Reply to ''Comment on 'Importance of electron time-of-flight measurements in momentum imaging of saddle-point electron emission' ''

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As pointed out in the preceding Comment, computer simulations presented by Irby [Phys. Rev. A **60**, 1135 (1999)] analyzed the effect of using constant rather than kinematically dependent values of the electron time of flight in assessment of ejected-electron momentum from recorded micro channel plate detector-impact positions. The article raised questions of possible error in the analysis used recently by Abdallah *et al.* [Phys. Rev. A **56**, 2000 (1997)]. In this reply, we present the results of more sophisticated Monte Carlo computer simulations, which show that the error due to the assumptions used in the analysis by Abdallah *et al.* are indeed quite miniscule. However, and equally as important, our simulations also *confirm* experimental projectile-charge dependent shifts reported earlier by Irby *et al.* [Phys. Rev. A **37**, 3612 (1988)] and Gay *et al.* [J. Phys. B **23**, L823 (1990)] in which conclusions opposite that of Abdallah *et al.* were reached. While still confirming the earlier experimental results, the simulations, on the other hand, support the conclusions of Abdallah *et al.* and not the conclusions of Irby *et al.* and Gay *et al.*

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Over the last decade, one particular device has played a major role in the advancement of many areas of the physical sciences, namely, the microchannel plate detector. Microchannel plate (MCP) detectors are typically utilized for the detection of charged subatomic particles and/or photons. Not only do MCP detectors signal the arrival of such entities, they also enable researchers to determine the precise position at which the charged particle/photon struck the detector.

MCP's have been utilized in numerous applications such as photon detectors, digital cameras, and infrared imaging, etc. These devices have also helped in broadening and challenging our understanding of ion-atom collisional dynamics. One powerful experimental technique that utilizes MCP technology is referred to as ''momentum imaging spectroscopy.'' (An excellent review article is given by Ullrich *et al.* [1].) This method enables scientists to not only detect all particles that are emitted in an ion-atom collision but to also obtain simultaneous measurements of the ejection velocities of these particles. In order to extract velocities of ejected electrons in ion-atom collisions, researchers have to detect both position and arrival times of the electrons. Depending upon the particular experimental setup, the electron times of flight can be difficult to measure. However, as pointed out in the preceding comment, electrons that are ejected in collisions involving low energy projectiles, are typically emitted with small velocities perpendicular to the incident beam direction. Thus, one may make the approximation that electron times of flight are essentially constant.

In a recent paper, Irby [2] presented computer simulation results that analyzed possible errors that could be introduced in the interpretation of momentum imaging data in which electron times of flight were not obtained. As stated in the preceding Comment, this paper can be easily read to imply that the analysis used in the reported data of Abdallah *et al.* [3] could suffer from possible error. In this reply, we present a further analysis of this situation by performing computer simulations similar to that of Irby but on a more rigorous basis. The results from these simulations strongly indicate that possible errors involved in the analysis of Abdallah *et al.* are indeed miniscule. However, the simulations also confirm, just as strongly, earlier experimental measurements of Irby *et al.* [4] and Gay *et al.* [5] in which conclusions opposite that of Abdallah *et al.* were reached. Although the simulations confirm the earlier experimental results, the simulations, however, support the conclusions of Abdallah *et al.* and not the previous conclusions of Irby *et al.* and Gay *et al.*

In the preceding Comment, the authors carefully pointed out that initial velocity distributions utilized in the computer simulations of Irby [2] may have not been all that realistic. We concur. Thus, we present the results of further and more sophisticated computer simulations involving more ''realistic'' velocity distributions in this reply.

It is important to note that the experimental electron-ejection-velocity data reported by Abdallah *et al.* [3] are *nothing but actual electron detector-impact positions*, divided by a constant time of flight. (The recent paper of Irby did not question the measurements of impact positions, but rather, the estimates of electron velocities by utilizing a constant time of flight.) Because detector impact positions can be easily obtained from data reported by Abdallah *et al.*, it is quite possible for one to deduce not only more realistic initial electron-velocity distributions from this data, but quite possibly, the *actual* three-dimensional (3D) initial ejection-velocity distributions. This is indeed what we have done. For simplicity, we chose the cases of both protons and alpha particles incident on neon at projectile velocities of 1.63 a.u.

