Shape of the "cusp" in He^{2+}-He and He^{+}-He collisions in the 0.6—1.6-MeV impact-energy region

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The shape of the distribution of electrons ejected into the forward direction in the He^{+}-He and He^{2+}-He collisions in the 0.6—1.6-MeV impact-energy region are investigated. In both cases the anisotropies observed in the measured double-differential electron spectrum are analyzed by the help of a series expansion and a fitting procedure for a better characterization of the cusp. The theoretical peak shapes are also analyzed by this method. In the case of He^{2+} the agreement between the measured and the calculated cusp shapes is especially poor.

I. INTRODUCTION

The study of the "cusp" in the spectrum of electrons ejected into the forward direction in ion-atom collisions seems to be an actual field of research in its own right nowadays.[1] In spite of the number of works on this phenomenon, however, there are quite a few problematic issues in this field. One of them is, without any doubt, the shape of the cusp.

The early theories predict nearly symmetric and identical cusp shapes for the electron capture to the continuum for bare projectiles (ECC)[2–5] and for the electron loss to the continuum for projectiles with accompanying electron (ELC).[6,7]

Disregarding the earliest results[8] where an asymmetric cusp shape skewed towards lower velocities was observed in both cases (i.e., in the case of ECC and ELC), the experimental evidence shows a significant difference in cusp shapes for the two cases. Studies carried out first with heavy-ion projectiles,[9,10] then with light projectiles[11] reliably showed an asymmetric shape (skewed towards lower velocities) for projectiles without electron(s), while for projectiles with accompanying electron(s) the cusp shape was found to be nearly symmetric.[12]

Several theoretical efforts were carried out to predict the asymmetric shape of the cusp for bare projectiles including the second Born term,[13–15] improving the first Born approximation calculations[16] and using the multiple-scattering theory.[17] The Jakubassa-Amundsen approach[18] for argon projectiles and helium targets seems to be successful in a rather special case by going beyond the second Born approximation and incorporating different effects as, e.g., those of large perturbing fields, but the explanation of the skewedness of the ECC cusp in general cannot be regarded as having been solved.

Concerning the experimental study of the cusp shape, a series expansion and a fitting procedure for a better characterization of the experimental data for the cusp were introduced.[19,20] It is a general, model-independent method, and different physical interpretations of the terms of the expansion can be given. Although any unique interpretation of the terms is now missing, the fact that a substantial "*p*-wave contribution" should be included for a good fit indicated qualitatively the presence of the second Born terms in the treatment of the cusp phenomena.[19,21]

It should be mentioned here, however, that in the case of projectiles with accompanying electron(s) there is no detailed comparison on the cusp shape between experimental evidence and the corresponding theories.[6,7] Meckbach *et al.*,[22] however, analyzed the contour lines of the cusp for H^{0}-He collision by using the series-expansion procedure. There are some other studies with qualitative statements.[11,23,24]

Recently a study has been carried out on the cusp features at simple collision systems by Kövér and co-workers.[11,23,25,26] In these published papers, however, no detailed evaluation of the experimental data was given on the shape of the cusp.

In this paper a detailed study of the cusp shape will be reported for He^{+}-He and He^{2+}-He collisions in the impact-energy range from 0.6 to 1.6 MeV, by using the experimental data obtained by Kövér *et al.*[23]

Such a study is well justified by the above-mentioned problems on the cusp shape. A similar detailed analysis has been published for simple collision systems only for the H^{+}-He collision between 40 and 240 keV.[20] Other publications on detailed analysis by the series expansion of the experimental data on the cusp shape are based on energetic heavy-ion impact[27,28] and on proton-foil collision[19,21,29] measurements.

In this paper we do not want to give any experimental details; they are reported in some earlier papers.[11,23,25,26] It should be mentioned here only that a 2.5-MV Van de Graaff generator was used by Kövér and co-workers to obtain the experimental data. The electron spectrum was taken by a special double-stage cylindrical mirror spectrometer of 0.3% resolution. The half angle of the angular acceptance cone at 0°, was 1.5° at the measurements concerned.

