About universal scalings in double K-shell photoionization

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Abstract

We discuss the problem of the universal scalings in the double ionization of atomic K-shell electrons caused by the absorption of a single photon. In particular, we envisage the following questions: Under which conditions and up to which accuracy are the universal scalings realized? Does it make sense to talk about different physical mechanisms in the double-ionization process? Finally, we also present the theoretical analysis of recent experimental measurements performed on neutral atoms. As a testing ground, QED perturbation theory is employed.

((Some figures in this article are in colour only in the electronic version)
leading order of the perturbation theory, $\varepsilon \gamma$ the double K-shell ionization can occur for the photon energy numerically for the particular case of the helium atom [20, 21]. In many-body perturbation theory, this has been demonstrated dependent and, therefore, are devoid of the physical meaning. 

For gauge-invariant set, the total contribution of which does not quantities, the diagrams contribute always coherently, giving final state turns out to be strongly suppressed, provided the diagram describing the electron–electron interaction in the dipole approximation is again legitimate. Due to the gauge electron and, therefore, can be neglected. Accordingly, the electron–nucleus bindings in the atomic system become insignificant, since another small parameter comes into play, due to the identity of electrons, $\varepsilon_f = \omega/k$. To leading order of the perturbation theory, $\Delta k = 2I$, that is, the double K-shell ionization can occur for the photon energy $\varepsilon_f \geq 2$. The dimensionless photon momentum $x = aZ\varepsilon_f/2$ serves as a quantitative measure of the non-dipolarity [15]. If $k \ll \eta$, the dipole approximation ($x = 0$) can be employed. Obviously, this holds true within the near-threshold energy domain, if $aZ \ll 1$.

In the asymptotic high-energy regime, some of the electron–nucleus bindings in the atomic system become insignificant, since another small parameter comes into play, namely $\varepsilon_f^{-1} \ll 1$. In this case, the main contribution to the double-ionization cross section arises in the following kinematics: $p_1 \sim q \sim \sqrt{2m\omega} \gg \omega = k$ and $p_2 \sim \eta$ (or due to the identity of electrons, $p_2 \sim q \sim \sqrt{2m\omega} \gg k$ and $p_1 \sim \eta$). In other words, one ejected electron is fast, acquiring almost all the incident photon energy. Another ejected electron turns out to be slow. The photon momentum $k$ is now small compared to the asymptotic momentum of the fast outgoing electron and, therefore, can be neglected. Accordingly, the dipole approximation is again legitimate. Due to the gauge invariance of QED, one can choose the appropriate gauge, which simplifies the numerical calculations. For example, the diagram describing the electron–electron interaction in the final state turns out to be strongly suppressed, provided the Coulomb gauge is used [12].

The Feynman diagrams depicted in figure 1 represent a gauge-invariant set, the total contribution of which does not depend on the gauge of the electron–photon interaction. The separate contributions of each diagram, which sometimes are referred to as dominant ‘physical mechanisms’, are gauge dependent and, therefore, are devoid of the physical meaning. In many-body perturbation theory, this has been demonstrated numerically for the particular case of the helium atom [20, 21]. In differential and total cross sections, which are observable quantities, the diagrams contribute always coherently, giving rise to the interference terms. The interference is sometimes neglected in the theoretical analysis, as if it would be of minor importance (see, for example, recent papers [7–10]). However, within the near-threshold energy domain, this assumption is definitely not correct, because all correlation contributions are of the same order of magnitude. Moreover, beyond the leading order, the electron–electron interactions in the initial and final states turn out to be generally entangled due to the crossed photon diagrams (the vertex correction), although the higher order correlation contributions are suppressed by the parameter $Z^{-1}$. As a consequence, the attempts to separate the ‘physical mechanisms’ fail. The discussion of the double photoionization in terms of ‘physical mechanisms’ is superfluous, because the concepts themselves are physically unfounded.

To leading orders of QED perturbation theory with respect to the parameters $aZ$ and $Z^{-1}$, the total cross sections for double and single K-shell photoionizations are given by [16, 17]

$$
\sigma^{++} = \sigma_0 Q(\varepsilon_f, \lambda)Z^4,
$$

$$
\sigma^+ = \sigma_0 F(\varepsilon_f, \lambda)Z^{-2},
$$

where $\sigma_0 = \alpha \pi a_0^2$ and $a_0 = 1/(m\alpha)$ is the Bohr radius. The dimensionless functions $Q(\varepsilon_f, \lambda)$ and $F(\varepsilon_f, \lambda)$ depend on the nuclear charge $Z$ via the incident photon momentum $\lambda$. The scalings (1) and (2) become to be universal, if one sets $x = 0$ only. Accordingly, the quantities $aZ, Z^{-1}$ and $x$ estimate the accuracy, with which the universal scalings take place. In the dipole approximation, the function $F(\varepsilon_f, \lambda)$ is known in the analytical form [22]:

