Two-center electron emission in collisions of fast, highly charged ions with He: Experiment and theory

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Electron emission cross sections differential in energy and angle of the ejected electrons were measured in collisions of 5-MeV/*u* C^{6+}, O^{8+}, and Ne^{10+} ions on He. The experimental results deviate substantially from calculations based on the plane-wave Born approximation indicating that the ejected electrons are significantly affected by the two-center field of the target and projectile ion. The two-center effects were confirmed by comparison with results from the continuum-distorted-wave–eikonal-initial-state (CDW-EIS) approximation that has recently been improved by using Hartree-Fock-Slater wave functions for the ejected electrons. It is shown for nearly complete energy and angular ranges that the improved CDW-EIS method predicts cross sections in excellent agreement with experiment.

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I. INTRODUCTION

Since several decades, studies of electron emission have provided important information about ionization mechanisms in fast ion-atom collisions. In the early 1960s, Rudd and collaborators [1,2] conducted pioneering experiments determining cross sections for electron emission within nearly complete electron energy and angular ranges. The measured electron spectra showed significant structures, such as the soft-collision peak and the binary-encounter peak that were found to be well described by calculations using the plane-wave Born approximation (PWBA) [1–3]. This agreement is primarily due to the fact that the PWBA describes one-center electron emission where the target interacts strongly with the electron whereas the projectile interaction enters as a first-order perturbation. Hence, theory and experiment are expected to agree well for soft-collision electrons that are due to weak projectile-electron interactions. This is not necessarily true for binary-encounter electrons that are essentially produced by violent projectile impact. Nevertheless, for binary collisions by bare projectiles, perturbative methods are adequate since they yield similar results as higher-order calculations [4].

The early experiments, performed by proton impact at intermediate projectile energies of a few hundred keV, exhibited characteristic discrepancies with theory. At forward angles certain experimental cross sections were found to be considerably higher than the predictions by the PWBA. These discrepancies were associated with two-center effects where the long-range Coulomb forces of both projectile and target atom play an important role [5]. In particular, additional projectile-electron interactions in the final state give rise to the cusp shaped peak due to electron capture to continuum (ECC) observed in the early 1970s [6–8]. Similar two-center effects were made responsible for discrepancies between theory and PWBA at forward observation angles. Once, these discrepancies were understood, they could be reduced by using projectiles of relatively high energies. Indeed, at forward angles, the agreement between experiment and theory improved essentially as protons with energies as high as a few MeV were used [9].

Significant discrepancies remained for the case of high-energy electron ejection at backward angles. In this case the electron initially receives a large momentum transfer in a binary projectile-electron collision followed by a backscattering of the electron in the field of the target atom. This target-backscattering [10] is due to a one-center phenomenon that is expected to be well described within the framework of the PWBA. Hence, at backward angles, rather than to attribute the missing agreement between theory and experiment to a failure of the PWBA, it should be associated with the use of an inadequate wave function for the active electron. In the early theoretical studies, hydrogenlike wave functions were applied to describe the final continuum state of the ejected electron [1,2]. Such wave functions are based

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on an effective target charge which is smaller than that of the corresponding bare nuclei so that the violent electron-target backscattering is underestimated by the theory.

The importance of the adequate description of the final continuum states was recognized by Madison [11] who was first to use Hartree-Fock-Slater wave function in the PWBA. With the inclusion of realistic bound and continuum wave functions, a crucial source for discrepancies between theory and experiment has been withdrawn. Indeed, the calculations were found to be in remarkable agreement with experimental cross sections for the ejection of high-energy electrons at backward angles [11]. In addition, as protons of a few MeV were used, an excellent description of the experiments was achieved within the almost complete angular range [9]. In this case, two-center effects are limited to an angular region of near zero degree where the ECC cusp occurs [12,13]. Hence, apart from extreme forward angles, the problems involved in the understanding of electron emission by fast incident ions of low charge appeared to be solved.

