01 Nov 1988

Excitation of the Lowest Autoionizing Levels in Lithiumlike Ions by Electron Impact

Rajesh C. Srivastava

Don H. Madison
Missouri University of Science and Technology, madison@mst.edu

Recommended Citation

R. C. Srivastava and D. H. Madison, "Excitation of the Lowest Autoionizing Levels in Lithiumlike Ions by Electron Impact," *Physical Review A - Atomic, Molecular, and Optical Physics*, vol. 38, no. 10, pp. 5419-5422, American Physical Society (APS), Nov 1988.
The definitive version is available at https://doi.org/10.1103/PhysRevA.38.5419

Excitation of the lowest autoionizing levels in lithiumlike ions by electron impact

R. Srivastava
Department of Physics, University of Roorkee, Roorkee 247 667, India

Don H. Madison*
Department of Physics, Drake University, Des Moines, Iowa 50311
(Received 18 January 1988)

We present theoretical, differential, and total cross sections for electron impact excitation of the lowest autoionizing levels of various lithiumlike ions (viz., Be^+, B^{2+}, C^{3+}, O^{5+}, and Ne^{7+}). For these ions, the autoionizing level of interest results from excitation of an inner-shell electron. A distorted-wave Born approximation (with exchange) is used for the calculation. The present results are compared with previous theoretical calculations and it is concluded that the Coulomb-Born approach is unreliable, particularly near threshold.

Recently, considerable attention has been given to studying the excitation of autoionizing levels of atoms or ions by electron impact. Since autoionizing levels have very short lifetimes, most states decay almost immediately with a net result in a contribution to ionization known as excitation autoionization (EA). Sometimes the EA contribution to ionization is significant and plays a dominant role in the clear understanding of electron-impact ionization measurements of ions (atoms).[1-3] It is also well known that the studies of autoionizing levels have direct applications to high-temperature, low-density plasmas occuring in controlled thermonuclear fusion and in the coronal regions of the sun.

An example of the importance of the EA phenomena may be seen in the problem of electron-impact ionization of lithiumlike ions.[3,4] For this case, it has been shown[4-8] that the inner-shell excitations decay totally (99% or higher) by autoionization and that the calculated inner-shell excitation cross sections for the process $1s^22s \rightarrow \sum_l 1s2s2l$ were roughly appropriate for the observed structure in the ionization cross sections. Tiwary *et al.*[9] recently performed a calculation using the distorted-wave Born approximation method for the electron-impact excitation of the lowest autoionizing level (viz., $1s^22s \rightarrow 1s2s^2$) of the neutral lithium atom. They found that the total cross section peaked for an incident electron energy near the threshold for the excitation process. This peak in the cross section was attributed primarily to a dominance of exchange scattering near threshold. The feature of peaking for the cross section near threshold was expected from the experimental measurements,[10] but previous similar calculations failed to reflect this feature.[9,11]

In this Brief Report, our aim is to examine the threshold behavior for an isoelectronic series within the framework of the distorted-wave Born approximation including exchange (DWBE). Instead of considering all the $1s2s2l$ excitations for a single lithiumlike ion to determine the excitation-autoionization contribution to ionization (which has already been reliably assessed for a couple of ions by many previous workers[4]), we rather confine ourselves in this report to studying the excitation of only the lowest autoionizing level (viz., $1s2s^2$) for several different ions. At the present, there are no experimental results with which we can directly compare, although such measurements are possible with present technology.[12-14] There are other theoretical results[4,6,15] available for comparison, however.

We have calculated differential and total cross sections for inner-shell excitation of the $1s2s^2$ autoionizing level from the ground state for the lithiumlike ions Be^+ to Ne^{7+} using the DWBE approximation.[9] For this calculation, the ionic target wave functions for the initial and final states were chosen to be of the Hartree-Fock type and they were obtained using Fischer's code.[16] The excitation energies for the transitions in the various ions were found to reproduce the values obtained by Henry.[6] After this work was prepared for publication, Itikawa *et al.*[15] reported a distorted-wave calculation with exchange which is very similar to the present calculation. The primary difference between the Itikawa *et al.*[15] work and the present calculation lies in the target ion wave functions. Itikawa *et al.*[15] used the ion wave functions adopted by Henry[6] while Hartree-Fock wave functions were used in this work.