II. METHOD OF THE PARTIAL-WAVE EXPANSION FITTING

It is well known from the earlier papers[15,17,21,22,30] that the cross sections for both the ELC and the ECC processes have the following form:

$$\frac{d\sigma}{d\mathbf{v}_e}=\frac{1}{|\mathbf{v}_e-\mathbf{v}_p|}F(v',v_p,\cos\theta')\ , \tag{1}$$

where $\mathbf{v}'=\mathbf{v}_e-\mathbf{v}_p$ and $\mathbf{v}_e,\mathbf{v}_p$ are the velocity of the electron and the ion in the laboratory frame, respectively, while θ' is the polar angle of the electron velocity in the projectile frame measured with respect to the direction of v_p. In Eq. (1) the first term is symmetric around $\mathbf{v}_e=\mathbf{v}_p$, so the observed asymmetry should be associated with $F(v',v_p,\cos\theta')$.

The asymmetric term in Eq. (1) can be described by a multipole expansion,[19,20] so the cross section is written as

$$\frac{d\sigma}{d\mathbf{v}_e}=\frac{1}{v'}\sum_{j=0}^{\infty}a_j(v')P_j(\cos\theta')\ . \tag{2}$$

It is assumed that all coefficients can be represented as Taylor's series in v':

$$a_j(v')=\sum_{n=0}^{\infty}B_{nj}(v_p)v'^n\ . \tag{3}$$

Equation (2) can be written

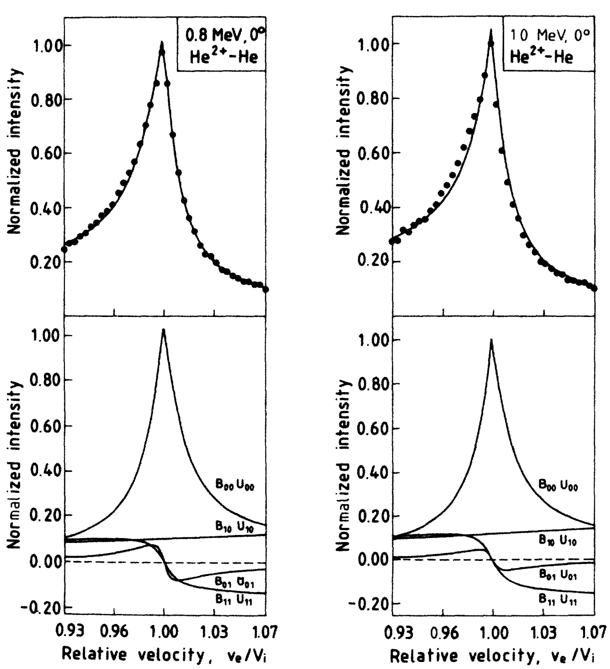

FIG. 1. Comparison of the experimental data on the cusp shape with the fitted spectrum by four coefficients of series expansion and the contribution of the different terms for 0.8 and 1.0 MeV He^{2+} impact on He target.

TABLE I. Coefficients B_{nj} from a fitting procedure for the cusp in He^{2+}-He collision.

E_b (MeV)	0.6	0.7	0.8	0.9	1.0	1.2	1.4	1.6
B_{01}/B_{00}	−0.36±0.01	−0.26±0.02	−0.18±0.02	−0.27±0.02	−0.11±0.02	−0.32±0.02	−0.31±0.02	−0.29±0.02
B_{10}/B_{00}	4.75±0.32	4.79±0.25	4.03±0.20	4.65±0.27	4.33±0.22	4.99±0.27	5.52±0.21	5.55±0.19
B_{11}/B_{00}	−4.26±0.32	−4.84±0.27	−4.58±0.22	−4.31±0.29	−4.98±0.23	−3.32±0.23	−3.84±0.60	−4.48±0.17
χ^2	1.8	1.2	1.2	2.1	1.7	3.9	2.9	1.4

$$\frac{d\sigma}{d\mathbf{v}_e}=\frac{1}{v'}\sum_{n,j}^{\infty}B_{nj}(v_p)v'^{n}P_j(\cos\theta') \ . \qquad (4)$$