More recently, current interest in two-center effects was created, since fast and highly charged ions were used in the experiments [14,15]. The experimental results were interpreted by means of continuum distorted-wave (CDW) theories where the final state is described by a two-center continuum wave function. A particular version, referred to as CDW-EIS, represents the projectile interaction in the initial state by an eikonal phase [16,17]. Thus, the CDW-EIS is suitable to describe electron emission in the combined Coulomb fields of the projectile and target. This theoretical approach has initially been put forward by Crothers and McCann [18] to analyze previous experimental results of total ionization cross sections [19]. The more recent experiments, devoted to the angular and energy distribution of ejected electrons, exhibited clear signatures for two-center effects. In particular, the data from high-energy collisions of 25-MeV/u Mo^{40+} on He indicated that two-center effects are important in the whole angular range of the ejected electrons [14]. Similar results have been obtained by Schneider *et al.* [20] and Pedersen *et al.* [21] investigating extended energy ranges of the ejected electrons. Also, two-center effects in the electron emission spectra have been studied at intermediate projectile energies by Bernardi *et al.* [22].

For high projectile energies, the analysis of absolute cross sections for electron emission suffered from inaccuracies of the CDW-EIS results which were due to the use of hydrogenlike wave functions for the ejected electrons [14,16,20,21]. Recently, this deficiency of the CDW-EIS has been removed [23,24]. Similar to the work by Madison [11] and Manson *et al.* [9], Hartree-Fock-Slater wave functions were implemented to describe the final continuum state centered at the target atom. The improved CDW-EIS was applied to electron emission from various collision systems. The theoretical description was refined, however, noticeable discrepancies remained between theory and experiment at intermediate projectile energies [23,24]. These discrepancies called for further studies.

In the present work, CDW-EIS calculations with Hartree-Fock-Slater wave functions are compared with electron emission cross sections measured with high-energy projectiles. In particular, we study the fully stripped ions C^{6+}, O^{8+}, and Ne^{10+} incident with 5-MeV/u on He, for which preliminary results have already been given by Platten *et al.* [15]. Here, we present a more detailed description of the experimental method including a refined analysis of the electron emission cross sections. Furthermore, theoretical cross sections using the PWBA and the CDW-EIS were evaluated. The PWBA results are found to deviate strongly from the experimental data indicating substantial two-center effects. On the other hand, between CDW-EIS and experiment an outstanding agreement is observed within the entire ranges of the measured electron emission angle and energy. From this agreement it is concluded that two-center phenomena in fast, highly charged ion-He collisions can essentially be understood.

In this work, Sec. II presents the experimental setup and the data analysis. Section III is devoted to the basic properties of the theoretical method. In Sec. IV the experimental results are compared with the theoretical data. A large number of data points were measured so that only a limited set of experimental cross sections can be given here. A complete compilation of the experiment data may be obtained on request [25].

II. MEASUREMENTS AND EXPERIMENTAL RESULTS

The experiments were performed using the cyclotron facility of the Ionenstrahl-Labor at the Hahn-Meitner Institut in Berlin. The experimental method is similar to that developed many years ago [26] so that here only the essential parts of the experimental set up will be described. The ion beam extracted from the accelerator was directed into a high-vacuum scattering chamber. The chamber has a diameter of about 1 m and was pumped by a set of four turbo pumps, each of which has a pumping speed of 1500 1/sec. A residual gas pressure of better than 10^{-6} mbar was achieved in the chamber. In the center of the chamber the ion beam was crossed by a gas beam produced by a nozzle of an inner diameter of 1 mm. It created a gas target whose average pressure was about 10^{-3} mbar over an extension of $\sim$5 mm. When the gas nozzle was operated, a homogeneous pressure of a few 10^{-5} mbar was produced in the rest of the scattering chamber. These gas densities in the chamber and in the target center are sufficiently low to achieve single-collision conditions.

The electrons ejected from the scattering center were measured by means of an electrostatic 45° spectrometer which consisted of a single stage. It was moved around the scattering center viewing different emission angles of the electrons. The single-stage spectrometer was used also at the observation angle of 0°. In this case the ion-beam passed through the deflection plates of the spectrometer. The angular resolution was $\Delta\theta = 5°$ and the energy resolution with $\Delta E/E = 0.075$. This moderate energy resolution was sufficient, as continuous electron spectra were studied in the present experiments.

