that the Glauber amplitude should simply be modified as follows:

$$f_{\mathrm{GM}}=f_G-f_{G2}+f_{B2}\,, \tag{1}$$

where f_G, f_{G2}, and f_{B2} are the Glauber amplitude, the second-order eikonal amplitude, and the second-order Born amplitude, respectively. It has recently been brought to our attention that Byron and Joachain[7] once tentatively substituted the direct scattering part of their eikonal-Born series (EBS) amplitude with this modified Glauber amplitude in an analysis of a particular electron-helium inelastic process with the EBS method, and found that it yielded results agreeing better with data than the EBS. The basis for our choice of this modified Glauber amplitude for electron-atom scatterings is, however, completely different from theirs.[1,5] As was well known, f_G of elastic electron-helium scattering is given by[8]

$$f_G = \frac{ik_\mu}{2\pi}\int d^2b\, d\vec{r}_1\, d\vec{r}_2 \,|u_0(\vec{r}_1,\vec{r}_2)|^2 \times\left[1-\left(\frac{|\vec{b}-\vec{b}_1|}{b}\right)^{2i\eta}\left(\frac{|\vec{b}-\vec{b}_2|}{b}\right)^{2i\eta}\right], \tag{2}$$

where $u_0(\vec{r}_1,\vec{r}_2)$ is the ground state of a helium atom. We shall represent this ground state by the product of Hartree-Fock wave functions

$$\varphi_{1s}^{\mathrm{He}} = (1/4\pi)(Ae^{-\alpha r} + Be^{-\beta r}) \tag{3}$$

with $A = 2.605\,05$, $B = 2.081\,44$, $\alpha = 1.41$, and $\beta = 2.61$. f_{G2} is the second-order term of an eikonal expansion of the corresponding Glauber amplitude. To calculate the second-order Born term of the elastic electron scattering by a helium atom in its ground state, we start with its exact form,

$$f_{B2} = 8\pi^2 \int d^3\vec{k} \sum_n \frac{\langle 0,\vec{k}_\nu | V | n,\vec{k}\rangle\langle n,\vec{k}|V|\vec{k}_\mu\rangle}{k^2-k_\mu^2+2(\omega_n-\omega_\mu)-i\epsilon} \tag{4}$$

in which the interaction potential is given by

$$V = \sum_{i=1}^{2}\frac{1}{r_{i3}} - \frac{1}{r_3} \tag{5}$$

with $r_{i3} = |\vec{r}_i - \vec{r}_3|$. The integration over the plane-wave parts of the matrix elements of Eq. (4) can be done easily, and one obtains

$$f_{B2} = \frac{2}{\pi^2}\int d^3\vec{k}\sum_n \frac{1}{K_\mu^2 K_\nu^2}\,\frac{\langle 0|\sum_{i=1}^{2}(e^{-i\vec{K}_\nu\cdot\vec{r}_i}-1)|n\rangle\langle n|\sum_{i=1}^{2}(e^{i\vec{K}_\mu\cdot\vec{r}}-1)|0\rangle}{k^2-k_\mu^2+2(\omega_n-\omega_\mu)-i\epsilon}, \tag{6}$$

where $\vec{K}_\mu = \vec{k}_\mu - \vec{k}$ and $\vec{K}_\nu = \vec{k}_\nu - \vec{k}$. As in the case of a hydrogen atom, the usual approximation to be made here is to carry out an average closure summation over the intermediate states n as was often considered for the second-Born theory.[9] By average summation, we mean that the closure summation is performed after the excited energy of the intermediate state has been replaced by an average value $\overline{\omega}$. Here $|0\rangle$ is the ground state of a helium atom and $p_\mu^2 = k_\mu^2 - 2\overline{\omega}$. The following expression for the approximate second-Born term will be obtained after the orthonormality of spin wave functions of the single-particle ground states of helium has been taken into consideration:

