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

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Xu and Shakeshaft [Phys. Rev. A **84**, 024701 (2011)] presented theoretical cross sections for excitation of the $2s$ and $2p$ states of He^+ at low collision energies, pointing out in particular the presence of cusps at the excitation threshold. We update their discussion of the comparison between theory and experiment, and confirm that results obtained using standard R-matrix and two-dimensional R-matrix propagation techniques also show such cusps.

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In a recent Brief Report [1], Xu and Shakeshaft applied their variant of the R-matrix approach [2] to the study of electron-impact excitation of the He^+ ion into the $2s$ and $2p$ states at collision energies ranging from 40.84 to 45.66 eV. The main purpose of their paper was to point out the presence of cusps in the integrated cross sections at the excitation threshold, similar to those seen in the cross sections for photoionization of helium leaving the residual ion in its $2s$ or $2p$ state [3]. They compare their results with those of an early close-coupling calculation [4] and a 15-state R-matrix study [5] as well as a hybrid multichannel algebraic variational calculation [6].

The authors start by describing the discrepancy of almost a factor two between various theoretical results and experiment [7–9], noting in particular that "no absolute measurements exist" and "The striking discrepancy with experiment remains a mystery." This was indeed the situation at the end of the 1990s. In 2001, however, Smith *et al.* published a set of absolute measurements of the combined cross sections for excitation into the $2s$ and $2p$ states close to threshold, obtained using a merged-electron-ion-beam energy-loss (MEIBEL) technique [10]. Their results are approximately 20% larger than those of a number of representative calculations [5,6,11,12], a large improvement compared to the difference of almost a factor two that existed before. The energy-loss spectroscopy used in this experiment cannot, of course, distinguish between the different final states, and so the theoretical cross sections for excitation into the $2s$ and $2p$ states must be summed in order to compare with experiment. As noted by Xu and Shakeshaft, the increase due to the cusp in the $2s$ cross section close to threshold is mostly compensated by the decrease in the $2p$ cross section, so that the sum of the two cross sections is relatively flat. It is therefore not surprising that there is no evidence of the cusps in the experimental results of Smith *et al.*

The authors "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." More precisely, none of the other theoretical studies apparently attempted to calculate cross sections close enough to threshold for the slope due to the cusp to become well pronounced. The results at threshold given by Burke and Taylor were based on an extrapolation rather than an explicit calculation [4] and thus do not exhibit any cusp. As noted by Xu and Shakeshaft, computing cross sections close to threshold requires integrating the equations out to large distances, which would have been computationally prohibitive particularly for the earlier calculations. To verify that other methods do indeed display cusps in the cross sections close to threshold, we have performed calculations using the standard R-matrix approach and the two-dimensional R-matrix propagation (RM2D) technique [13].

Our R-matrix calculations extend the 15-state results of Aggarwal *et al.* [5] and have, in fact, already been presented in our previous paper where the cusp behavior is indeed visible [12]. The parameters of the calculation are the same as those used by Aggarwal *et al.* with an internal region of 43 a.u. The only difference is in the treatment of the external region: In the original calculation, long-range couplings were taken into account using a perturbation technique, while here we employ the FARM package [14], which solves the set of coupled equations describing an electron moving in the long-range multipole potential (including the Coulomb and dipole interactions) of the target using a combination of one-dimensional R-matrix propagation and an asymptotic expansion. We have verified that the results obtained using FARM and the older code are the same, differing at most by 0.5% close to threshold and generally by less than 0.1% elsewhere.

The RM2D calculation, described in detail in our earlier paper [12], propagates a global two-electron R-matrix in the two radial directions from the origin through a number of sectors out to some distance r_{out}, which here is taken to be 60 a.u. A set of target states and pseudostates is defined by diagonalizing the one-electron Hamiltonian in the global sector $[0,r_{out}]$: This gives a discrete set of basis functions, of which the lowest correspond to the lowest exact hydrogenic bound states, while the rest are pseudostates representing more highly excited states and the continuum. Beyond r_{out}, the scattering problem is solved within the close-coupling formalism expressed in this basis using the same combination of one-dimensional R-matrix propagation and an asymptotic expansion as used in FARM. In the current calculation, we employ a basis consisting of 90 target states and pseudostates (20 s, 19 p, 18 d, 17 f, 16 g), including very good representations of all the $n \leqslant 5$ states of He^+.

In order to obtain converged cross sections very close to threshold, in both calculations the asymptotic expansion had to be evaluated at a distance of at most several hundred atomic

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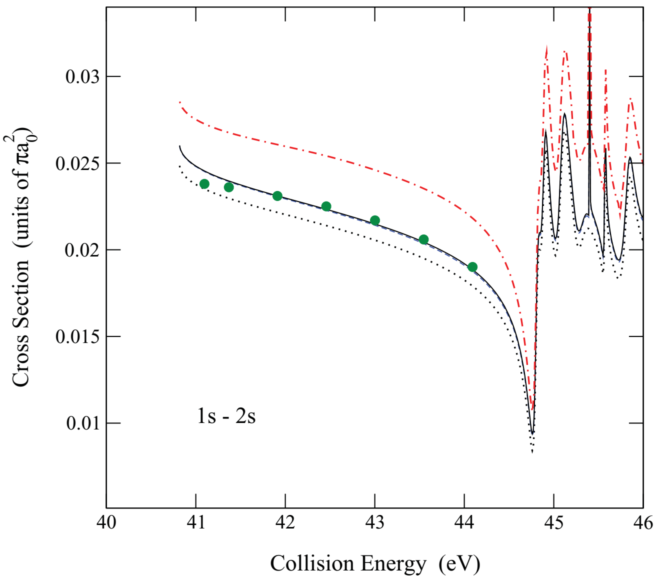

