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Near-threshold behavior of electron-impact excitation of $He^+(2s)$ and $He^+(2p)$

Hao Xu and Robin Shakeshaft[*]
Physics Department, University of Southern California, Los Angeles, California 90089-0484, USA

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We present results for cross sections summed over partial waves $L = 0$–2 for electron-impact excitation of the $2s$ and $2p$ states of He^+ in the energy range of 40.84 to 45.66 eV. We find that these cross sections exhibit cusps at the excitation threshold of 40.81 eV.

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Excitation of He^+ to the $n = 2$ level by electron impact at low energies (roughly, within a few eV above the excitation threshold) has presented a challenge to both theorists and experimentalists. There are noticeable discrepancies among the various theoretical results [1–11] in this energy range. Furthermore, no absolute measurements exist. If the experimental data [12–14] are normalized to the theoretical results in the high-energy limit (where the Born approximation is considered to be accurate) the various measured cross sections for $2s$ excitation agree well with each other over the entire range of low to high energies, but they are roughly a factor of two smaller than the theoretical results at low energies.

In this Brief Report we present results for the $2s$ and $2p$ excitation cross sections summed over partial waves $L = 0$–2 and in the energy range of 40.84 to 45.66 eV. Our results were obtained by using a variant of the traditional R-matrix approach; one which incorporates the proper boundary conditions so that both the wave function and its derivative are continuous at the boundary of the interior and exterior regions at all energies [15]. We believe that our results (for the partial waves $L = 0$–2) have a relative error of no more than 1%. Furthermore, we find excellent agreement with the results obtained more than thirty years ago by Burke and Taylor [7] (who used the close-coupling approach) and by Morgan [9] (who used a multichannel extension of a hybrid algebraic variational method). The striking discrepancy with experiment remains a mystery—one which we do not attempt to resolve here.

In fact, the primary purpose of this Brief Report is not to address existing discrepancies among different results for electron-impact excitation of He^+ but rather to report on an investigation of the threshold behavior of the cross sections (integrated over all angles) for $2s$ and $2p$ excitation. We find that these cross sections are finite (nonzero) at the excitation threshold, as expected, but they exhibit cusp-like behavior. This contrasts with the case of electron-impact excitation of H where, as shown by Gailitis and Damburg, the cross sections for $2s$ and $2p$ excitation are also finite at the threshold, but they oscillate with the logarithm of the excess energy just above the threshold [16,17]. Both the oscillations and the cusps originate from an attractive long-range dipole interaction between the scattered electron and the excited H or He^+ target. The excited target has a permanent dipole moment because the $2s$ and $2p$ states are degenerate and, if this dipole is parallel to the direction of motion of the scattered electron, the interaction is attractive. The cross sections for both processes are finite at threshold because the scattered electron experiences a significant time delay, which results in an enhancement of the excitation probability. The threshold behavior of the (angle-integrated) cross sections for electron-impact excitation of H can be attributed almost entirely to the time delay in the attractive dipole potential, but to understand the threshold behavior for electron-impact excitation of He^+ the exchange of population between the $2s$ and $2p$ states of the ion must be taken into account. The primary difference in the two processes is that, in the latter one, it is the attractive Coulomb potential which governs the motion of the scattered electron at large distances.

Once the scattered electron is at a sufficiently large distance from the target that further excitation of the target is negligible, population moves back and forth between the $2s$ and $2p$ states due to mixing by the dipole interaction. The period at which the population oscillates is determined by the splitting of the $2s$ and $2p$ energies, which is induced by the dipole interaction. We restrict ourselves to electron-impact excitation of He^+, and we assume that the asymptotic speed v of the scattered electron is very small. On the initial leg of its outward journey the scattered electron moves rapidly—too fast for the $2s$ and $2p$ populations to oscillate more than a few times. On the final leg of its journey, after it has slowed down in the Coulomb field of the ion, the scattered electron moves with a speed close to v. However, on this final leg the $2s$–$2p$ energy splitting is so small, and hence the period of oscillation so large, that the $2s$ and $2p$ populations cannot undergo a full oscillation. Rather, on the final leg the $2s$ and $2p$ populations change by an amount proportional to v; accordingly, the excitation cross sections have cusps.