In order to compare $(d\sigma/dv_e d\Omega)=v_e^2(d\sigma/d\mathbf{v}_e)$ with the measured distribution $Q(v_e,\theta)$ of the ejected electron (θ is the angle between $\mathbf{v}_e$ and $\mathbf{v}_p$), it must be convoluted with the spectrometer transmission function $S(v_e,\Omega)$ and also integrated over the experimental acceptances in velocity and angle,

$$Q(v_e,\theta)=\int_{v_e}\int_{\Omega}v_e^2\frac{d\sigma}{d\mathbf{v}_e}S(v_e,\Omega)dv_e d\Omega \ . \qquad (5)$$

By substituting Eq. (4) into Eq. (5) we obtain

$$Q(v_e,\theta)=\sum_{n,j}^{\infty}B_{nj}U_{nj} \ , \qquad (6)$$

where

$$U_{nj}=\int_{v_e}\int_{\Omega}v_e^2(v')^{n-1}P_j(\cos\theta')S(v_e,\Omega)dv_e d\Omega \ .$$

The spectrometer transmission function $S(v_e,\Omega)$ was determined according to the geometrical conditions of our spectrometer.[11,23] Its value was calculated for a rectangular-shaped slit. The result was the same as for a circular-shaped slit if the same solid angle was taken. After the appropriate transformation of variables from the projectile frame to the laboratory frame, the integrals in Eq. (6) could be calculated numerically.

The B_{nj} coefficients in Eq. (6) limited for $n=0,1$ and $j=0,1,2$ can be obtained by a least-squares-fitting routine. In our procedure the experimental error at the individual values in the electron distribution was about 3%. The error of the fitted parameters indicated in Tables I and III includes the experimental error and the error of the fitting procedure.

III. RESULTS AND CONCLUSIONS

A. He^{2+}-He collisions

As it was mentioned above, detailed cusp-shape investigations by series expansion for bare ions have been carried

TABLE II. Value of χ^2 at the inclusion of different coefficients in the fitting procedure of the experimental value for He^{2+}-He.

E_b (MeV)	B_{00}	B_{01}	B_{10}	B_{11}	B_{02}	χ^2
0.7	×					193
	×	×				28
	×	×	×			21
	×	×		×		28
	×	×	×	×		1.2
	×	×	×	×	×	1.1
1.2	×					221
	×	×				69
	×	×		×		70
	×	×	×	×		3.9
	×	×	×	×	×	2.7

TABLE III. Coefficients B_{nj} from a fitting procedure for the cusp in He^{+}-He collision.

E_b (MeV)	0.6	0.7	0.8	0.9	1.0	1.2	1.4	1.6
B_{01}/B_{00}	0.00±0.03	0.00±0.02	−0.07±0.1	0.00±0.02	0.00±0.02	−0.02±0.02	−0.01±0.01	−0.06±0.02
B_{10}/B_{00}	2.66±0.18	2.42±0.13	1.68±0.01	2.68±0.13	2.59±0.11	4.17±0.20	3.92±0.18	2.60±0.14
B_{11}/B_{00}	−1.44±0.08	−1.35±0.07	−0.90±0.05	−1.39±0.07	−1.39±0.06	−1.07±0.12	−0.20±0.10	−1.19±0.10
χ^2	1.3	1.9	0.8	1.7	1.8	3.8	3.0	4.1

out for H^+ projectiles[20] and for incident heavy ions (C^{6+}, O^{8+}, Ne^{10+}, Ar^{16+}).[27,28] For He^{2+}, which is the next simplest projectile succeeding H^+, no similar shape study is available, and so, in this case, it was interesting to study the cusp shape in detail.