Initially, we made appropriate ''guesses'' at the initial 3D velocity distributions. After comparison of the associated detector-impact positions computer generated from these distributions with the actual positions obtained from Abdallah *et al.* [3], we then ''tweeked'' (through many hours of trial and error) the initial distributions so that they eventually gave the same results for detector-impact positions as that reported by Abdallah *et al.* Specifically, the transverse velocity distributions, v_x and v_y, were initially generated by using

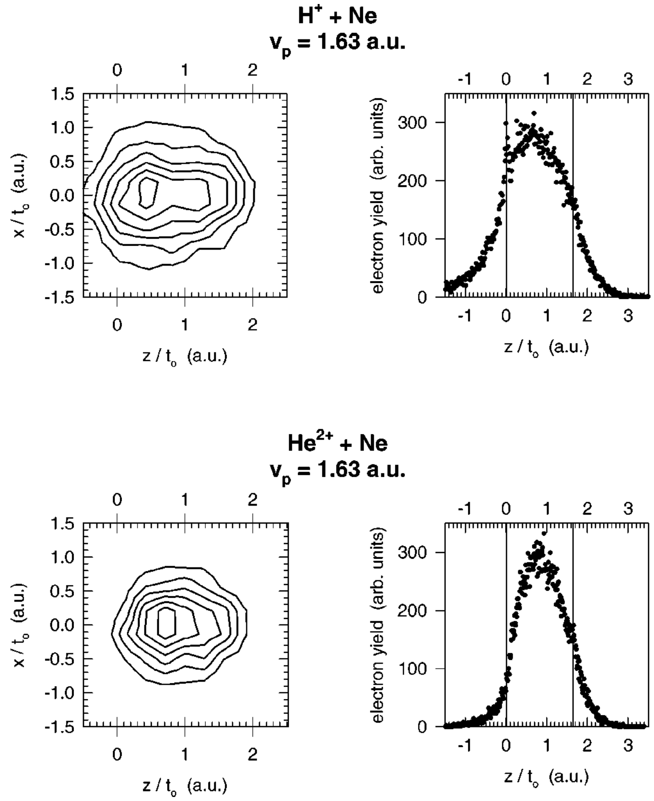

FIG. 1. Detector response functions obtained from computer simulations for 1.63 a.u. H^+ and He^{2+} projectiles incident on neon. Detector response functions are obtained from the computed detector-impact positions by dividing by a constant time of flight $t_o = 3.2$ ns. The results are plotted in this fashion for easy comparison to the data of Abdallah *et al.* (see Ref. [3]).