$$
F(\varepsilon_f) = \frac{2^{10}\pi}{3} \exp(-4\xi \cot^{-1} \frac{3\xi}{4}) \left[1 - \exp(-2\pi\xi)\right],
$$

where $\xi = 1/\sqrt{\varepsilon_f - 1}$. The universal function $Q(\varepsilon_f)$ can be obtained by the numerical integration only (see figure 2). The calculations performed by independent theoretical groups are consistent with each other [16–18]. Note also that the maxima of the universal functions $Z^2\sigma^{++}$ and $Z^2\sigma^+/\sigma^+$ peak at different values of the photon energy, namely at $\varepsilon_f \approx 2.5$ and 4, respectively. In the asymptotic non-relativistic range characterized by the condition $2 \ll \varepsilon_f \ll 2(aZ)^{-2}$, the double-to-single photoionization ratio does not depend on the photon energy [12]. To a given order of the non-relativistic perturbation theory with respect to the electron–electron interaction, it is represented as the Padé approximant [19]. The ratio $\sigma^{++}/\sigma^n$ can be less sensitive to the correlation effects rather than the cross sections themselves, when the higher order corrections to $\sigma^{++}$ and $\sigma^n$ have the same signs. In the relativistic limit, which is characterized by $\varepsilon_f \gtrsim 2(aZ)^{-2}$, the double-to-single photoionization ratio again depends on the incident photon energy [13, 14].

In the case of neutral atoms, the universal scaling behaviour deduced for helium-like targets still remains to be valid, if one takes into account the screening effect of the outer-shell electrons [16]. This can be achieved by the substitution of the true nuclear charge $Z$ by its effective value $Z_{\text{eff}}$, which is defined via the experimentally observable (or Hartree–Fock) ionization potential $I_{\text{exp}} = m(aZ_{\text{eff}})^2/2$. In addition, the photon energy $\omega$ should be calibrated in units of
The obvious consequence of the universal scalings consists in the following. For neutral atoms, at any fixed value of the dimensionless photon energy $\varepsilon_\gamma$, the double-to-single photoionization ratio $\sigma^{++}/\sigma^+$ should decrease, if the effective nuclear charge $Z_{\text{eff}}$ (and, respectively, the value of $Z$) increases. Indeed, at any particular value $\varepsilon_\gamma$, the ratio is given by $\sigma^{++}/\sigma^+ = C Z_{\text{eff}}^{-2}$, where $C$ is a constant. However, if we compare, for example, the experimental ratio $\sigma^{++}/\sigma^+$ for Mo [23] and Cu [24] near the maxima of the double K-shell photoionization cross sections, it turns out to be significantly larger for heavier Mo rather than that for Cu. A similar conclusion can also be drawn for measurements performed on Ag atoms [7]. Accordingly, the experimental data [7, 23] seem to be not quite reliable. One of the possible reasons, which could perhaps explain the strong discrepancy between theory and experiment, might be the contribution of some other (indirect) ionization channels.

In paper [8], the near-threshold energy behaviour for the double-to-single K-shell photoionization cross section ratios is studied for neutral atoms with nuclear charges within the range $23 \leq Z \leq 30$. These experimental results, however, raise more new questions, rather than giving affirmative answers. One part of the results is in fair agreement with the theoretical universal scaling, while another part of the measurements is in disagreement with it (see figure 3). Since the disagreements are quite significant, they cannot be explained by taking into

\[ I_{\exp} = \frac{\omega}{I_{\exp}}. \]

This procedure was also adopted by Hoszowska et al [10, 11], although not properly cited.

In works [16–18], the theoretical analysis is made for the experimental data on the double K-shell photoionization available until 2004. A satisfactory agreement of the universal scaling and experimental results is found in the majority of cases. However, for neutral molybdenum ($Z = 42$), the measurements performed at $\omega = 50$ keV give the double-to-single photoionization ratio $\sim 3.4 \times 10^{-4}$ [23], which is more than three times as large as the theoretical prediction $\sim 0.87 \times 10^{-4}$ [16–18]. Recently, a similar disagreement between the theory and experimental data has also been found for silver atoms ($Z = 47$) [7]. Of course, for such heavy targets, the corrections with respect to the parameters $\alpha Z$ and $\kappa$ can become significant. However, the disagreement of the universal scaling with the experimental results of papers [7, 23] cannot be explained by taking into account higher order corrections, because the disagreement is much larger than the parametrical values $\alpha Z$, $Z^{-1}$ and $\kappa$. In addition, as we argue below, the results of works [7, 23] are in contradiction not only with the theory, but also with other experimental measurements, for example, with work [24], where the double K-shell photoionization is measured for Cu atoms. Note that the results of Diamant et al [24] are consistent with the universal curve [16–18]. Therefore, this remains as a challenge for further experimental and theoretical investigations.
account higher order corrections with respect to the small parameters $\alpha Z, Z^{-1}$ and $\chi$. The slope of the experimental curves for the neighbouring elements changes drastically at all the characteristic parameters corrections are significant in the second case. The universal corrections are the most suitable targets to test the universality. In the first case, the higher order correlation corrections should be taken into account, while the relativistic and non-dipole distort the universal behaviour of the ionization cross sections.