Electron spectra of ejected electrons were measured in collisions of 5-MeV/u C^{6+}, O^{8+}, and Ne^{10+} with He target atoms. The spectra were acquired in the angular range from 0° to 160° in steps of 10°. The measured electron energies covered the range from 1 eV to a maximum value of 5000 eV. Within this interval, 100 data points were measured in logarithmic increments. In general, the lower limit for measuring reliable double differential cross sections was 10^{-24} cm^2/eV sr. At backward angles this value was already reached at an electron energy of about 1000 eV so that no measurements were performed above this limit.

The measured data were converted to absolute cross sections using methods described previously [26]. Before the experiments at the cyclotron, the spectrometer efficiency was calibrated by means of auxiliary measurements at a low-energy accelerator providing 300-keV H^+ ions. For this projectile, absolute cross sections have been measured previously with reliable accuracy [27] so that these values were used to calibrate the spectrometer efficiency. Then, the experiments at the high-energy accelerator were performed. It was not possible to measure directly absolute cross sections with the gas target from the nozzle as its density was not well known. In this case absolute cross sections were obtained by normalizing to results obtained without the gas nozzle using a homogeneous gas pressure in the scattering chamber. To produce the homogeneous pressure in the scattering center, the gas nozzle was lifted up by 7 cm. Hence the pressure in the scattering center was reduced to a known value, without changing any other instrumental parameter. This technique has also been described in more detail previously [26].

In the data analysis a few revisions were made since our preliminary publication [15]. It is well known that the soft-collision electrons are easily influenced by instrumental effects. For instance, spurious magnetic and electric fields in the scattering region may cause an efficiency loss of the spectrometer. We presume that the measurements of low-energy electrons were affected by electric fields due to charge up of the nozzle as the corresponding intensities decrease rapidly at electron energies lower than ~3 eV [15]. Therefore, in the present analysis, the low-energy data from 1–20 eV, measured with the gas nozzle, were replaced by the corresponding data obtained with homogeneous pressure (where the nozzle was lifted up). It is noted that corresponding spectra measured with and without nozzle agree (by normalization) at energies >20 eV, however, differences occur at energies <20 eV. Also, the spurious background due to detector noise was carefully subtracted from the measured data. Thus, small intensities corresponding to cross sections of a few 10^{-24} cm^2/eV sr were reduced. This reduction affected primarily data obtained at backward angles. Other more specific revisions are indicated in conjunction with the tabulated cross sections [25].

Figure 1 shows the measured cross sections for electron emission in 5-MeV/*u* Ne^{10+}+He collisions. Similar results were obtained for 5-MeV/*u* C^{6+} and O^{8+}+He impact. The data indicate a strong decrease over several orders of magnitude as the electron energy increases. At the low energy limit of a few eV the cross section curves reach a maximum due to the occurrence of the soft-collision electrons. The curves for emission angles of 40°, 50°, and 60° exhibit structures which are due to binary-encounter electrons.

The uncertainty of the absolute cross section is ±30% originating primarily from the error in the determination of the detector efficiency. The relative error with regard to a variation of the electron energy is about ±20% due to limited counting statistics and the spatial fluctuations of the ion beam hitting the gas target at varying thicknesses. The low-energy electrons (1–10 eV) are to be associated with higher uncertainties which, however, are difficult to determine. For example, 1-eV electrons have uncertainties as high as ±50%. Furthermore, statistical errors are significant for small cross sections where the background plays an important role. The errors of the small cross sections near 10^{-24} cm^2/eV sr were estimated to be as high as ±50%. It should be noted that the data measured at an observation angle of 0° may have additional errors due to spurious electrons created by ions hitting slit edges on their way through the spectrometer. Finally, it is noted that the C^{6+} data are less accurate than those for O^{8+} and Ne^{10+} impact as in the first case beam instabilities occurred during the experiments.