$$\overline{f}_{\mathrm{SB2}} = \frac{4}{\pi^2}\int d^3\vec{k}\,\frac{1}{K_\mu^2K_\nu^2}\,\frac{1}{k^2-p_\mu^2-i\epsilon}\Big[\langle\varphi_{1s}^{\mathrm{He}}|e^{i\vec{q}\cdot\vec{r}} - e^{i\vec{K}_\mu\cdot\vec{r}} - e^{-i\vec{K}_\nu\cdot\vec{r}} + 1|\varphi_{1s}^{\mathrm{He}}\rangle + \langle\varphi_{1s}^{\mathrm{He}}|e^{i\vec{K}_\mu\cdot\vec{r}}-1|\varphi_{1s}^{\mathrm{He}}\rangle\langle\varphi_{1s}^{\mathrm{He}}|e^{-i\vec{K}_\nu\cdot\vec{r}}-1|\varphi_{1s}^{\mathrm{He}}\rangle\Big], \tag{7}$$

where $\varphi_{1s}^{\mathrm{He}}$ is given by Eq. (3). Equation (7) will be used to obtain the approximate value for f_{B2} of helium in our calculation. Another approximate form for f_{B2} will be obtained if one treats the ground state of helium different from the rest of a cluster of other intermediate states in the average closure summation. This approximate amplitude will be denoted by $\overline{f}_{B2}$ and is given by

$$\overline{f}_{B2} = \frac{4}{\pi^2}\int d^3\vec{k}\,\frac{1}{K_\mu^2K_\nu^2}\,\frac{1}{k^2-p_\mu^2-i\epsilon}\Big[\langle\varphi_{1s}^{\mathrm{He}}|e^{i\vec{q}\cdot\vec{r}} - e^{i\vec{K}_\mu\cdot\vec{r}} - e^{-i\vec{K}_\nu\cdot\vec{r}} + 1|\varphi_{1s}^{\mathrm{He}}\rangle - \langle\varphi_{1s}^{\mathrm{He}}|e^{i\vec{K}_\mu\cdot\vec{r}}-1|\varphi_{1s}^{\mathrm{He}}\rangle\langle\varphi_{1s}^{\mathrm{He}}|e^{-i\vec{K}_\nu\cdot\vec{r}}-1|\varphi_{1s}^{\mathrm{He}}\rangle\Big] + \frac{8}{\pi^2}\int d^3\vec{k}\,\frac{1}{K_\mu^2K_\nu^2}\,\frac{1}{k^2-k_\mu^2-i\epsilon}\langle\varphi_{1s}^{\mathrm{He}}|e^{-i\vec{K}_\nu\cdot\vec{r}}-1|\varphi_{1s}^{\mathrm{He}}\rangle\langle\varphi_{1s}^{\mathrm{He}}|e^{i\vec{K}_\mu\cdot\vec{r}}-1|\varphi_{1s}^{\mathrm{He}}\rangle\,. \tag{8}$$

However, for a possible favorable theoretical interpretation of the approximation, in our model, we would prefer to choose Eq. (7) for f_{B2}, although we shall also perform the calculations with $\overline{f}_{B2}$ for comparison with other methods. It should be stressed that the main conclusions of our work presented here are not affected by the choice of either form of approximation for f_{B2}. The differential cross section is given by

$$\frac{d\sigma}{d\Omega} = |f_{\mathrm{GM}}|^2\,. \tag{9}$$

Also, for the purpose of making a comparison with results of other theoretical calculations, the exchange effect may tentatively be included through the consideration of an Ochkur amplitude.[10] In this case, the differential cross sections will be given by

$$\left(\frac{d\sigma}{d\Omega}\right)_{WE} = |f_{GM} - g^{He}_{Och}|^2 , \tag{10}$$

where g^{He}_{Och} is

$$g^{He}_{Och} = -\frac{8}{k_\mu^2}\left(\frac{\alpha A^2}{(q^2+4\alpha^2)^2} + \frac{(\alpha+\beta)AB}{[q^2+(\alpha+\beta)^2]^2} + \frac{\beta B^2}{(q^2+4\beta^2)^2}\right). \tag{11}$$

Atomic units have been used throughout in this paper.