Total cross-section results for the case of excitation of C^{3+}, N^{4+}, and O^{5+} ions are presented and compared where available with the close-coupling approximation (CCA) of Henry[6], the Coloumb-Born approximation (CBA) of Magee *et al.*,[17] and the distorted-wave-exchange approximation (DWXA) of Itikawa *et al.*[15] in Figs. 1(a)–1(c), respectively. Itikawa *et al.*[15] pointed out an error in the CCA results of Henry[6] for the O^{5+} ion. Consequently, the CCA results for O^{5+} are the corrected results as obtained by Itikawa *et al.*[15] From Figs. 1(a)–1(c), we see that our DWBE results for C^{3+}, N^{4+}, and O^{5+} are about 10–15 % higher than the CCA results of Henry,[6] while the DWXA results of Itikawa *et al.*[15] lie in between CCA and DWBE results. Since the difference between the DWBE and DWXA results are primarily due to the different choices for the target ion wave functions in the two calculations, it is seen that the total cross

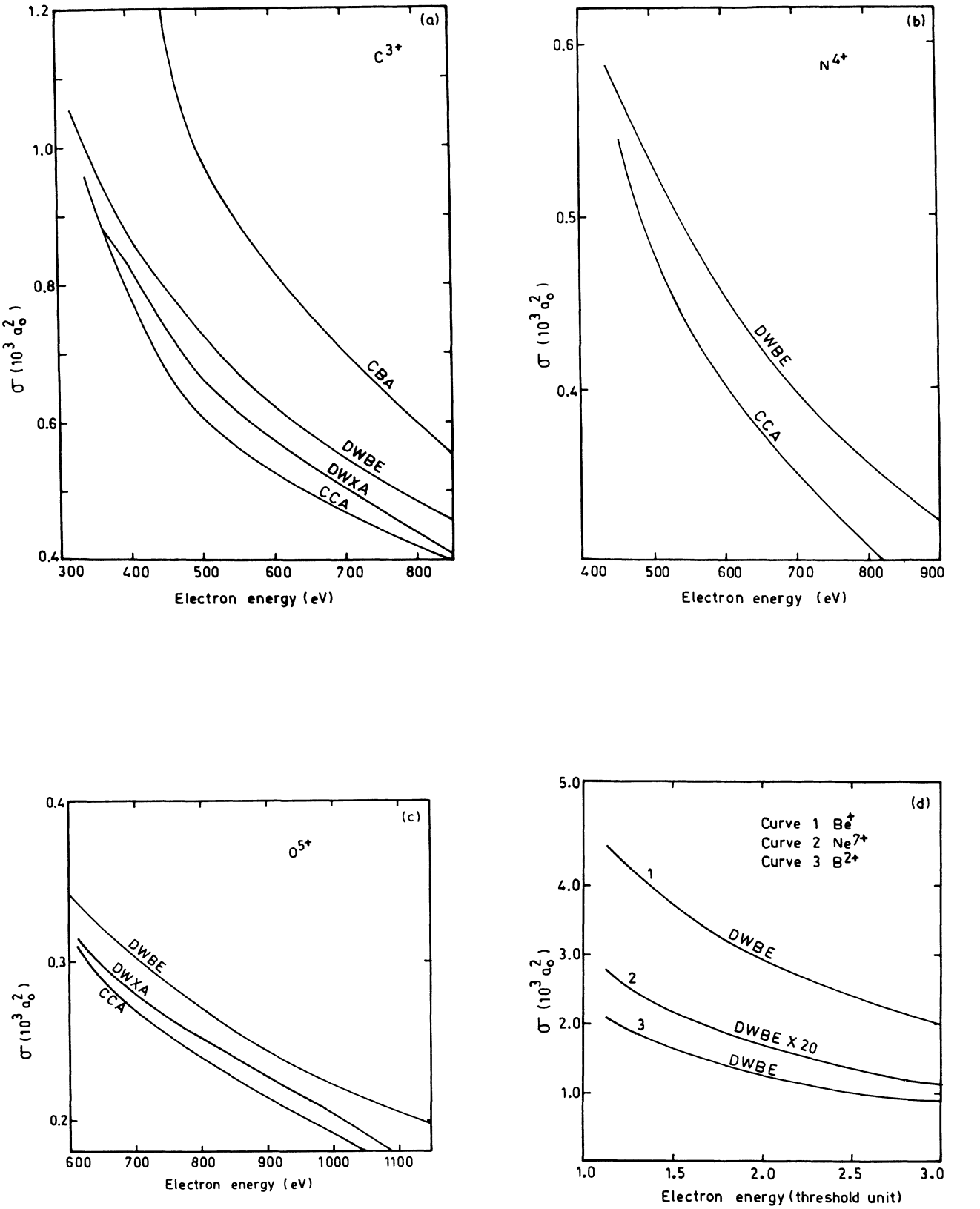

FIG. 1. Total excitation cross sections for electron excitation of the $1s2s^2$ state of various lithiumlike ions. The present results are labeled DWBE, the CCA results are those of Henry (Ref. 6), the DWXA results are of Itikawa *et al.* (Ref. 15), and the CBA results are those of Magee *et al.* (Ref. 17).