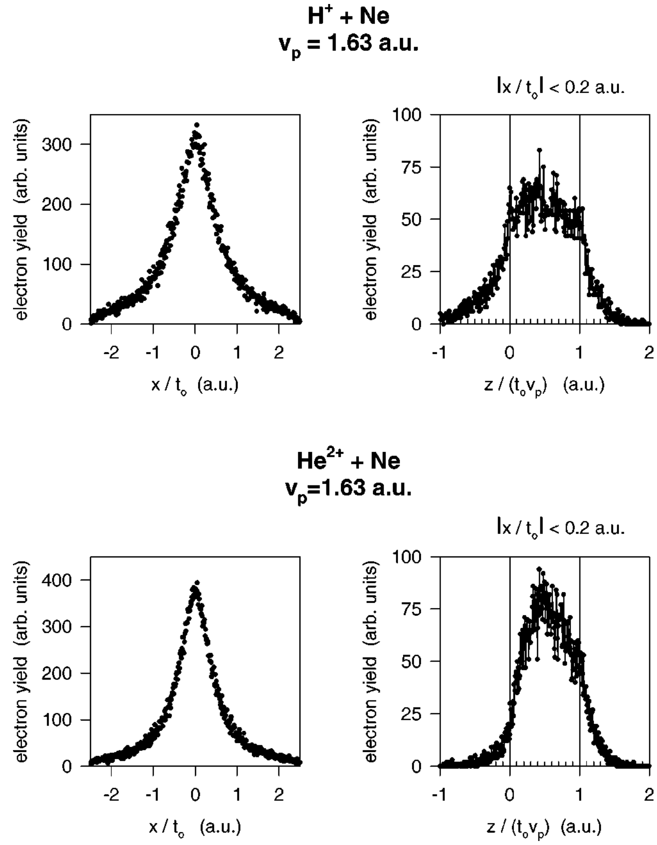

FIG. 2. Detector response functions projected along the transverse axis (left-hand side) are plotted along with the longitudinal response function for small transverse velocities (right-hand side).

Lorentzian probability distributions. The full widths at half maximum were chosen directly from the reported v_y distributions of Abdallah *et al.* Longitudinal distributions were generated using Gaussian distributions. In order to obtain better agreement with the measured data, cusp electrons were also generated utilizing Lorentzian distributions with a FWHM of 0.25 a.u. for all velocity components. (Cusp electrons comprised 1.8% of the total.) Again, the overall 3D distributions were continuously adjusted to obtain better agreement with the associated detector-impact position data of Abdallah *et al.*

For the sake of easy comparison, we also define the ''detector response'' function as the final detector-impact positions divided by a constant time of flight, as in the preceding comment. The detector-response functions for proton and alpha particles resulting from our simulations are illustrated in Figs. 1 and 2. The results reproduce quite well the experimental distributions found for these cases by Abdallah *et al.* [3], but are different from the target-centered ones used earlier by Irby [2]. In addition, the velocity distributions yield much better results with the reported data of Abdallah *et al.* than do the distributions utilized in the preceding Comment.

The next step in the analysis was to compare the response functions in Figs. 1 and 2 with the actual v_x and v_z source distributions. The response functions in Figs. 1 and 2 were found to be identical to the actual source distributions. (In fact, because they are so similar, we chose not to plot these distributions in order to save page space.) A more rigorous analysis of time-of-flight error can be made by comparing source and response distributions for small transverse v_x speeds. Figure 3 illustrates the results for small values of v_x. As one can readily see, although there does exist some error, overall it is quite small. Thus, as these simulations strongly indicate, possible error involved in the analysis of Abdallah *et al.* [3] is quite negligible.

A second issue raised by Irby [2] and Abdallah *et al.* [3] is whether measurements of only 2D electron spectra provide enough information for researchers to ascertain the physical dynamics involved in ionizing collisions. As an example, one may be inclined to conclude, based on the 2D distributions illustrated in Figs. 1 and 2, that electrons are typically emitted with higher ejection speeds from alpha particles than they are from protons of the same velocity. This observation certainly seems to be in disagreement with earlier results reported by Irby *et al.* [4] and Gay *et al.* [5] in which electrons were observed to be ejected at smaller speeds from alpha particle projectiles. In order to make a comparison with the earlier data of Irby *et al.* and Gay *et al.*, actual ejection speeds, $v = \sqrt{v_x^2 + v_y^2 + v_z^2}$, were calculated from the 3D source distributions used in our time-of-flight error analysis. Total ejection speed distributions, integrated over all ejection angles, are illustrated in Fig. 4. Figure 5 illustrates electron emission between 10° and 20° for both protons and alpha

