Time Delay of Slow Electrons by a Diatomic Molecule Described by Non-Overlapping Atomic Potentials Model

M. Ya. Amusia\textsuperscript{a,b,*} and A. S. Baltenkov\textsuperscript{c}

\textsuperscript{a} Racah Institute of Physics, the Hebrew University, Jerusalem, 91904 Israel
\textsuperscript{b} Ioffe Institute, St. Petersburg, 194021 Russia
\textsuperscript{c} Arifov Institute of Ion-Plasma and Laser Technologies, Tashkent, 100125 Uzbekistan

*e-mail: Miron.Amusia@mail.huji.ac.il, amusia@vms.huji.ac.il, Miron.Amusia@mail.ioffe.ru

Received May 15, 2020; revised June 12, 2020; accepted June 16, 2020

Abstract—The Wigner time delay in the processes of elastic scattering of slow electrons by two-atomic molecule has been studied within the frame of non-overlapping atomic potentials model. The molecular continuum wave function is represented as a combination of a plane wave and two spherical s-waves, generated by the centers of atomic spheres. The asymptotic of this function determines in closed form the amplitude of elastic electron scattering. It has been shown that at asymptotically great distances from the molecule the continuum wave functions can be presented as an expansion in a set of other than spherical, orthonormal functions. The coefficients of the scattering amplitude expansion in a series of these functions determine the scattering phases for the molecular system under consideration. With these molecular phase shifts the Wigner time delay for slow electron scattered by two-atomic target has been calculated. As a concrete example of a molecule we consider $\text{C}_2$.

DOI: 10.1134/S10637761200100015

1. INTRODUCTION

Experiments with atomic photoionization under the action of attosecond laser pulses provided qualitatively new information on the real time dynamics of this process. The accepted interpretation of these experimental data relies on the EWS-time delays originally introduced by Eisenbud, Wigner, and Smith [1–3]. As compared to atomic photoionization, the molecular time-delay case is much more complex due to anisotropic nature of the molecular scattering potential. Temporal analysis of molecules photoionization leads to so-called angular time delay [4–9] as a function depending on the orientation of photon polarization $\mathbf{e}$ and photoelectron momentum $\mathbf{k}$ vectors, relative to the molecular axes $\{\mathbf{R}_i\}$. The time delay, as a quantum dynamical observable, is extremely sensitive to the phase shifts of photoelectron wave function, or, more precisely, to its energy derivative. Therefore, analysis of the correctness of methods for calculating phase functions for nonspherical targets, such as molecules, is very important. When calculating the delay times of photoelectrons in the processes of molecular photoionization, the continuum wave functions and their phases should be calculated numerically.

For these calculations usually the complex of mathematical programs \textit{ePolyScat} [10–12] (see Lucchese Group Website, 2015) is used [6–9]. Within the framework of these programs the continuum electron functions are similar to those for electron-atom scattering [12]. The asymptotic form of the wave function far from the molecule (beyond the molecular sphere\textsuperscript{1}) is a sum of a plane wave and spherical waves emitted by the molecular center. In fact, we have a picture of 

\textit{diffr action of an electron wave by an isolated molecular sphere}. The continuum wave function is a linear combination of regular and irregular solutions of the wave equation. The coefficients of this linear combination determine the molecular phases of electron scattering. The phases derivatives with respect to energy give partial Wigner times delay. This recipe to build a molecular continuum wave function and to calculate molecular phase shifts are considered as a matter-of-course and, as far as we know, are assumed to be beyond any doubt.

A different and more realistic approach in describing scattering of an electron wave by a molecule is considered in an article by Cohen and Fano [14], where the diffraction pattern of an electron wave scattered by a molecule is a result of the interference of spherical waves generated by spatially separated sources. In this approach, the target is considered as a cluster of non-

\textsuperscript{1} We have demonstrated quite a while ago [13] that the introduction of a molecular sphere into the muffin-tin-potential model leads to some non-physical features in the molecular continuum wave functions.
overlapping atomic spheres, and the spherical waves emitted by them produce an interference pattern whose properties depend periodically on the ratio of the inter-nuclear distance to the photoelectron wavelength. This article is devoted to the answer to the question whether molecular phases exist in this scattering picture, and if so, how can they be calculated.