The evaluation of our earlier experimental data from this point of view was carried out in the present study for He^{2+} impact in the bombarding energy region from 0.6 to 1.6 MeV (from 2.45 to 4.00 a.u.). It represents a velocity region partly overlapping with that of Meckbach *et al.*[20] and, in general, much lower than the region described in the work of Berry *et al.*[27,28] Figure 1 shows the results of the fitting procedure and the contributions of the different terms of the expansion for 0.8 and 1.0 MeV impact energy. The values of the coefficients are given in Table I, relative to B_{00} which is the dominant term and represents the simplified symmetric approach according to, e.g., Dettman *et al.*[5]

The figure shows a rather good agreement between the experimental data and the fitted values by a four-term expansion at 0.8 and 1.0 MeV impact energy. The agreement is also acceptable as a function of the impact energy (cf. the values of the reduced χ^2 in Table I).

By increasing the number of coefficients in the fitting procedure, it was found that the fitting is not improved by the additional parameters (see Table II) or these coefficients are equal to 0 within the limit of the error (B_{02}).

Looking at the table of coefficients, however, the most striking feature is the *approximate* constancy of the values mainly for B_{10} and B_{11}. For B_{01}, however, there is a rather large fluctuation in the energy range studied. At the same time there is no tendency for a unique increase or decrease of the coefficients with energy in any case, which indicates that the cusp shape does not depend strongly on the impact energy at the He^{2+}-He collision in the impact-energy region concerned, or at least there is no tendency for a unique change with impact energy, respectively.

Comparing, however, other details of the results (i.e., the values of the parameters) from previous works with our corresponding values, the following can be stated: Both the relative B_{10} and B_{11} values seem to be much higher in our case than in Refs. 20, 27, and 28. Their velocity regions, however, are different from ours as are their experimental conditions.

The $B_{01}U_{01}$ term is mainly responsible for the asymmetry of the cusp close to the top of the peak. Berry *et al.*[28] found that this coefficient is approximately constant or has a small increase in a broad impact-energy interval (from 8.6 to 18.1 a.u.) for C^{6+}-, O^{8+}-, Ne^{10+}-, and Ar^{18+}-He collisions similarly to our findings (He^{2+} projectile, 2.45—4.00 a.u.). A similar phenomenon has also been observed, for the H^+-He collision in the 2.04—3.11 a.u. region.[20]

Regarding the coefficient B_{10} and the corresponding term, it characterizes a "background" (the continuous part of the spectrum under the cusp) contribution to the cusp. Its contribution is nearly constant in the present measurements as a function of the energy of the electron (see Fig. 1) similarly as is in Refs. 20 and 28. The much higher value of the coefficients in our study, however, might be explained by the fact that in the work of Meckbach

TABLE IV. Value of the χ^2 at the inclusion of different coefficients in the fitting procedure of the experimental value for He^+-He.

E_b (MeV)	B_{00}	B_{01}	B_{10}	B_{11}	B_{02}	B_{12}	χ^2
0.7	×						52
	×	×					19
	×		×				43
	×			×			25
	×				×		45
	×					×	38
	×	×	×				4.0
	×	×			×		7.1
	×	×		×			19
	×	×	×	×			1.9
	×	×	×	×	×		1.6
	×	×	×	×	×	×	1.6
1.2	×						61
	×	×					58
	×		×				15
	×			×			65
	×				×		19
	×					×	13
	×	×	×				6.1
	×	×		×			59
	×	×			×		11
	×	×	×	×			3.8
	×	×	×	×	×		2.3

et al.[20] and Berry *et al.*,[28] the projectile beam was formed with better quality and a "real" background was subtracted in both cases. (However, the measurements of the background were different in the two studies.)