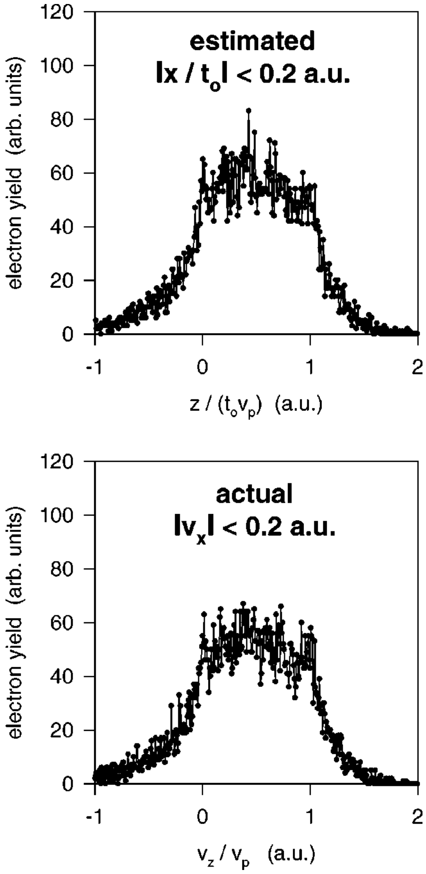

FIG. 3. Upper plot is the detector response function for H^+ incident on neon (same as in Fig. 2). Lower plot is the ''actual'' longitudinal v_z distribution of velocities for small transverse ejection velocities v_x. Any errors involved with using a constant time of flight would be manifested by differences between these graphs.

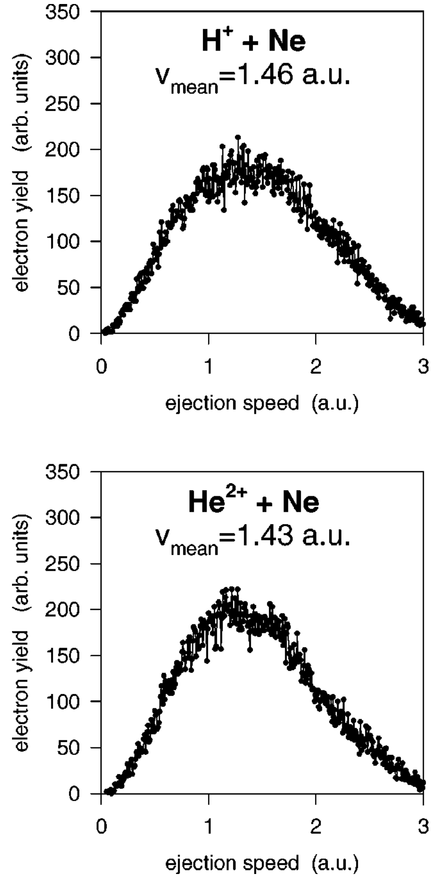

FIG. 4. Comparison of electron speed distributions $v = \sqrt{v_x^2+v_y^2+v_z^2}$ obtained from the actual 3D velocity distributions used in the generation of Figs. 1, 2, and 3.

particles. If one assumes that the source functions used in this analysis are correct, then the results in Fig. 5 *confirm* the earlier controversial ''saddle-point'' shift measurements of Irby *et al.* [4] and Gay *et al.* [5]. (In this case, electron times of flight are absolutely necessary for experimental confirmation utilizing momentum imaging techniques).

What is one to make of these results? The apparent contradiction between the experimental data of Abdallah *et al.* [3] and Irby *et al.* [4] and Gay *et al.* [5] may be reconciled in the following fashion. The ejection-velocity distribution of electrons may be approximated utilizing Gaussian distributions [as in Eq. (1) of the preceding comment]. This distribution can be rewritten in terms of the ejection angle θ and ejection speed $v=\sqrt{v_x^2+v_y^2+v_z^2}$. That is,

$$d^3p/dv_x dv_y dv_z = N \exp[-(v \sin\theta)^2/\sigma_t{}^2 - (v\cos\theta - v_c)^2/\sigma_l{}^2], \tag{1}$$

where σ_t is the transverse spread in ejection velocity, σ_l is the longitudinal spread, and v_c is the spectral peak in the longitudinal distribution. Taking the derivative of Eq. (1) with respect to v, setting equal to zero, and solving for v allows us to obtain the speed at which a spectral maximum appears v_{peak} as a function of ejection angle θ,

$$v_{peak} = \frac{v_c \cos\theta}{(\cos\theta)^2 + (\sigma_l/\sigma_t)^2 (\sin\theta)^2}. \tag{2}$$