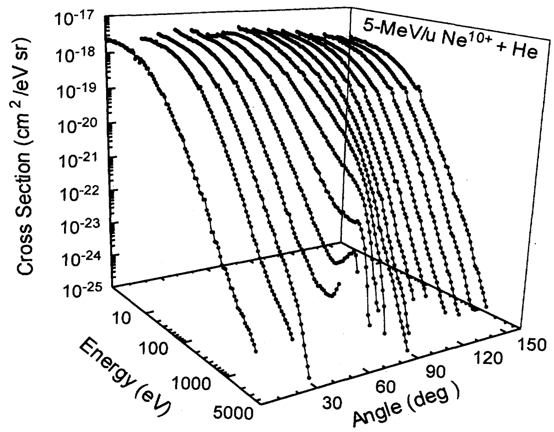

FIG. 1. Double differential cross sections for electron emission in 5-MeV/*u* Ne^{10+}+He collisions as a function of the electron energy and observation angle.

III. THEORETICAL METHOD

Since the present theoretical results are based on new developments of the CDW-EIS approximation [23,24], a few details of that method shall be given here. Within the theoretical framework it is assumed that one active electron is located on the target, while the others remain frozen during the collision. This allows us to reduce the problem to that of a single-electron defined by the Hamiltonian:

$$H_{\rm el}=T_{\rm el}+V_T+V_P=H_0+V_P, \qquad (1)$$

where $T_{\rm el}$ refers to the kinetic energy of the electron and V_T and V_P denote the target and projectile potential, respectively. In the PWBA the initial and final states are chosen as solutions of H_0, whereas in the CDW-EIS approximation they are taken as products of the PWBA wave function and a distortion that takes into account the long range projectile-electron interaction. In the initial state this distortion is chosen as an eikonal phase while in the final state it is chosen as a Coulomb continuum function. The distorted waves verify the correct asymptotic conditions for the Coulomb potential. Once the initial and final distorted waves are defined, they can be used to calculate the perturbation which, in turn, allows us to calculate the transition amplitude in first order of the distorted-wave series. A more detailed description of the theory can be found in a recent review [17].

In an application of this approach, Fainstein *et al.* [16] used hydrogenic wave functions for the continuum states of H_0 with an effective charge for the target continuum states. It was determined from the binding energy of the active electron in the initial state represented by a Roothaan Hartree-Fock wave function [28]. This scheme allows us to obtain analytical expressions for the transition amplitude which can readily be computed. The main drawbacks of this earlier method are that the initial and final target wave functions are not orthogonal and that the effective charge is a free parameter in the theory.

Recently, Gulyás *et al.* [24] improved the CDW-EIS model evaluating bound and continuum eigenstates of H_0 by numerical integration of the stationary Schrödinger equation with the Numerov algorithm. The interaction of the ejected electron with the projectile is described by a Coulomb continuum function as in the earlier CDW-EIS version [16]. This method provides a general framework which can be put in a single computer program to treat any target atom by inserting the corresponding target potential V_T. Thus, Gulyás *et al.* [24] developed a CDW-EIS code which was applied to evaluate the present theoretical results. The PWBA results were also obtained from the new code [24] using a negligibly small projectile charge of 10^{-4}. We verified that the present PWBA results accurately reproduce those by Manson *et al.* [9].

The improved CDW-EIS method is appropriate to correct previous limitations of the model. In particular, the incorporation of the continuous Hartree-Fock-Slater wave functions centered at the target allows an adequate description of electrons ejected at the backward angles. There is no ambiguity in the use of a hydrogen wave function describing the final projectile-electron interaction for a bare ion moving with a high velocity. In this case the ion remains bare as the electron capture probability is small. Also the high projectile velocity justifies the perturbative approach inherent in the CDW-EIS model.

IV. COMPARISON BETWEEN THEORY AND EXPERIMENT

For a detailed comparison of the experimental and theoretical results, it is advantageous to consider angular distributions rather than energy distributions. As already seen from Fig. 1 the double differential cross sections change by orders of magnitude in the measured electron energy range. In this case discrepancies between theory and experiments are often lost in the graphical display of the cross sections. However, the cross sections vary less with the electron emission angle so that a sensitive graphical comparison is possible in this case [9].