To do this, it is reasonable to consider a model molecular system that allows an exact solution [15]. In the present paper, we will do this using as an example a target formed by two spatially separated by distance \( R \) non-overlapping short-range atomic potentials. The calculation of the elastic scattering amplitude \( F(\mathbf{k}, \mathbf{k}', \mathbf{R}) \) of slow electrons by such a target (in Section 2 of this paper) is a good example that has an analytical solution.

The problem of elastic scattering of a particle on a non-spherical target and S-matrix method for this case was developed in [16], where it was shown that asymptotically at great distances from the molecule the continuum wave function can be presented as an expansion in a set of other, than spherical, orthonormal functions \( Z_\lambda(\mathbf{k}) \). These functions depend, in particular, on the number of atoms forming the target and on the relative orientation of the scattering centers in space, etc. In Section 3 we briefly discuss the main ideas of the method [16] and apply them to amplitude \( F(\mathbf{k}, \mathbf{k}', \mathbf{R}) \).

The expansion of amplitude \( F(\mathbf{k}, \mathbf{k}', \mathbf{R}) \) into a series of functions \( Z_\lambda(\mathbf{k}) \) performed in Section 4 determines the set of phases, called in [16] the “proper molecular phases.” The latter are used for numerical calculations of the scattering cross sections of slow electrons by molecules with different \( R \). The radial parts of the molecular continuum wave functions \( R_\lambda(r) \), that are accurate at asymptotically large distances from the target, determine the electron fluxes through the surface of a sphere with a large radius surrounding the molecule. According to [3], these flows determine the Wigner times delay of the slow electron by the target. In Section 5 the “proper phases” (hereinafter we will call them simply “molecular phases”) are used for numerically calculations of two partial Wigner times delay of the slow electron by the target.

Here \( \delta_\lambda(k) \) is the s-phase shift of electron elastic scattering by isolated atomic potential; \( C_1 \) and \( C_2 \) are some constants.

One should have in mind that this wave function is actually incorrect inside the atomic spheres, since the regular s-type wave function near the centers of each atomic sphere is a constant. However, this does not play any role in solving the problem of elastic electron scattering by the target. It is physically obvious that a complete knowledge in all the space of the molecular continuum wave function is not necessary for a satisfactory description of the scattering amplitude. It is enough to have the asymptotic wave functions, which are directly related to the phase shift.

Applying formulas (2) to the function (1) we obtain the exact general solution of the Schrödinger equation that describes the multiple scattering of electron by two-center target [17, 18]. Indeed, if we substitute function (1) in the wave equation we obtain in its right hand side the sum of two delta-functions \( \delta(r \pm R/2) \), because the second and third terms in (1) coincide up to constants with the Green functions of the wave equation for free particle motion. Delta-functions are equal to zero in all space except the points \( r = R/2 \). So, beyond the atomic spheres (where \( r \neq \pm R/2 \) the function (1) obeys the wave equation for free electron motion.

The amplitude of slow electron scattering by the target is obtained by considering the asymptotic behavior of the wave function (1). As a result, we obtain the following exact amplitude of the electron multiple scattering by given two-center target \([17, 18]\)

\[
F(\mathbf{k}, \mathbf{k}', \mathbf{R}) = \frac{2}{a^2 - b^2} \left[ b \cos \left( \mathbf{k} - \mathbf{k}' \right) \cdot \frac{R}{2} \right] - a \cos \left( \mathbf{k} + \mathbf{k}' \right) \cdot \frac{R}{2}.
\]

2 Atomic units are used throughout this paper.

3 Note, that in [18] a similar function was used to describe scattering of slow mesons by deuteron.
As in [17], we use here the following notation: \( k \) and \( k' \) are the electron linear momentums before and after scattering, respectively; \( b = k(i - \cot \delta_0) = -1/f_s(k) \) and \( a = \exp(ikR)/R \). Here \( f_s(k) \) is the \( s \)-partial amplitude of electron elastic scattering by isolated atomic potential.