As one can readily see, the ejection speed at which a maximum occurs will depend not only on v_c and ejection angle θ but also on the ratio of longitudinal versus transverse velocity spread σ_l/σ_t. [Note: if $\sigma_l = \sigma_t$, then Eq. (2) reduces to $v_{peak} = v_c \cos\theta$.] Even though electrons may be ejected at higher speeds for alpha particles, at small ejection angles, they are ejected at smaller speeds than that of protons at larger angles. This is due entirely to the differences in the ratio of longitudinal to transverse spreads in ejection speeds for protons and alpha particles. As a specific example, comparisons of ejection speeds at which maxima occur in ejected-electron spectra for protons and alpha particles incident on helium are plotted versus ejection angles in Fig. 6. Another comparison can be made with our Monte Carlo simulations for neon targets. In this case, the differential probability distribution is given by

$$d^3p/dv\, d\Omega = N v^2 \exp[-(v\sin\theta)^2/\sigma_t{}^2 - (v\cos\theta - v_c)^2/\sigma_l{}^2] \tag{3}$$

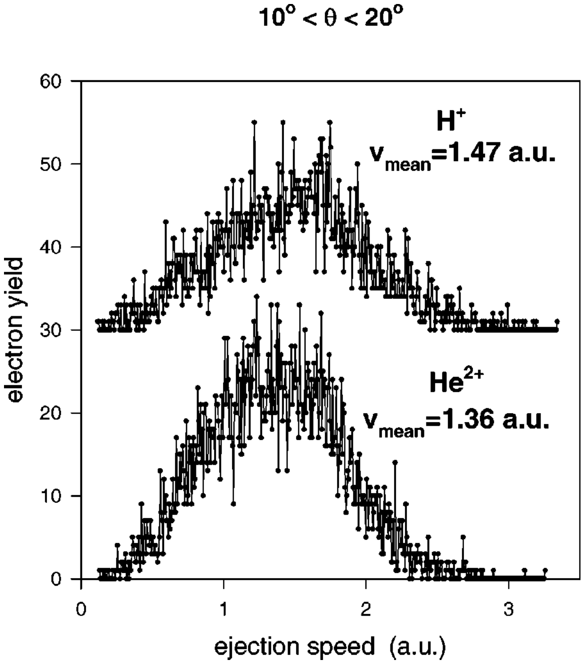

FIG. 5. Comparisons of electron speed distributions for electron ejection angles between 10° and 20°, obtained from actual velocity distributions.

[which is simply Eq. (1) multiplied by v^2]. The values for σ_t, σ_l, and v_c were chosen *directly from the reported distributions* of Abdallah *et al.* [3] (see Fig. 5 of their paper) and the results are presented (for an ejection angle of $\theta = 15°$) in Fig. 7. Note the similarities between Figs. 7 and 5.

If one considers *only* the earlier measurements of Irby *et al.* [4] and Gay *et al.* [5], it is perfectly natural to form the

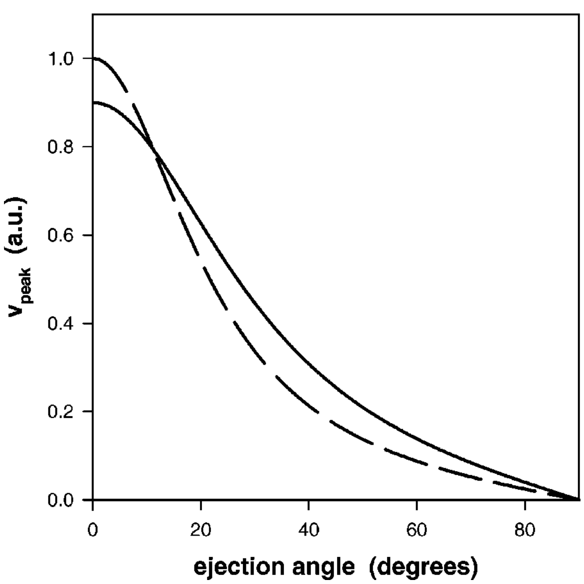

FIG. 6. Comparisons of maxima in electron-speed distributions. The dashed line indicates results from Eq. (2), for alpha particles incident on helium ($v_c = 1$ a.u., $\sigma_l = 0.8$ a.u., and $\sigma_t = 0.3$ a.u.). Solid line indicates results for protons incident on helium ($v_c = 0.9$ a.u., $\sigma_l = 0.8$ a.u., and $\sigma_t = 0.4$ a.u.).