Figures 2 and 3 show comparisons between experimental and theoretical cross sections as a function of electron emission angle for C^{6+} and Ne^{10+} impact, respectively. The theoretical results are obtained using PWBA and CDW-EIS. For all electron energies it is seen that the PWBA underestimates the experimental data at forward angles and overestimates them at backward angle. To explain these discrepancies it is recalled that the PWBA describes accurately one-center effects. Hence, the observed discrepancies can be associated with two-center effects where the projectile is likely to per-

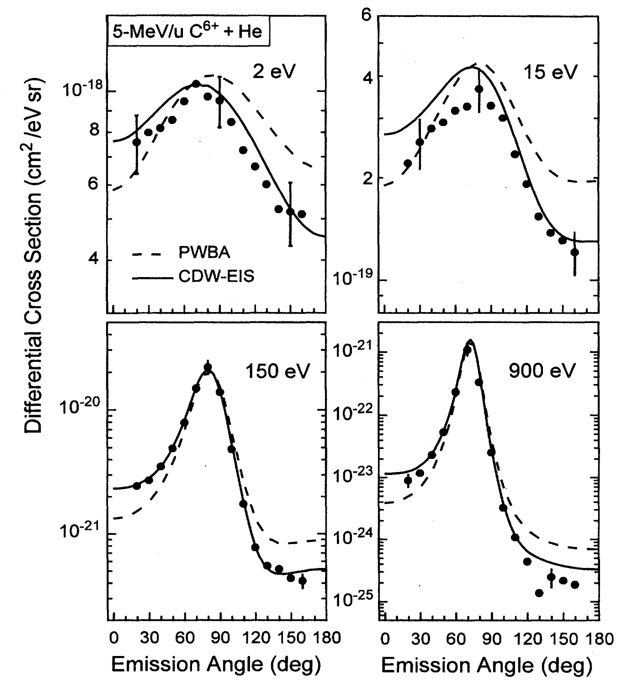

FIG. 2. Double differential cross sections for electron emission in 5-MeV/*u* C^{6+}+He collisions as a function of the electron observation angle. A few electron energies are selected as indicated. The experimental results are compared with calculations using the PWBA and the CDW-EIS.

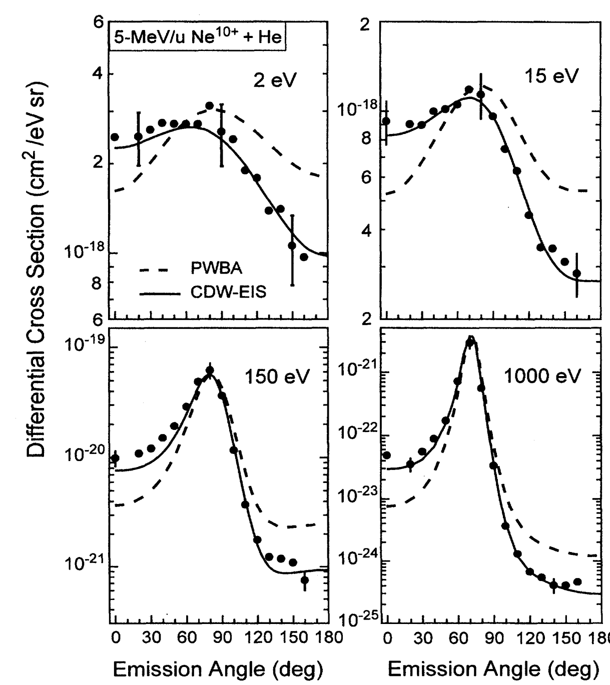

FIG. 3. Double differential cross sections for electron emission in 5-MeV/*u* Ne^{10+}+He collisions. Further legend as in Fig. 2.

turb the active electron in the final state [14,20,21].

In contrast to the PWBA, the CDW-EIS shows excellent agreement with the experiment in the complete angular range and at all energies. It is noted that electron energies are selected within a range covering three orders of magnitude (Figs. 2 and 3). Such an agreement between absolute cross sections in nearly complete regions of both the electron emission angle and energy is remarkable. It shows that the present theoretical CDW-EIS approach describes well the specific features of the two-center effects occurring at high projectile velocities.