III. RESULTS AND DISCUSSION

We have performed the calculations[11] of differential cross sections of elastic scattering of electrons by helium in its ground state at energies equal to 100, 200, 300, 400, and 500 eV, using the modified Glauber amplitude as proposed in the previous section [Eq. (1)] and with f_{B2} approximated to be $\bar{f}_{SB2}$ [Eq. (7)]. These results are shown in Figs. 1–7. Also shown are data obtained recently by various experimental research groups,[12] as well as theoretical values of the first Born and conventional Glauber approximations.

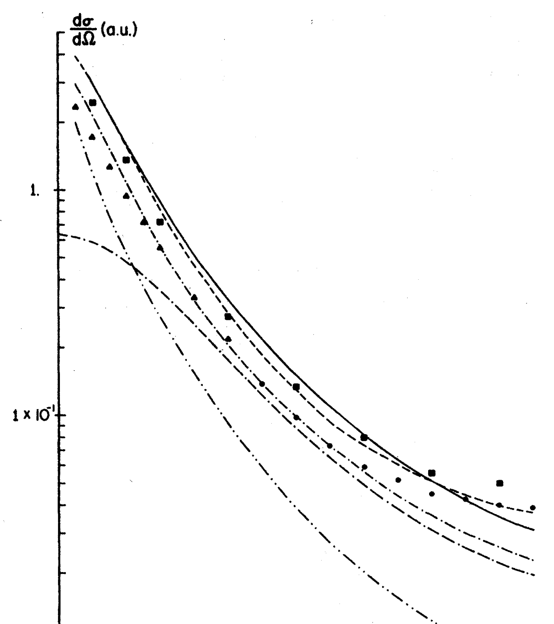

FIG. 1. Differential cross sections of elastic scattering of electrons by helium atoms in their ground states at 100 eV. •— •—, present calculation without exchange; —, present calculation with Ochkur exchange; ----, EBS; ••— ••—, conventional Glauber; •— — •— —, first Born approximation. ▲, experimental data by Jensen *et al.*; ●, experimental data by Sethuraman *et al.*; ■, experimental data by Crooks *et al.* Atomic units are used here.

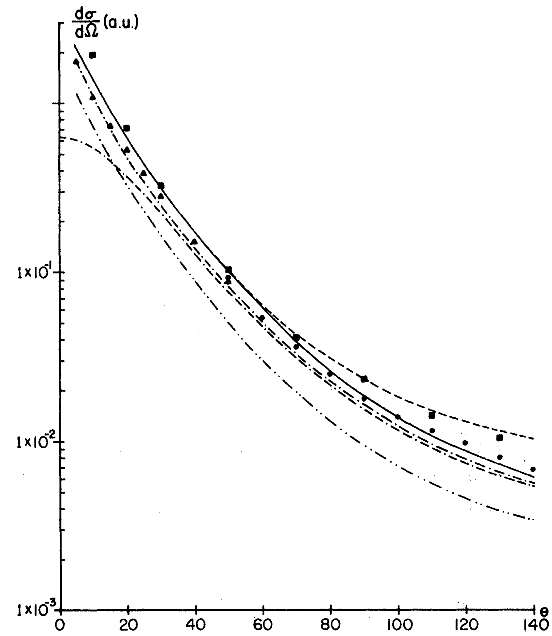

FIG. 2. Same as in Fig. 1 at 200 eV.

We found that values calculated with our modified Glauber amplitude are in good agreement with data at all angles. Among the new sets of experimental data, our results tend to be in better agreement with those by Jansen *et al.*[12] at smaller angles of scattering and with those by Sethuraman *et al.*[12] at larger angles of scattering. Our theo-