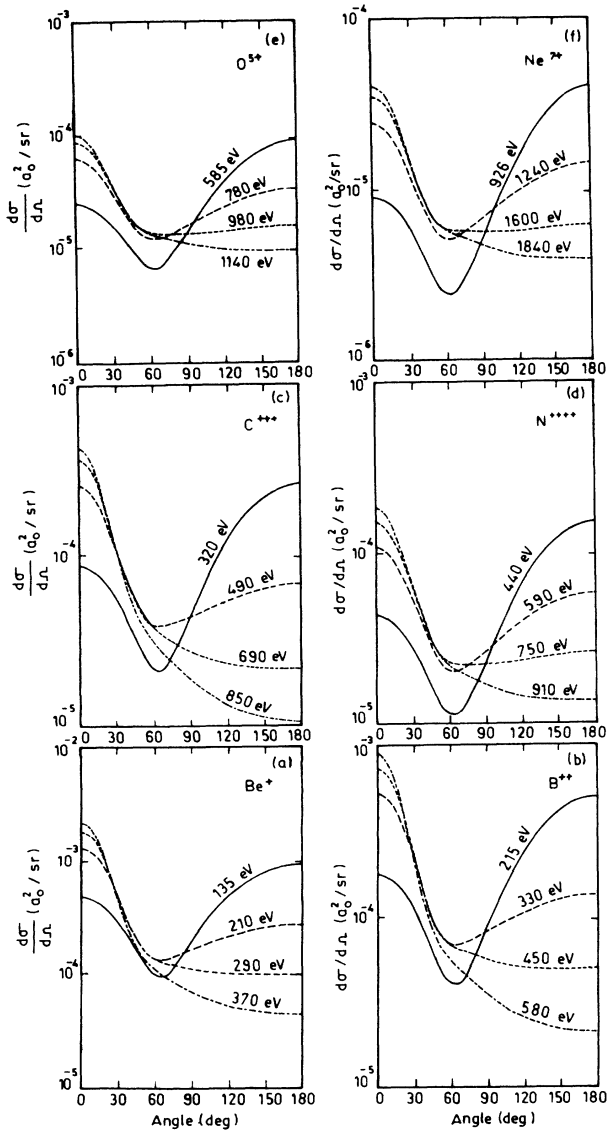

FIG. 2. DWBE differential excitation cross sections for electron excitation of the $1s2s^2$ state of various ions. The curves are for different incident electron energies.

sections are fairly sensitive to this choice. The CBA results for C^{3+} are significantly larger over the entire energy range and the CBA predicts a very large threshold excitation cross section. Since the DWBE, DWXA, and CCA results are similar and would, in general, be expected to be more accurate, we would conclude that the CBA significantly overestimates these cross sections and that the CBA is therefore, unreliable. In general, we can say that the agreement between our DWBE results and CCA results (and the DWXA results), tend to improve with increasing nuclear charge of the ion.

In Fig. 1(d) total-cross-section results are shown for the ions Be^+, B^{2+}, and Ne^{7+}. For Be^+ and B^{2+}, CCA results[4] are only available for a couple of energies up to 1.3 times threshold, and these CCA results are lower than the DWBE results.