The total scattering cross section we obtain from the amplitude (3) using the optical theorem \([19]\)

\[
\sigma(k, R) = \int \frac{d\sigma}{d\Omega} \frac{d\Omega}{d\varepsilon} = \frac{4\pi}{k} \text{Im} F(k) = \frac{4\pi}{k} \text{Im} \left[ \frac{b - a \cos(k \cdot R)}{a^2 - b^2} \right]
\]

The vectors \( k \) and \( R \) as the argument of the cross section (4) emphasize that we are dealing with fixed in space molecule. The total cross section (4) averaged over all the directions of the incident electron momentum \( k \) relative to the vector \( R \) has the form:

\[
\sigma(k) = \frac{4\pi}{k} \sum \sigma(k, R) d\Omega_k
\]

\[
= \frac{4\pi}{k^2} \left[ 1 + \frac{(qR + \cos(kR))}{kR + \sin(kR)} \right]^{-1}
\]

\[
= \frac{1}{k^2} \left[ 1 + \frac{(qR - \cos(kR))}{kR - \sin(kR)} \right]^{-1},
\]

where \( q = -k\cot \delta_0(k) \). The cross section (5) contains \( \sin kR/kR \) that characterizes diffraction phenomena. Its appearance is a consequence of the interference of two \( s \)-waves in the continuum wave function (1).

### 3. METHOD OF PARTIAL WAVES FOR NON-SPHHERICAL TARGETS

A molecular potential as a cluster of non-overlapping atomic potentials centered at the atomic sites is nonspherical. The solution \( \psi^*_m(r) \) of the Schrödinger equation with this potential is impossible to present at an arbitrary point of space as an expansion in spherical functions \( Y_{lm}(r) \). However, asymptotically at great distances from the molecule, according to \([16]\), the wave function can be presented as an expansion in a set of other orthonormal functions \( Z_\lambda(k) \):

\[
\psi^*_m(r \rightarrow \infty) = 4\pi \sum Z_\lambda(k) Z^*_\lambda(k)
\]

with the radial part of the wave function determined by the following expression

\[
R_{\lambda\lambda}(r \rightarrow \infty) = e^{i\left[\eta_\lambda f_{\lambda\lambda} \right]} \left( kr - \frac{\pi}{2} \omega_\lambda + \eta_\lambda \right)
\]

Here the index \( \lambda \) numerates different partial wave functions similar to the quantum numbers \( l \) and \( m \) for the central field; \( \omega_\lambda \) is the quantum number that is equal to the orbital moment \( l \) for the spherical symmetry case; \( \eta_\lambda(k) \) are the molecular phases. The explicit form of functions \( Z_\lambda(k) \) (in terminology of \([16]\) they are “characteristic amplitudes”) depends upon the specific type of the target field, particularly on the number of atoms forming the target and on mutual disposition of the scattering centers in space, etc. Functions \( Z_\lambda(k) \), like the spherical functions \( Y_{lm}(k) \), create an orthonormal system. The elastic scattering amplitude for a non-spherical target, according to \([16]\), is given by the following expression

\[
F(k, k') = \frac{2\pi}{ik} \sum_{\lambda} (e^{2\eta_\lambda} - 1) Z^*_\lambda(k) Z_\lambda(k').
\]

The cross section averaged over all directions of momentum of incident electron \( k \) is connected with the molecular phases \( \eta_\lambda(k) \) by the following expression

\[
\sigma(k) = \frac{4\pi}{k^2} \sum \sin^2 \eta_\lambda.
\]

The partial wave (7) and molecular phases \( \eta_\lambda(k) \) are classified, according to \([16]\), by their behavior at low electron energies, i.e. at \( k \rightarrow 0 \). In this limit the particle wavelength is great as compared to the target size and the function \( Z_\lambda(k) \) tends to some spherical function \( Y_{lm}(k) \). In this limit the corresponding phase is characterized by the following asymptotic behavior: \( \eta_\lambda(k \rightarrow 0) \approx k^{2\lambda + 1} \).

We apply the formulas of this section to calculate the elastic electron scattering by a target formed by two non-overlapping atomic potentials.

### 4. EXPANSION OF THE SCATTERING AMPLITUDE (3) IN A SERIES OF FUNCTIONS \( Z_\lambda(k) \)

According to formulas in Section 3, the amplitude (3) should be represented as a partial expansion in a series of functions \( Z_\lambda(k) \). For a given molecular system the molecular phase shifts \( \eta_\lambda(k) \) and the functions \( Z_\lambda(k) \) can be calculated explicitly \([17]\). Following this paper let us rewrite the scattering amplitude (3) in the following form

\[
F(k, k', R) = -\frac{2}{a + b} \cos(k \cdot R/2) \cos(k' \cdot R/2)
\]

\[
+ \frac{2}{a - b} \sin(k \cdot R/2) \sin(k' \cdot R/2).
\]