The observed enhancement at forward angles and the reduction at backward angles can be understood as a deflection of the outgoing electron in the receding field of the projectile nucleus [14]. The distortion of the electronic state by the projectile may occur during the interaction with the target nucleus. Hence, two-center effects are produced which are dominant in regions where the cross sections are relatively small. Other regions, with larger cross sections, are governed by the soft-collision and binary-encounter electrons which are essentially due to one-center phenomena. For instance, the pronounced binary encounter peak located near 75° (Figs. 2 and 3) is well described by the PWBA. It is noted that the best agreement between PWBA and experiment is observed for relatively high electron energies of 150 eV and 1000 eV.

At lower energies (15 eV) the binary encounter peak is shifted with respect to the PWBA results. This angular shift is analogous to the energy shift of the binary-encounter peak which has recently been studied in terms of two-center effects [29–31]. Also, Figs. 2 and 3 show that the peak of low-energy (2 eV) electrons is affected by an angular shift which, in turn, produces an asymmetry of the angular distribution with respect to 90°. Hence, two-center effects cannot be ignored for soft-collision electrons. More details about these effects on low-energy electrons have recently been reported by Suarez *et al.* [32]. It should be realized, however, that two-center effects are relatively weak for soft-collision electrons. In the present collision systems, they do not exceed 40% for 2 eV electrons whereas they are as large as a factor of 5 for 1000 eV electrons (Fig. 3).

In view of the excellent overall agreement between experiment and the CDW-EIS theory it is interesting to search for remaining discrepancies. The 150-eV data for the collision system Ne^{10+}+He shows at forward angles from 0° to 60° that the experimental data are noticeably higher than CDW-EIS results (Fig. 3). Similar discrepancies are observed in the plot of 1000-eV electrons. To verify this phenomenon in more detail, cross section ratios rather than absolute values are considered. Figure 4 shows experimental data and theoretical CDW-EIS cross sections for the collision system 5-MeV/*u* Ne^{10+}+He in relation to the corresponding PWBA results. In general, good overall agreement is found between theory and experiment. However, for energies above ~100 eV the CDW-EIS theory underestimates the experimental data at an observation angle of 30°. Moreover, at 90° the theory overestimates the experimental data for energies higher than ~200 eV.

The discrepancies between experiment and CDW-EIS, which are slightly outside the experimental uncertainties for Ne^{10+}, are barely observable for the lighter projectiles C^{6+} and O^{8+}. Hence, it is interesting to verify the results for heavier projectiles. We performed PWBA and CDW-EIS calculations for the collision system 25-MeV/*u* Mo^{40+}+He studied previously [14]. It is noted that the theoretical cross section ratios do not differ much from those obtained from the previous CDW-EIS version involving hydrogenic continuum wave functions [14,16]. In Fig. 5 the theoretical cross section ratios are compared with the corresponding experimental data. The raw data for the 25-MeV/*u* Mo^{40+}+He system have slightly been revised at low electron energies of 1–20 eV affecting a few forward angles. (Also in this case, tabulated cross sections may be obtained on request [25].) From Fig. 5 it is seen that the theoretical underestimation of the cross sections at the observation angle of 30° and the overestimation at 90° are enhanced. In addition, discrepancies occur at 150°. It is pointed out, however, that the 150° data are rather uncertain above ~100 eV due to errors in the background subtraction.

It is noteworthy that the 90° data approach the PWBA at energies close to ~200 eV (Fig. 5). This finding may be explained by the one-center phenomenon of electron-target scattering creating a considerable contribution of binary-encounter electrons near 200 eV. These electrons are initially produced in binary projectile-electron collisions at angles <90° and subsequently defected to 90° by interaction with the target center.