Differential cross sections are shown in Fig. 2 for various electron energies for excitation of the ions Be^+ through Ne^{7+}. For each of the ions, we observed the following characteristic shapes: For electron energies near threshold, the differential cross sections had a minimum near 60° with a peak in the backward direction. For higher energies, the minimum disappears and the differential cross sections become peaked in the forward direction. As was mentioned above, Tiwary *et al.*[9] showed that the peaking in the total cross sections near threshold was a consequence of exchange. Since the angular distributions near threshold peak in the backward direction, it would be logical to assume that exchange caused this peaking, particularly in light of the fact that most angular distributions peak in the forward direction and exchange is normally most important for backward scattering. However, a study of the effects of exchange revealed that this is not the case. In fact, exchange has a small effect on the large-angle cross section and significantly increases the small-angle cross section. It is this increase at small angles which causes the threshold peaking in the total cross section, and without exchange the angular distributions are even more strongly peaked at back angles near threshold. While theoretical and experimental interest in the problem of differential cross sections for excitation of ions is recently being reported,[18–21] our results are what we believe to be the first to be reported for this particular isoelectronic series and autoionizing level. We expect increased interest in this type of work in the future.

This work was supported by the National Science Foundation (NSF) under Grant No. PHY-8607989.

*Present address: Department of Physics, University of Missouri–Rolla, Rolla, MO 65401.

[1]D. C. Gregory, in *Invited Papers of the Fourteenth International Conference on the Physics of Electronic and Atomic Collisions,* edited by D. C. Lorents, W. E. Meyerhof, and J. R. Peterson (North-Holland, Amsterdam, 1985), p. 205.

[2]D. H. Crandall, in *Invited Papers of the Twelfth International Conference on the Physics of Electronic and Atomic Collisions, Gatlinburg, 1981,* edited by S. Datz (North-Holland, Amsterdam, 1982), p. 595.

[3]D. H. Crandall, Phys. Scr. **23**, 153 (1980).

[4]D. H. Crandall, R. A. Phaneuf, D. C. Gregory, A. M. Howald, D. W. Mueller, T. J. Morgan, G. H. Dunn, D. C. Griffin, and R. J. W. Henry, Phys. Rev. A **34**, 1757 (1986), and references therein.

[5]D. Sampson and L. Golden, J. Phys. B **12**, L785 (1979).

[6]R. J. W. Henry, J. Phys. B **12**, L309 (1979).

[7]D. Sampson and L. Golden, J. Phys. B **14**, 903 (1981).

[8]J. Jakubowicz and D. Moores, J. Phys. B **14**, 3733 (1981).

[9]S. N. Tiwary, J. Macek, and D. H. Madison, Phys. Rev. A **32**,

2541 (1985).
[10]K. J. Nygaard, Phys. Rev. A **11**, 1475 (1975).
[11]R. Srivastava, C. S. Singh, and D. K. Rai, J. Phys. B **15**, 1899 (1982).
[12]V. Pejcev and K. J. Ross, J. Phys. B **10**, L291 (1977).
[13]W. B. Westerveld, F. B. Kets, and H. G. M. Heideman, J. Phys. B **12**, 2575 (1979).
[14]W. Rave, E. Herr, S. Zuccatti, A. Binder, A. Gutehkunst, and W. Mehlhorn, in *Abstracts of the Fifteenth International Conference on the Physics of Electronic and Atomic Collisions, Brighton, 1987,* edited by J. Geddes, H. B. Gilbody, A. E. Kingston, and C. J. Latimer (Queen's University, Belfast, 1987), p. 638 and references therein.
[15]Y. Itikawa, K. Sakimoto, and S. Nakazaki, Phys. Rev. A **36**, 1088 (1987).
[16]C. Froese-Fischer, Comput. Phys. Commun. **4**, 107 (1972).
[17]N. H. Magee, J. B. Mann, A. L. Merts, and W. D. Robb, Los Alamos Scientific Report No. LA6691MS, 1977.
[18]A. Z. Msezane and R. J. W. Henry, Phys. Rev. A **33**, 1636 (1986).
[19]R. Srivastava and A. K. Katiyar, Phys. Rev. A **35**, 1080 (1987).
[20]Y. Itikawa and K. Sakimoto, in *Abstracts of the Fifteenth International Conference on The Physics of Electronic and Atomic Collisions, Brighton, 1987,* edited by J. Geddes, H. B. Gilbody, A. E. Kingston, and C. J. Latimer (Queen's University, Belfast, 1987), p. 359.
[21]I. D. Williams, A. Chutjan, and R. J. Mawhorter, J. Phys. B **19**, 2189 (1986).