On the other hand, the constancy of the coefficient B_{10} somewhat reflects the stability of our measuring system, mainly that of the beam parameters (see Ref. 28).

Let us consider now the coefficient B_{11}. This coefficient and the corresponding term partly contribute in reflecting the asymmetry. At the same time the B_{11} coefficient is also important for the peak tails[28] and is also related to the background under the cusp. The relative large spread in the value of B_{01} may be caused by B_{11} due to the similar effect in the fitting procedure.

To check how the values of the coefficients (B_{01}, B_{10}, B_{11}) depend on the range of fitting, the procedure was carried out for different regions: from $(1\pm0.03)v_p$ to $(1\pm0.15)v_p$ at six different regions. If the region is higher than ±0.05 around the peak, the values of the parameters are practically constant, but if the region is smaller than ±0.05 around the top of the cusp, some changes can be observed. A probable reason for this is that the results become very sensitive to the accuracy and the density of the points measured around the top of the peak when the fitting procedure is performed very close to the top of the peak.

The theoretical investigations can give some asymmetric shape of the cusp[13,14,17,18] only if the interaction between the outgoing electron and the projectile ion is tak-

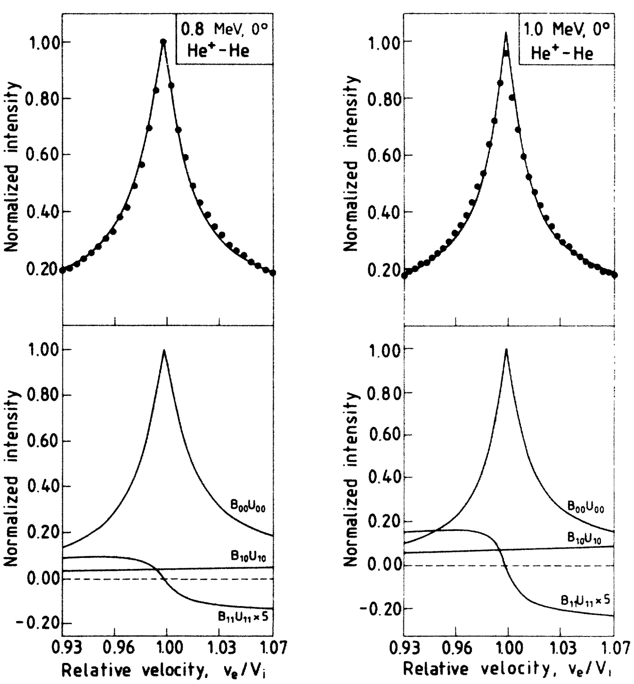

FIG. 2. Comparison of the experimental data on the cusp shape with the fitted spectrum by four coefficients of series expansion for 0.8 and 1.0 MeV He^{+} impact on He target. In the case of 0.8 MeV we do not show the contribution from $B_{01}U_{01}$ because the B_{01} parameter equals 0 between the experimental error.

TABLE V. Coefficients B_{nj} from the fitting procedure of the spectrum according to the first-order Born approximation for He^{+}-He collision.

E_b (MeV)	0.6	0.7	0.8	0.9	1.0	1.2	1.4	1.6
B_{01}/B_{00}	0.00±0.02	0.00±0.02	0.03±0.01	0.00±0.02	0.00±0.02	0.00±0.01	0.00±0.02	0.00±0.01
B_{10}/B_{00}	4.71±0.17	3.72±0.14	3.49±0.32	3.14±0.12	2.68±0.11	3.06±0.07	2.20±0.11	1.53±0.06
B_{11}/B_{00}	0.00±0.08	0.00±0.07	0.00±0.15	0.00±0.06	0.00±0.05	0.00±0.09	0.00±0.03	0.00±0.04
χ^2	12	11	11	10	11	9	11	10

en into consideration in higher orders.