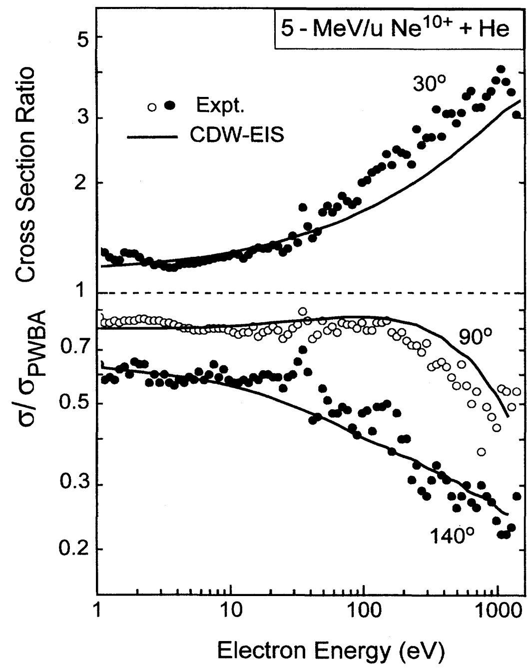

FIG. 4. Experimental and theoretical CDW-EIS cross sections for electron emission in 5-MeV/*u* Ne^{10+}+He collisions. The data are displayed in relation to the corresponding PWBA results as a function of the electron energy. Observation angle is 30°, 90°, and 140° as indicated. The peak structures at 35 eV are due to autoionization electrons from He.

V. CONCLUSIONS

In summary, significant two-center effects are detected by comparison of double differential cross sections for electron

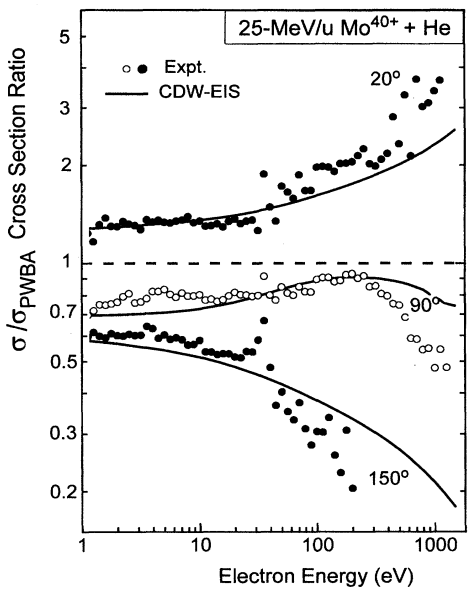

FIG. 5. Experimental and theoretical CDW-EIS cross sections for electron emission in 25-MeV/*u* Mo^{40+}+He collisions. Further legend as in Fig. 4.

emission with calculations using the PWBA. Besides an enhancement at forward angles, a reduction at backward angles is observed with respect to PWBA calculations. In accordance with previous work [14], the reduction at backward angles is found to be more pronounced than the enhancement at forward angles. In particular, it is shown that the cross sections for intermediate angles such as 90° are also affected by reductions with respect to the PWBA.

When Hartree-Fock-Slater wave functions are incorporated in CDW-EIS calculations, outstanding agreement between experiment and theory is achieved within large ranges of electron energy and angle. This finding is similar to that encountered several years ago by Madison [11] and Manson *et al.* [9] when they started to use realistic wave functions in the PWBA. The present analysis, however, provides additional information about two-center effects on the ejected electrons. It is recalled that CDW-EIS theory accounts for two-center effects in first order of a distorted-wave series. From the present agreement between theory and experiment it is concluded that this distorted-wave treatment of the two-center effects is adequate for the high-energy projectiles considered in this work.

Finally, we searched for remaining deviations between the experiment and CDW-EIS calculations. Such deviations are expected since the theory accounts for two-center effects in a perturbative approach. Although, differences between experiment and theory are small for the present cases, we detected certain discrepancies at high electron energies which increase with increasing projectile charge. Similar discrepancies have been seen previously for strong interactions in the final state [24]. It appears for high incident charge states or low projectiles energies that post-collisional effects of the projectile are underestimated by the CDW-EIS approximation. Further work is suggested to study higher-order terms for two-center effects using projectiles with increasing charge state.

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