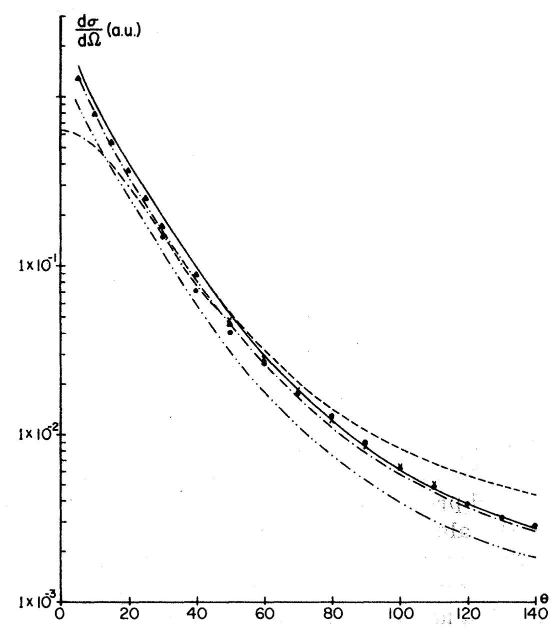

FIG. 3. Same as in Fig. 1 at 300 eV. ×, experimental data by Bromberg.

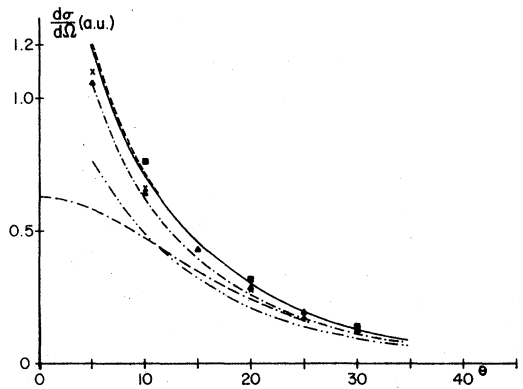

FIG. 4. Same as in Fig. 1 at 400 eV (small scattering angles). ×, experimental data by Bromberg.

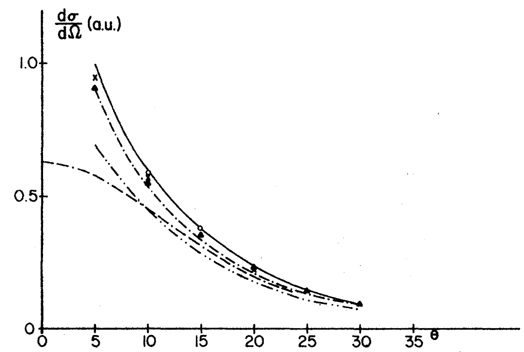

FIG. 6. Same as in Fig. 1 at 500 eV (small scattering angles). ×, experimental data by Bromberg; ○, experimental data by Oda *et al.*

retical values can also be regarded as in fair agreement with the set of data by Bromberg.[12] The first Born approximation of course yields values too small at small scattering angles, while theoretical points calculated with the conventional Glauber amplitude stay much lower than experimental data as well as those obtained in our method at all angles. The inclusion of an exchange effect, tentatively through an Ochkur term, would make our theoretical points deviate somewhat from data by Jansen *et al.*[12] at small angles. Relatively speaking, the new set of values obtained with the inclusion of the Ochkur term still can be regarded as in fair agreement with experimental data.

For the purpose of making a comparison with our modified Glauber method, we have also recalculated the differential cross sections within the eikonal-Born series (EBS) method[13] with the use of the same approximation for the second-Born term, first as $\bar{f}_{SB2}$ and subsequently as $\bar{f}_{B2}$. Also, to make the comparison more meaningful, the same wave functions of the helium atom are used, and the same value of the average excitation energy is chosen, i.e., $\bar{\omega} = 1.3$ a.u., in both calculations (modified Glauber and EBS). The results of EBS with $\bar{f}_{SB2}$ are also shown in these figures. While our modified Glauber results do not differ significantly from those obtained in the EBS at small and intermediate angles of scattering, they appear to systematically lie below the values of the EBS at larger angles. Although the basis for our choice of the modified Glauber amplitude is completely different from that of the EBS, on the computation side, our modified Glauber amplitude differs from the EBS by the presence of higher-order eikonal terms implicitly