The numerical method that we used in our calculations has been fully described elsewhere [15,18]. In Fig. 1 we show the cross section for excitation of He^+ from the $1s$ to the $2s$ state, summed over the lowest three partial waves, $L = 0$–2. Our results (solid line) agree almost perfectly with those of Burke and Taylor (circles) and Morgan (not shown) except very close to the threshold at 40.81 eV where our results turn sharply upward, indicating the presence of a cusp. We presume that the reason Burke and Taylor—and other theorists—did not find this cusp is that they did not integrate sufficiently far into the asymptotic region to account for the influence of the dipole interaction on the threshold behavior. In our R-matrix-type approach we built in the long-range dipole interaction exactly by matching the wave function at the boundary of

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[*] robins@usc.edu

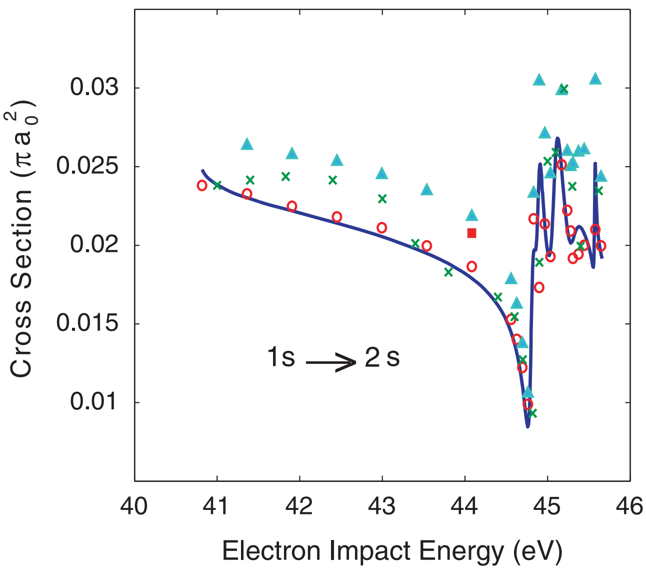

FIG. 1. (Color online) Spin-averaged cross section for electron-impact excitation of He$^+(2s)$. Solid line shows the present results ($L \leqslant 2$), circles show Burke and Taylor [7] ($L \leqslant 2$), square shows Aggarwal *et al.* [10] ($L \leqslant 2$), triangles show Aggarwal *et al.* [10] (all L), and crosses show Bray *et al.* [11] (all L). The rapid variation of the cross section at energies above 44 eV is due to a series of resonances accumulating below the $n = 3$ threshold.

the interior and exterior regions (at 50–70 a.u.) to the exact analytic wave function for an electron moving in both the Coulomb and dipole fields of a He$^+$ ion whose state is a superposition of $2s$ and $2p$ states [19]. We have verified that the excellent agreement between our results and those of Burke and Taylor and Morgan holds not just for the sum but also for the individual partial waves for each value of L from 0 to 2.

We show two other sets of results in Fig. 1: those of Aggarwal *et al.* (triangles), obtained using the traditional R-matrix approach, and those of Bray *et al.* (crosses), obtained using the the convergent close-coupling method. The results of Aggarwal *et al.* and Bray *et al.* include all partial waves, and they differ noticeably from ours, both qualitatively and quantitatively. In particular, the results of Bray *et al.* slope down as the threshold is approached. The numerical discrepancies are as large as 20%. However, it is doubtful that the contribution from partial waves $L > 2$ can account for these discrepancies in the low-energy range considered here. The scattered electron cannot excite the ion while close to the ion unless its angular momentum is small since its linear momentum in its final state is less than 0.5 a.u. for impact energies less than 44.1 eV. However, as the scattered electron departs and the ion oscillates between the $2s$ and $2p$ states, one unit of angular momentum is exchanged between the scattered electron and the ion. Therefore, during the scattering process the significant values of the angular momentum quantum numbers for both the ion and the scattered electron are 0 and 1, implying that the significant values of the total angular momentum quantum number L are 0, 1, and 2. The rate of convergence with respect to L was studied by Aggarwal *et al.* at the particular impact energy of 44.08 eV. They found that the net contribution from partial waves $L > 2$ at 44.08 eV is about 5%, with almost all of this coming from partial waves $L = 3$–5; the contribution from $L > 5$ is negligible. The square in Fig. 1 is the cross section for $2s$ excitation at 44.08 eV that Aggarwal *et al.*, obtained when they summed over only the lowest three partial waves. Presumably the net contribution from partial waves $L > 2$ is much smaller than 5% at energies within 1 eV or so above threshold.