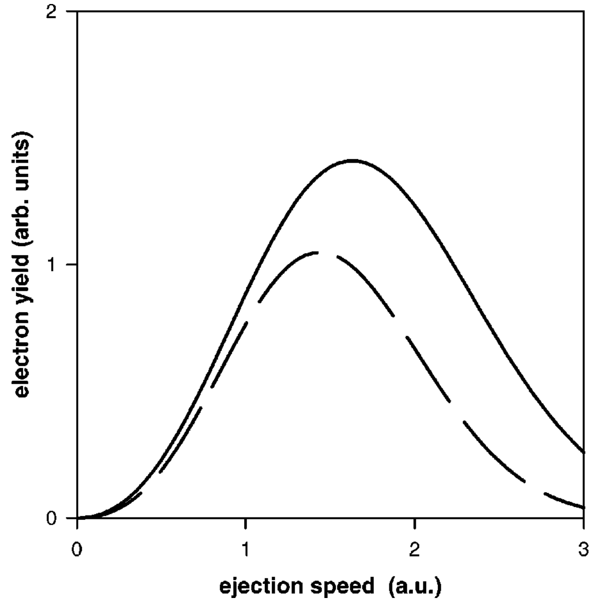

FIG. 7. Comparisons of estimated electron-speed distributions (ejected at $\theta = 15°$) for 1.63 a.u. proton and alpha particles incident on neon, utilizing Gaussian distributions. The dashed line indicates results from Eq. (3) for alpha particles incident on neon (N=1, $v_c = 1$ a.u., $\sigma_l = 1.1$ a.u., and $\sigma_t = 0.5$ a.u. These parameters are from experimental data presented by Abdallah *et al.*, see Ref. [3]). Solid line indicates results for protons incident on neon (N=1, $v_c = 0.8$ a.u., $\sigma_l = 1.3$ a.u., and $\sigma_t = 0.8$ a.u.).

conclusion that electrons are somehow ''stranded'' on the saddle-point or equiforce position of the collision system. Based on this assumption, one then would expect that higher charged projectiles would cause further saddle-point shifts resulting in slower moving electrons being ejected from the collision. However, the experiments of Irby *et al.* and Gay *et al.* were restricted to fairly large ejection angles and small solid angles of acceptance. The momentum-imaging measurements of Abdallah *et al.* [3], on the other hand, yield detail associated with smaller ejection angles although restricted to two dimensions.

Can the ''saddle-point'' mechanism still be considered as a dominant channel in single ionization? If an electron is truly associated with the saddle-point of the system, which necessarily travels only in the longitudinal direction, any projectile-charge dependent shift that is actually associated with the saddle-point mechanism should, most certainly, manifest itself in the longitudinal z component of the electron velocity (or small ejection angles). Since we have established that the z component distributions measured by Abdallah *et al.* are correct, and no such saddle-point shifts are observed in those distributions, the conclusions presented by Abdallah *et al.* are perfectly valid and more correct than earlier conclusions involving the saddle-point theory. (This observation is substantially strengthened by the subsequent data for higher charges.)

Even though measurements made at larger ejection angles may exhibit what ''appears'' to be saddle-point shifts, it now becomes apparent that these type of measurements simply do not yield sufficient information to form such a general conclusion. However, and equally as important, one should not conclude that the 2D distributions of Abdallah *et al.* invalidate the earlier reported experimental data of Irby *et al.* [4] and Gay *et al.* [5]. On the contrary, the data of Abdallah *et al.* actually *confirm* the earlier and controversial data of Irby *et al.* and Gay *et al.* although the interpretation and conclusions of Irby *et al.* and Gay *et al.* should be considered as invalid.

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