FIG. 1. (Color online) Cross sections for excitation of the ground state of He^+ into the $2s$ state. Two-dimensional R-matrix propagation: dotted curve, $L \leqslant 2$; dashed curve, $L \leqslant 3$; full curve, $L \leqslant 5$. Other theories: chain curve, 15-state R-matrix calculation [5]; circles, hybrid multichannel algebraic variational calculation [6].

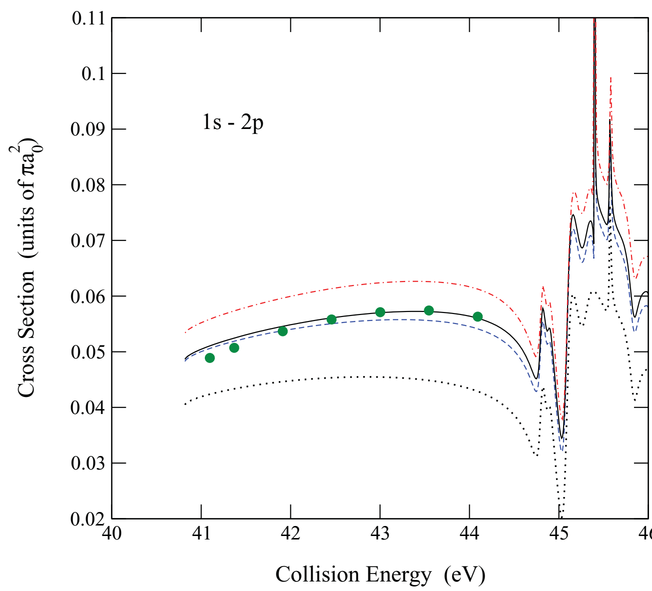

FIG. 2. (Color online) Cross sections for excitation of the ground state of He^+ into the $2p$ state. Two-dimensional R-matrix propagation: dotted curve, $L \leqslant 2$; dashed curve, $L \leqslant 3$; full curve, $L \leqslant 5$. Other theories: chain curve, 15-state R-matrix calculation [5]; circles, hybrid multichannel algebraic variational calculation [6].

units, and the R-matrix thus had to be propagated out this far. Away from threshold, the R-matrix had to be propagated only a short distance, if at all, before matching to the asymptotic solutions.

In Figs. 1 and 2, we present the total cross sections for excitation of the He^+ ground state into the $2s$ and $2p$ states, respectively, obtained using the two approaches described above and including total angular momenta L up to 5, as well as the results of a hybrid multichannel algebraic variational calculation by Morgan [6]. To illustrate the convergence of the cross section with increasing total angular momentum L, we also show RM2D cross sections obtained by including $L \leqslant 2$ and $L \leqslant 3$. Cross sections including $L \leqslant 4$ are essentially the same as those with $L \leqslant 5$ and are not shown in the figures. In view of the critique made by Morgan of Burke and Taylor's $L = 4$ partial cross sections for the $1s$-$2s$ transition [4], we choose not to compare the fully converged cross sections with theirs. We note that there is excellent agreement between the RM2D results and those of Morgan. The 15-state R-matrix results are 10%–15% larger, since this calculation does not include any representation via pseudostates of short-range interactions with highly excited states and the target continuum, which play a role in determining the final distribution of flux in the open channels. On the other hand, the resonance positions and widths agree well [12].

The cross sections for excitation of the $2s$ state obtained from the RM2D and 15-state R-matrix calculations both display a sharp upward turn just above threshold, similar to that reported by Xu and Shakeshaft. This behavior comes essentially from the $^1D^e$ partial wave and is not obscured by other contributions. Similarly, the cross sections for excitation into the $2p$ state show the same slight downturn approaching threshold as described by Xu and Shakeshaft and again is mostly due to the $^1D^e$ contribution.

Finally, we would like to comment on the statements "Presumably the net contribution from partial waves $L > 2$ is much smaller than 5% at energies within 1 eV or so above threshold" (for excitation into the $2s$ state) and "we do not expect the partial waves $L > 2$ to yield a large contribution at energies within 1 eV or so above threshold" (for excitation into the $2p$ state). As can be seen from Figs. 1 and 2, the contribution from $L = 3$ is actually relatively large, even close to threshold. More precisely, for the $1s$-$2s$ transition, the $L = 3$ partial waves still contribute approximately 4% to the total cross section for energies within 1 eV of threshold, while for the $1s$-$2p$ transition they contribute 16%, and almost 20% comes from the combination of $L = 3$ and 4. Hence even so close to threshold, it is necessary to include more partial waves than suggested by Xu and Shakeshaft in order to obtain fully converged results.

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