Therefore, neither the neutral helium nor very high-$Z$ atoms seem to be too small. One should stress again that further taking into account the relativistic, correlation and non-dipole corrections will distort the universal behaviour of the ionization cross sections. Therefore, neither the neutral helium nor very high-Z atoms are the most suitable targets to test the universality. In the first case, the higher order correlation corrections should be taken into account, while the relativistic and non-dipole corrections are significant in the second case. The universal scalings have the highest accuracy for atomic systems with moderate values of the nuclear charge $Z$, because in this case, all the characteristic parameters $\alpha Z, Z^{-1}$ and $\chi$ are small enough. The helium-like multicharged ions would be the simplest targets, which are clean from the screening effect of the outer-shell electrons. Up to now, such measurements are not available in the literature. Recently, the ratios of double-to-single K-shell photoionization cross sections have been reported for neutral Mg, Al and Si atoms [9, 10]. As seen in figure 4, these measurements confirm the universal scaling deduced to leading orders of QED perturbation theory. However, more experimental information is required in order to elucidate the generic features of the double ionization of innermost bound electrons.

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References

[1] McGuire J H, Berrah N, Bartlett R J, Samson J A R, Tanis J A, Cocke C L and Schlachter A S 1995 J. Phys. B: At. Mol. Opt. Phys. 28 913
[2] Briggs J S and Schmidt V 2000 J. Phys. B: At. Mol. Opt. Phys. 33 R1
[3] Spielberger L et al 1995 Phys. Rev. Lett. 74 4615
[4] Levin J C, Armen G B and Sellin I A 1996 Phys. Rev. Lett. 76 1220
[5] Dörner R et al 1996 Phys. Rev. Lett. 76 2654
[6] Samson J A R, Stolte W C, He Z-X, Cutler J N, Lu Y and Bartlett R J 1998 Phys. Rev. A 57 1906
[7] Kanter E P, Ahmad I, Dunford R W, Gemmell D S, Krässig B, Southworth S H and Young L 2006 Phys. Rev. A 73 022708
[8] Huotari S, Hamiläinen K, Diamant R, Sharon R, Kao C C and Deutsch M 2008 Phys. Rev. Lett. 101 043001
[9] Fennane K, Dousse J-CI, Hoszowska J, Berset M, Cao W, Maillard Y-P, Szlachetko J, Szlachetko M and Kavčič M 2009 Phys. Rev. A 79 032708
[10] Hoszowska J et al 2009 Phys. Rev. Lett. 102 073006
[11] Kheifets A S, Bray I and Hoszowska J 2009 Phys. Rev. A 79 042504
[12] Amusia M Ya, Drukarev E G, Gorshkov V G and Kazachkov M P 1975 J. Phys. B: At. Mol. Phys. 8 1248
[13] Drukarev E G and Karpelesh P F 1976 J. Phys. B: At. Mol. Phys. 9 399
[14] Mikhailov A I and Mikhailov I A 1998 Zh. Eksper. Teor. Fiz. 114 1537
[15] Mikhailov A I and Mikhailov I A 1998 JETP 87 833
[16] Mikhailov A I, Mikhailov I A, Moskalov A N, Nefiodov A V, Plunien G and Soff G 2003 Phys. Lett. A 316 395
[17] Mikhailov A I, Mikhailov I A, Nefiodov A V, Plunien G and Soff G 2003 Phys. Lett. A 316 141
[18] Mikhailov A I, Mikhailov I A, Nefiodov A V, Plunien G and Soff G 2003 Phys. Lett. A 316 211
[19] Dalgarno A and Sadeghpour H R 1992 Phys. Rev. A 46 R3591
[20] Hino K, Ishihara T, Shimizu F, Toshima N and McGuire J H 1993 Phys. Rev. A 48 1271
[21] Akhiezer A I and Berestetskii V B 1974 Quantum Electrodynamics (New York: Wiley)
[22] Kanter E P, Dunford R W, Krässig B and Southworth S H 1999 Phys. Rev. Lett. 83 508
[23] Diamant R, Huotari S, Hamiläinen K, Kao C C and Deutsch M 2000 Phys. Rev. A 62 052519
[24] Oura M et al 2002 J. Phys. B: At. Mol. Opt. Phys. 35 3847