Comment on "Observation of oscillatory (interference?) structure in the forward peak from fast-projectile electron loss"

Joel I. Gersten* and Maurice Cohen†
Institute for Advanced Studies, The Hebrew University, Jerusalem, Israel
(Received 14 December 1978)

The observation of oscillatory structure in the forward peak from fast-projectile electron loss observed by M. Suter *et al.* is interpreted as being due to autoionization of highly stripped ions.

The study of collisional phenomena involving energetic highly ionized atoms has been of considerable interest in recent years. In particular, the problem of charge exchange to the continuum has been studied both experimentally and theoretically.[1] Recently, structure in the forward peak from fast-projectile electron loss has been observed.[2] The structure was tentatively interpreted as being due to an interference phenomenon associated with alternative channels for populating projectile-centered continuum states. In this paper, we argue that collisional excitation to autoionizing states accounts for the observed features. Autoionization of moving helium atoms after their passage through thin foils has previously been observed experimentally.[3] In that case the autoionization was attributed to *KLL* and *KLM* Auger transitions. In the present paper we consider a different type of Auger mechanism which we shall call a core-shift autoionization process.

The reported structure was observed to have the following attributes. It was present only in the case where the ion had two or more electrons. The structure was independent of the target gas and independent of the projectile energy. The widths of the structural features were observed to be comparable to the instrumental resolution, perhaps indicating a narrow linewidth. The feature locations scaled with increasing atomic number Z. The energies of the features in the electronic structure corresponded to a center-of-mass energy range of between 2 and 20 eV.

As a highly stripped ion traverses a target gas one may expect excitation, stripping, or pickup reactions to occur. Thus the charge state of the exiting ion may be different from that of the incident ion. In our model we assume that the exiting ion is collisionally promoted to a doubly excited electronic state. One of the excited electrons occupies a Rydberg state, whereas the second electron occupies a low-lying excited state.

In particular, we consider a berylliumlike ion, whose ground-state configuration $1s^2 2s^2\,{}^1S_0$. After excitation, we assume it is promoted to the state $1s^2 2pnl^{2S+1}L$.

This state autoionizes to a lithiumlike ion, with ground configuration $1s^2 2s\,{}^2S_{1/2}$, plus an electron. Let ΔE indicate the energy difference between the autoionizing state and the lithiumlike state. The magnitude of the wave vector of the ejected electron (in a.u.) is

$$k = (2\Delta E)^{1/2}. \tag{1}$$

If the speed of the ion in the laboratory is k_0, we would predict peaks in the forward direction at energies

$$E_{\pm} = \tfrac{1}{2}(k_0 \pm k)^2. \tag{2}$$

Generally, one would expect to observe an angular distribution of the structure given by

$$E = E_0 + \Delta E + 2(E_0 \Delta E)^{1/2}\cos\theta, \tag{3}$$

where $E_0 = k_0^2/2$ and θ is the angle the ejected electron makes with the incident ion. The experiments[2] monitored only those electrons emerging in the forward direction, so Eq. (2) should be the appropriate description.

The rate for autoionization is determined by the Coulomb matrix element

$$M = \langle 2s, C|1/r_{12}|2p, nl\rangle, \tag{4}$$

where the continuum orbital is denoted by C. Since the atom is highly ionized, the size of the wave functions $\langle r|2s\rangle$ and $\langle r|2p\rangle$ are rather compact, being proportional to Z^{-1}, where Z is the nuclear charge. If the continuum state is to have an appreciable overlap with these wave functions it must have low orbital angular momentum, i.e., be an S wave or a P wave. Similarly, the orbital angular momentum of the Rydberg electron should probably be low, e.g., $l=0$ or $l=1$.

Let us now see if the model can explain the data. Firstly, if the electronic spectrum is indeed due to autoionization it should be present only for ions containing at least two electrons. A bare ion would not have any electrons to emit and a hydrogenic ion cannot autoionize spontaneously. We expect the structure to be independent of the target gas

TABLE I. Predicted peak locations in highly ionized silicon based on Eqs. (1), (2), and (5). Here $Z=14$.

Transition	n	E_+(eV)	E_-(eV)
$1s^22pns \rightarrow 1s^22s$	9	1502	1261
	10	1578	1194
	11	1619	1159
	12	1649	1134
	13	1667	1119
	∞	1764	1041
$1s^22pnp \rightarrow 1s^22s$	9	1511	1253
	10	1583	1189
	11	1622	1156
	12	1649	1134
	13	1670	1116
	∞	1764	1041
$1s2pns \rightarrow 1s2s$ (singlet)	15	1440	1320
	16	1479	1282
	17	1502	1261
	∞	1619	1159
$1s2pnp \rightarrow 1s2s$ (singlet)	15	1443	1317
	16	1479	1282
	17	1502	1261
	∞	1619	1159