According to \([16]\), the amplitude (10) should be considered as a sum of two partial amplitudes. The first of them is written as

\[
\frac{4\pi}{2ik} \left( e^{2\eta_0} - 1 \right) Z_0(k) Z_0^*(k')
\]

\[
= -\frac{2}{a + b} \cos(k \cdot R/2) \cos(k' \cdot R/2).
\]
The second one is defined by the following expression

\[
\frac{4\pi}{2ik}(e^{2\text{im}} - 1)Z_1(k)Z^*_1(k') = \frac{2}{a - b} \sin(k \cdot R/2)\sin(k' \cdot R/2).
\] (12)

After elementary transformations of (11) and (12), we obtain two molecular phases

\[
\cot \eta_0 = -qR + \cos kR, \quad \cos \eta_1 = -qR - \cos kR
\]

where \( q = -k\cot \delta_0(k) \), and two “characteristic amplitudes”

\[
Z_0(k) = \frac{\cos(k \cdot R/2)}{\sqrt{2\pi S_+}}, \quad Z_1(k) = \frac{\sin(k \cdot R/2)}{\sqrt{2\pi S_-}}.
\] (14)

Here \( S_\pm = 1 \pm \sin kR/kR \). It is easy to demonstrate that the functions \( Z_0(k) \), like the spherical functions \( Y_{lm}(k) \), create an orthonormal system.

Evidently, the functions (14) are defined by the geometrical target structure, i.e. by the direction of the molecular axis \( R \) in the arbitrary coordinate system, in which the electron momentum vectors before and after scattering are \( k \) and \( k' \), respectively. The transition to the limit \( k \to 0 \) in formulas (14) gives instead of the functions \( Z_0(k) \) the well-known spherical functions

\[
Z_0(k)_{k \to 0} \to \frac{1}{\sqrt{4\pi}} \equiv Y_{00}(k),
\]

\[
Z_1(k)_{k \to 0} \to \frac{3}{\sqrt{4\pi}} \cos 0 \equiv Y_{10}(k).
\] (15)

Here \( \theta \) is the angle between the vector \( k \) and axis \( R \). So, only in the limit \( k \to 0 \) it becomes correct to replace a non-spherical molecular field by a spherical one.

The molecular phases \( \eta_\alpha(k) \) in (13) can be classified by considering their behavior at \( k \to 0 \) [16]. In this limit the electron wavelength is much greater than the target size and the picture of scattering should approach that in the case of spherical geometry. Considering the transition to this limit in the formulas (13), we obtain: \( \eta_0(k \to 0) \sim k \) and \( \eta_1(k \to 0) \sim k^3 \).

Thus, the molecular phases at \( k \to 0 \) behave similar to the \( s \)-and \( p \)-phases in the spherically symmetrical potential, which explains the choice of their indexes.

As expected, the sum of the partial cross sections of elastic scattering, calculated with phases (13)

\[
\sigma_0(k) = \frac{4\pi}{k^2} \sin^2 \eta_0 \quad \text{and} \quad \sigma_1(k) = \frac{4\pi}{k^2} \sin^2 \eta_1
\] (16)

coincides with the total cross section (5) that follows from the optical theorem. The results of numerical calculations of the electron scattering cross sections by molecule \( C_2 \) using formulas (16) are shown in Fig. 1. The presence of terms \( \sin kR/kR \) in (16) leads to oscillations in the cross sections associated with diffraction effects, arising from the interference of two spherical \( s \)-waves, generated by spatially separated sources. The diffraction effects, of course, are impossible if we assume that far from the molecule there is only one spherical wave, as it is assumed in the approach that substitute a multicenter molecule by a molecular sphere [10–12].

5. WIGNER TIME DELAY

The developed in Section 3 method of partial waves for non-spherical targets separates in a natural way the kinematics of the scattering process, which is defined by the functions \( Z_\alpha(k) \), from the dynamical part that is determined by the molecular phases \( \eta_\alpha(k) \). The partial waves with indexes \( \lambda = 0 \) and \( 1 \) have the following asymptotic forms [17]

\[
R_\alpha(r \to \infty) = e^{i\eta_\alpha \frac{\pi}{2}} \sin kr + \eta_\alpha;
\]

\[
R_\alpha(r \to \infty) = e^{i\eta_\alpha \frac{\pi}{2}} \sin kr - \frac{\pi}{2} + \eta_\alpha,
\] (17)

and they determine the particle fluxes through the surface of a sphere with a large radius surrounding the molecule. According to [3], these flows determine the following two delay times of the slow electrons by the target. The first Wigner time delay is:

\[
\tau_0(k) = 2 \frac{d\eta_0}{dE} = \frac{2}{k} \eta_0(k)
\]

\[
= -\frac{2}{k} RF_0(k)[(qR + \cos kR)^2 + (kR + \sin kR)^2]^{-1},
\] (18)

where the function \( F_0(k) \) is

\[
F_0(k) = (1 + \cos kR)(qR + \cos kR) - (q - \sin kR)(kR + \sin kR).
\] (19)