Macek et al.[21] strongly indicated that the second-order Born term plays an important role in the description of ECC processes. The above-mentioned theories are valid only for H-like target atoms and for asymptotically high velocities. In other cases there are no theoretical investigations because of the rather difficult numerical calculations.

The distribution calculated by us is based on the work of Shakeshaft and Spruch[13] who worked out a high-velocity approximation for the second-order Born term. (We used for He, $Z_{eff}=1.7$.) It is analyzed in the same way as the experimental one by series expansion. The B_{01} and B_{11} coefficients determined in this way are far less than the coefficients determined for the experimental distribution. It is not surprising, however, because the calculations were carried out in a high-velocity approximation.

B. He^+-He collision

A detailed analysis of the shape of the cusp for collisions, where the projectile carries electrons (presence of ELC mechanism), was carried out by Meckbach et al.[22] in the case of the H^0-He collision. They took a three-dimensional cusp spectrum at 105 keV impact energy and studied the contour lines of the cusp at the prefixed fractional levels of the peak height by a series expansion limited to the inclusion of two terms, namely, $n=0$ and $j=0$ and 2. The other studies on the cusp for projectiles carrying electrons are rather qualitative in character (cf., e.g., Refs. 11, 12, 23, and 24).

In the present work the cusp shape in the collision He^+-He has been studied as a function of the impact energy in the region from 0.6 to 1.6 MeV (from 2.45 to 4.00 a.u.). Figure 2 shows the results of the fitting procedure for 0.8 and 1.0 MeV impact energy and the coefficients of the series expansion from the fitting procedure is given in Table III. The effect of increase and decrease of the number of coefficients was checked in details. Table IV shows, as for He^{2+}, that the four-parameter expansion seems to be acceptable, all the more because with the fitting procedure of five coefficients, the error of the fifth coefficient is very high. It seems correct that two coefficients alone are not sufficient, especially B_{00} and B_{02}; these were used by Meckbach to interpret the contour line.

The values of the coefficient B_{10} which characterizes first of all the background contribution, are rather similar to those for He^{2+}-He collision (see Sec. III A), but they are somewhat smaller here. The coefficient B_{01}, however, which is responsible for the major asymmetric term, is practically zero in this case. The largest difference can be observed (see Tables I and III) in the case of B_{11}. The values of the coefficient concerned are lower approximately by a factor of 5 here than those for the He^{2+} projectile. This coefficient and the corresponding term also reflect the asymmetry of the cusp shape.

In other shape studies for projectiles carrying electron(s), the shape is only qualitatively symmetric (e.g., Refs. 11, 21, 22, 24, and 29). The theory of Drepper and Briggs,[6] however, gives a practically symmetric shape. A similar result is determined from our first-order Born calculation which differs from that in Ref. 6 mostly in the calculation of the elastic scattering form factor. We used Roothaan-Hartree-Fock wave functions[23] here.

To compare the experimental and theoretical cusp shape in this case, the theoretical distribution (first-order Born approximation[23]) was analyzed in the same way as the experimental cusp shape, i.e., by series expansion. Here the coefficients B_{01} and B_{11} happened to be zero (see Table V) which is to be expected because this theory cannot describe the observed slight asymmetry. This asymmetry may be caused by the possible ECC process shown in our earlier work.[23]

C. Conclusions

The series-expansion procedure used to characterize the shape of the cusp was formerly carried out for H^+ and for heavier ions (C^{6+}, O^{8+}, Ne^{10+}, and Ar^{18+}). Now it was performed for He^{2+} at several impact-energy values from 2.45 to 4.00 a.u. For projectiles carrying electron(s), the present study is the first detailed investigation of the cusp shape by series expansion for He^+ projectiles. A definite deviation from the strict symmetric shape and that from the one predicted by the theory of Drepper and Briggs[6] was found.

Furthermore, in the present study the necessary number of coefficients at series expansion was optimized together with the effect of the range of the fitting around the top of the cusp.

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