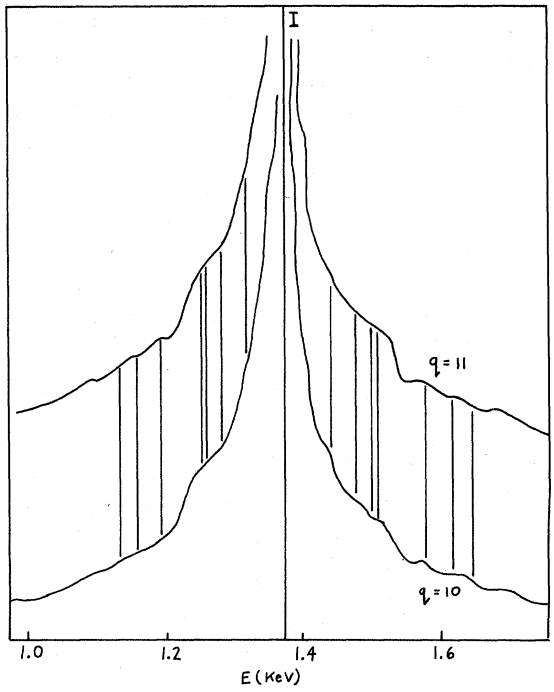

FIG. 1. Comparison of theoretical peak locations (vertical lines) with experimental data for 10 times ionized silicon and 11 times ionized silicon. Owing to the possibility of pickup and stripping there is a correspondence of features for these two cases.

identity and the projectile energy. These serve only to prepare the projectile ion in the autoionizing state. The widths of the autoionizing states are expected to be narrow, and this is observed experimentally.

Now let us examine the detailed structural features. In order to estimate the quantity ΔE of Eq. (1) we have computed the level terms of the relevant highly ionized atoms using a nonrelativistic $1/Z$ expansion method. Analytic expressions for the two-electron integrals were obtained from the formulas of Coulson and Sharma.[4] The resulting matrix elements were then fitted to a polynomial expression in $1/n$, where n is the principal quantum number of a Rydberg electron. The multiplet splittings were found to be quite small (much less than 1 eV) and were neglected for the purposes of this analysis.

When the leading nonrelativistic terms of the core energy shift[5,6] are included, we obtain the following expressions for $\Delta E_{\rm nr}$ (in a.u.):

For $(1s^22p\ ^2P)ns \rightarrow (1s^22s\ ^2S)+e$,

$$\Delta E_{\rm nr}=0.0707Z-0.1190-\left(\frac{(Z-3)^2}{2n^2}+\frac{1.3918Z}{n^3}+\frac{0.2471Z}{n^4}\right); \tag{5a}$$

for $(1s^22p\ ^2P)np \rightarrow (1s^22s\ ^2S)+e$,

$$\Delta E_{\rm nr}=0.0707Z-0.1190-\left(\frac{(Z-3)^2}{2n^2}+\frac{0.6805Z}{n^3}+\frac{0.2445Z}{n^4}\right); \tag{5b}$$

for $(1s2p^{1,3}P)ns \rightarrow (1s2s^{1,3}S)+e$,

$$\Delta E_{\rm nr}=\begin{cases}0.0280Z-0.0425-\left(\dfrac{(Z-2)^2}{2n^2}+\dfrac{1.0174Z}{n^3}+\dfrac{0.1993Z}{n^4}\right)\ \text{(singlet)}\\ 0.0378Z-0.0256-\left(\dfrac{(Z-2)^2}{2n^2}+\dfrac{1.0174Z}{n^3}+\dfrac{0.1993Z}{n^4}\right)\ \text{(triplet)};\end{cases} \tag{5c}$$

for $(1s2p^{1,3}P)np \rightarrow (1s2s^{1,3}S)+e$,

$$\Delta E_{\rm nr}=\begin{cases}0.0280Z-0.0425-\left(\dfrac{(Z-2)^2}{2n^2}+\dfrac{0.5605Z}{n^3}+\dfrac{0.2364Z}{n^4}\right)\text{(singlet)}\\[2ex] 0.0378Z-0.0256-\left(\dfrac{(Z-2)^2}{2n^2}+\dfrac{0.5605Z}{n^3}+\dfrac{0.2364Z}{n^4}\right)\text{(triplet)}\,.\end{cases}\tag{5d}$$

We note that the limiting values of $\Delta E_{\rm nr}$ as given by Eqs. (5c) and (5d) are in good agreement, for Si XIII with the precise nonrelativistic calculations of Ermolaev and Jones.[7a] Their calculated relativistic term values have been reproduced by Lin *et al.*,[7b] but differ somewhat from the observations tabulated by Bashkin and Stoner.[8] It turns out that the relativistic correction to $\Delta E_{\rm nr}$ is negligible for singlets, but may be of the order 1.5–2.5 eV for triplets, depending on which term values we adopt. We have therefore not presented peak positions for the triplets, but speculate that much of the remaining structure close to the center of the forward peak may be resolved when more reliable term values become available. The values of the expected peaks in the forward electron distribution are presented in Table I. In Fig. 1, we reproduce the experimental[2] electron distribution for highly ionized silicon[9] and indicate the location of the expected autoionization peaks. The value k_0 = 10.07 a.u. was used, as determined from the location of the charge-exchange-to-the-continuum peak. We see that the correlation between theory and experiment is very good.

In a recent note,[10] the authors of Ref. 2 have independently given the same explanation for similar features in some new and better resolved data on oxygen. The peak locations in that case were assigned on the basis of quantum defect theory, also with very good agreement between theory and experiment. These results on oxygen, taken together with the results on silicon, would appear to substantiate the theory completely.

While the present theory predicts the *location* of the peaks rather well, we can make no statement as to their relative magnitudes. To do this one must make a detailed calculation of the cross sections for excitation, stripping, and pickup reactions.

ACKNOWLEDGMENTS

We acknowledge computational assistance from Shlomit Felix.

*Permanent address: Dept. of Physics, City College of New York, New York, N.Y. 10031.

†Permanent address: Dept. of Physical Chemistry, The Hebrew University, Jerusalem, Israel.

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