The second Wigner time delay is

\[
\tau_1(k) = 2 \frac{d\eta_1}{dE} = \frac{2}{k} \eta_1(k)
\]

\[
= -\frac{2}{k} RF_1(k)[(qR - \cos kR)^2 + (kR - \sin kR)^2]^{-1},
\] (20)

where the function \( F_1(k) \) is of the form

\[
F_1(k) = (1 - \cos kR)(qR - \cos kR) - (q + \sin kR)(kR - \sin kR).
\] (21)

In these formulas the functions \( q(k) \) and \( \dot{q}(k) \) are, respectively

\[
q(k) = -k \cot \delta_0(k);
\]

\[
\dot{q}(k) = -\frac{\sin \delta_0 \cos \delta_0 - k \delta_0}{\sin^2 \delta_0},
\] (22)

Operator \( \frac{\partial}{\partial k} \) in formulas (18)–(22) is denoted by a dot.
Figure 2 presents the times delays $\tau_0(k)$ and $\tau_1(k)$ for molecule $C_2$ in the model of two non-overlapping atomic spheres for four fixed values of inter-atomic distances $R$. In the real molecule $R_C = 2.479$ atomic units [17]. In these calculations with formulas (18)–(22) the atomic phase shift $\delta_0(k)$ was described by the following analytical expression $\delta_0(k) \approx 2\pi - 1.912k$. In the left upper panel of Fig. 2 the Wigner time delay for electron scattering by the single carbon atom $\tau_{0\text{at}}(k)$ is presented together with the molecular times $\tau_0(k)$ and $\tau_1(k)$. Atomic time delay $\tau_{0\text{at}}(k)$ goes to minus infinity as electron wave vector $k$ goes to zero

$$\tau_{0\text{at}}(k \to 0) = \frac{2}{k} \frac{d}{dk} (2\pi - 1.912k) \to -3.824/k.$$  

(23)
The molecular function $\tau_0(k)$ behaves in a qualitatively similar way. Large negative delays are in apparent contradiction with the causality principle. From the classical viewpoint a large negative time delay means that the electron appears to be ejected before the external action on the molecule takes place. We can estimate the ability of an electron to penetrate the potential field of a molecule by observing the behavior of the second time delay $\tau_1(k)$. According to Fig. 2, with increase of interatomic distance $R$, the minimum value of the function $\tau_0(k)$ increases i.e. an increase in the interatomic distance $R$ of the molecule is accompanied by a more intense expulsion of the electron from the inner region of the molecule.

A similar picture is given in the article [20] in Fig. 4, which shows the dependence of the photoelectron time delay by $H_2$ molecule as a function of the interatomic distance. The time delay becomes negative at $R > 2.6$ at. units and deepens with growth of $R$ in molecule $H_2$.

Both molecular curves in Fig. 2 with growth of $R$ rapidly oscillate, which is associated with the presence...
in the scattering phases of terms \( \sin kR/kR \) that are typical for interference of two \( s \)-waves in the continuum wave function (1).

6. CONCLUSIONS

As a rule, in studies of electron-molecule scattering, the continuum electron is usually treated as moving in a spherically averaged molecular field [10–12]. The wave functions describing the scattering of an electron by a polyatomic molecule outside the so-called molecular sphere are considered as a linear combination of regular and irregular solutions of the wave equation. The phase shifts of molecular wave function are determined from the matching condition for the solutions of the wave equation inside and beyond this sphere [21] or in the calculations of radial integrals up to distances defining a range of the interaction (\( r_{\text{max}} = 10 \, \text{Å} \) [7]). The pattern of diffraction of an electron wave on a molecule (see Fig. 1c in [22]) corresponding to these ideas is the diffraction of a wave on an isolated molecular sphere.