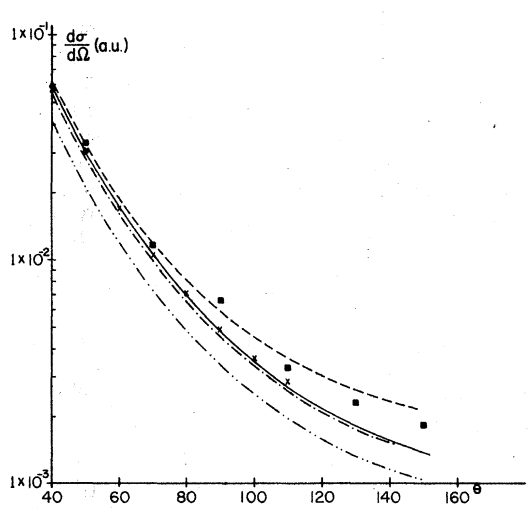

FIG. 5. Same as in Fig. 4 (large scattering angles).

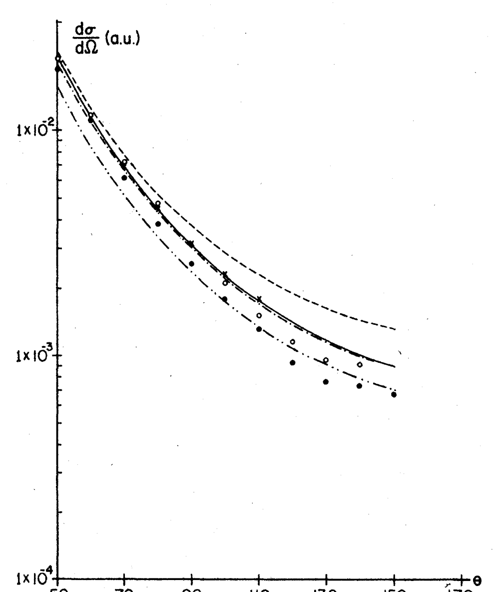

FIG. 7. Same as in Fig. 6 (large scattering angles).

contained in f_G. Thus, contrary to the popular belief that higher-order eikonal terms are completely dominated by the EBS terms in the entire range of momentum transfer, the results shown here indicate that these higher-order terms do seem to play some significant role at large scattering angles. This is possible, since although the magnitude of each of these higher-order terms might be small, the number of these terms are, however, infinite; hence, their effect as a whole on the scattering amplitude might not be negligible. As for the differential cross sections calculated with the second-Born term approximated to be $\bar{f}_{B2}$ [Eq. (8)], the same conclusions can be reached. In fact, we found that our modified Glauber results again systematically lie below those of the EBS at large scattering angles. Thus, these higher-order eikonal terms do seem to play some significant role there. To justify the neglect of these higher-order terms from the EBS, the authors of the EBS model[13] had to rely on a conjecture of a partial cancellation, which they contended probably exists between these eikonal terms ($n>3$) and the remaining part of the higher-order Born terms, missing from the Glauber amplitude due to eikonization—although there is not any proof that this kind of cancellation actually occurs for all terms and at all angles. While calculations with the second-Born term approximated to be $\bar{f}_{B2}$ decrease somewhat the modified Glauber values at larger scattering angles, both results (calculated with $\bar{f}_{SB2}$ and $\bar{f}_{B2}$) can be used to confirm that the deficiency of the Glauber amplitude stems mainly from the inadequacy of its second-order eikonal term. In fact, the replacement of f_{G2} in the Glauber amplitude by an approximate second-Born term (either $\bar{f}_{SB2}$ or $\bar{f}_{B2}$) improves significantly the values of differential cross sections at all angles.

IV. CONCLUSION

In this paper, we have applied the so-called modified Glauber amplitude (in which, the second-order term of the eikonal expansion is already corrected with its counterpart prior to eikonization) to the study of elastic scattering of electrons by a helium atom in its ground state at several intermediate energies. Our theoretical values obtained in the calculation are found to agree well with experimental data. Thus, one can draw from this work a few conclusions. First, the results obtained here confirm reasonably clearly that the deficiency of the Glauber amplitude in dealing with electron-atom scattering indeed originates mainly from its second-order eikonal term. Second, a comparison between the results of the modified Glauber and EBS methods with the use of exactly the same wave functions and the same approximations for the second-Born term indicates that higher-order terms in the eikonal expansion do seem to play some significant role at large scattering angles. Therefore, the neglect of these terms from the scattering amplitude appears not to be very well justified.