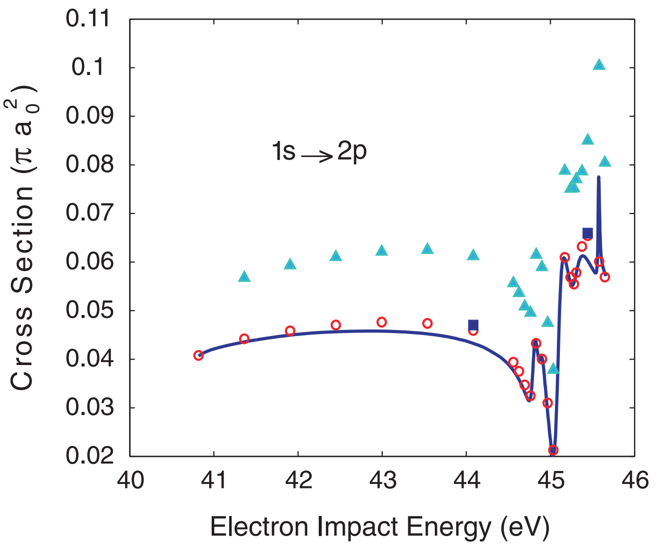

FIG. 2. (Color online) Spin-averaged cross section for electron-impact excitation of He$^+(2p)$. Solid line shows present results ($L \leqslant 2$), circles show Burke and Taylor [7] ($L \leqslant 2$), squares show Aggarwal *et al.* [10] ($L \leqslant 2$), and triangles show Aggarwal *et al.* [10] (all L).

In Fig. 2 we show the cross section for $2p$ excitation, again summed over partial waves $L = 0$–2. Once more our results (solid line) agree nearly perfectly with those of Burke and Taylor (circles) and Morgan (not shown). There is a cusp at threshold, which slopes downward to offset the rise in the cross section for $2s$ excitation. However, this cusp is not nearly as sharp as the one for $2s$ excitation. A look at the individual partial waves reveals the reason. Near threshold the major contribution to the (spin-averaged) cross section for $2p$ excitation, more than 50%, comes from the spin-singlet $L = 2$ partial wave; this contribution does have a prominent cusp, as shown in Fig. 3, and its downward turn roughly cancels the upward turn in the cusp shown in Fig. 1. The other partial waves, taken together, give a contribution that is almost flat

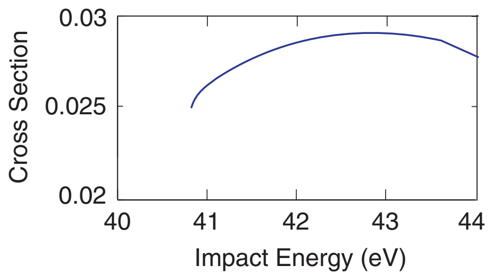

FIG. 3. (Color online) Contribution from the spin-singlet $L = 2$ partial wave to the (spin-averaged) cross section (in units of πa_0^2) for electron-impact excitation of He$^+(2p)$.

near the threshold, so they dilute the cusp in the cross section for $2p$ excitation.

Results for $2p$ excitation obtained by Aggarwal *et al.* are also shown in Fig. 2, including the results (squares) they obtained at the two energies 44.08 and 45.44 eV when they summed over only the lowest three partial waves. The angular momentum quantum number of the scattered electron in its final state is $L \pm 1$ or L when the final state of the ion is the $2p$ or $2s$ state, respectively. The possibility for the scattered electron to have a final angular momentum quantum number of $L-1$ if $L \geqslant 1$ implies that the rate of convergence of the cross section with respect to L is slower in the case of $2p$ excitation than in the case of $2s$ excitation. Nevertheless, we do not expect the partial waves $L > 2$ to yield a large contribution at energies within 1 eV or so above threshold—not large enough to qualitatively alter the threshold behavior of the $2p$ excitation cross section.

The cross section for photoionization of He accompanied by excitation of He^+ to the $2s$ or $2p$ state also has a cusp at the excitation threshold. This was shown in a previous paper, where a detailed explanation was given [18]. As in our earlier work, we employed a hybrid basis consisting of radial Sturmian and Riccati-Bessel functions, and we included the variational correction to our first-order estimate of the K matrix. Various criteria were used to assess the accuracy of our results. Typically, the variational correction was less than 1%. After the variational correction was included, our values for the K matrix were symmetric to at least 6 figures. We varied the size of the basis and the distance of the boundary and observed changes of no more than 0.1%.

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