The scattering pattern, in which far from the target there is a set of spherical waves generated by spatially separated centers (Fig. 1a in [22]), is much closer to the reality. In this paper, it was shown that S-matrix method of partial waves can also be developed for the latter scattering picture. This method allows separating the kinematics of the scattering process from the dynamical part that is determined by the molecular phases. The energy derivatives of \( \eta_\lambda(k) \) are the partial Wigner times delay of slow electron by the molecule.

A straightforward application of the classical S-matrix method based on the spherical functions \( Y_{\lambda m}(k) \) to non-spherical targets leads to irreparable internal contradictions and therefore cannot be considered as satisfactory. We came to this conclusion based on the consideration of the simplest model system (1). It was demonstrated in [23] (Section 3.1) that a set of molecular scattering phases capable of reproducing the elastic scattering cross section (5) resulting from an analytical solution to the problem in the frame of the classical S-matrix method does not exist.

As in the case of considered two-atomic system, the amplitude of electron elastic scattering by a cluster of \( N \) non-overlapping atomic potentials can be represented in the form of a series of orthonormal functions \( Z_\ell(k) \) specific to a given system (“characteristic scattering amplitudes”). The coefficients of this expansion determine a unique (again for a given target) set of molecular scattering phases (“proper phase shifts”). These phases also determine the Wigner times delay of an electron by a given molecule.

We do believe that the developed approach will open new horizon in studies of electron–molecule collisions, including their temporal picture.

ACKNOWLEDGMENTS

A.S. Baltenkov thanks for support the Uzbek Fund, grant OT-F2-46, and Dr. I. Woiciechowski for useful discussions.

REFERENCES

1. L. E. Eisenbud, Ph. D. Thesis (Princeton Univ., Princeton, 1948).
2. E. P. Wigner, Phys. Rev. 98, 145 (1955).
3. F. T. Smith, Phys. Rev. 118, 349 (1960).
4. P. M. Kraus, A. Rupenyub, and H. J. Wörner, Phys. Rev. Lett. 109, 233903 (2012).
5. A. Chacon, M. Lein, and C. Ruiz, Phys. Rev. A 89, 033427 (2014).
6. P. M. Kraus, D. Baykusheva, and H. J. Wörner, Phys. Rev. Lett. 113, 023001 (2014).
7. P. Hockett, E. Frumker, D. M. Villeneuve, and P. B. Corkum, J. Phys. B 49, 095602 (2016).
8. M. Huppert, I. Jordan, D. Baykusheva, A. von Conta, and H. J. Wörner, Phys. Rev. Lett. 117, 093001 (2016).
9. D. Baykusheva and H. J. Wörner, J. Chem. Phys. 146, 1 (2017).
10. F. A. Gianturco, R. R. Lucchese, and N. Sanna, J. Chem. Phys. 100, 6464 (1994).
11. A. P. P. Natalense and R. R. Lucchese, J. Chem. Phys. 111, 5344 (1999).
12. F. A. Gianturco and A. Jain, Phys. Rep. 143, 347 (1986).
13. M. Ya. Amusia and A. S. Baltenkov, Centr. Eur. J. Phys. 8, 825 (2010).
14. H. D. Cohen and U. Fano, Phys. Rev. 150, 31 (1966).
15. A. S. Baltenkov, S. T. Manson, and A. Z. Msezane, J. Phys. B 51, 205101 (2018).
16. Yu. N. Demkov and V. S. Rudakov, Sov. Phys. JETP 32, 1103 (1971).
17. A. S. Baltenkov and A. Z. Msezane, Eur. Phys. J. D 71, 305 (2017).
18. K. A. Brueckner, Phys. Rev. 89, 834 (1953).
19. L. D. Landau and E. M. Lifshitz, Course of Theoretical Physics, Vol. 3: Quantum Mechanics, Non-Relativistic Theory (Pergamon, Oxford, 1965; Nauka, Moscow, 1989).
20. V. V. Serov, V. L. Derbov, and T. A. Sergeeva, Phys. Rev. A 87, 063414 (2013).
21. D. Dill and J. L. Dehmer, J. Chem. Phys. 61, 692 (1974).
22. A. S. Baltenkov, S. T. Manson, and A. Z. Msezane, J. Phys. B 45, 035202 (2012).
23. M. Ya. Amusia and A. S. Baltenkov, arXiv: 2001.03652 (2020).