ACKNOWLEDGMENT

I wish to thank the National Research Council of Canada for its financial support of this work.

---

*Work supported in part by the National Research Council of Canada (Operating Grant No. A-3962).

[1]T. T. Gien, J. Phys. B 9, 3203 (1976).
[2]R. J. Glauber, *Lectures in Theoretical Physics*, edited by W. E. Brittin and L. G. Duncan (Interscience, New York, 1959), Vol. 1, pp. 315–444.
[3]See a rather clear and complete review article by E. Gerjuoy and B. K. Thomas, Rep. Phys. 37, 1345 (1974), and references therein.
[4]V. Franco, Phys. Rev. Lett. 20, 709 (1968).
[5]T. T. Gien, Phys. Rev. A 16, 123 (1977).
[6]P. J. O. Teubner, C. R. Lloyd, and E. Weigold, J. Phys. B 6, L134 (1973); C. R. Lloyd, P. J. O. Teubner, E. Weigold, and B. R. Lewis, Phys. Rev. A 10, 175 (1974); J. F. Williams, J. Phys. B 8, 2191 (1975).
[7]F. W. Byron, Jr. and C. J. Joachain, J. Phys. B 8, L284 (1975).
[8]V. Franco, Phys. Rev. A 1, 1705 (1970); Phys. Rev. Lett. 26, 1088 (1971); Phys. Rev. A 8, 2927 (1973); B. K. Thomas and F. T. Chan, Phys. Rev. A 8, 252 (1973); H. Tai, R. H. Bassel, E. Gerjuoy, and V. Franco, Phys. Rev. A 1, 1819 (1970).
[9]S. P. Khare and B. L. Moiseiwitsch, Proc. Phys. Soc. London 85, 821 (1965); S. P. Khare, Proc. Phys. Soc. London 86, 25 (1965); Phys. Lett. A 29, 355 (1969); A. R. Holt and B. L. Moiseiwitsch, J. Phys. B 1, 36 (1968); A. R. Holt, J. Hunt, and B. L. Moiseiwitsch, J. Phys. B 4, 1318 (1971); J. Phys. B 4, L241 (1971); C. R. Garibotti and P. A. Massaro, J. Phys. B 4, 1270 (1971); M. J. Woolings and M. R. C. McDowell, J. Phys. B 5, 1320 (1972); M. J. Woolings, J. Phys. B 5, L164 (1972).
[10]V. I. Ochkur, Zh. Eksp. Teor. Fiz. 45, 734 (1963) [Sov. Phys. JETP 18, 503 (1964)]; V. I. Ochkur and V. F. Brattsev, Opt. Spektrosk. 19, 490 (1965) [Opt. Spectrosc. 19, 274 (1965)].
[11]Calculations performed on an IBM 370-158 of the NLCS, a joint computer service of Memorial University of Newfoundland and the Newfoundland Provincial Government.
[12]J. P. Bromberg, J. Chem. Phys. 61, 963 (1974); G. B. Crooks and M. E. Rudd, Bull. Am. Phys. Soc. 17, 131

(1972); G. B. Crooks, Ph.D. thesis (University of Nebraska, Lincoln, 1972) (unpublished); N. Oda, F. Nishimura, and S. Tahira, J. Phys. Soc. Jpn. 33, 462 (1972); S. K. Sethuraman, J. A. Rees, and J. R. Gibson, J. Phys. B 7, 1741 (1974); R. H. J. Jansen, F. J. DeHeer, H. J. Luyken, B. VanWingerden, and H. J. Blaauw, J. Phys. B 9, 185 (1976); R. H. J. Jansen, thesis (Amsterdam University, 1975) (unpublished).

[13]F. W. Byron, Jr. and C. J. Joachain, Phys. Rev. A 8, 1267 (1973); 8, 3266 (1973).