Bound-to-bound and bound-to-continuum optical transitions in negative quasi-molecules

A Z Devdariani¹,²

¹St. Petersburg State University, Peterhof, Ul’yanovskaia St. 3, 198504, St.Petersburg, Russia
²The Herzen State Pedagogical University of Russia, nab. Reki Moiki, 48, 191186, St.Petersburg, Russia

E-mail: snbrn2@yandex.ru, a.devdariani@spbu.ru

Abstract. Optical transitions between both discrete and continuum states are considered in the frame of the model of two delta potentials. The wave functions of the definite parity are utilized for both discrete and continuum states cases.

1. Introduction
This work presents the theory of optical transitions formed in low-energy symmetrical collisions of atoms with negative ions

\[ A + A^- \rightarrow A + A^- + \omega, A^- + \omega \]
\[ A + A^- + \omega \rightarrow A + A + e, A^- + e \] (1) (2)

These processes can be of interest for studies of the molecular hydrogen formation in the early Universe [1], for the studies of the formation and stability of molecular ion \( H_2^- \) [2], and for studies of oscillations appearing in photoionization cross-sections of diatomic molecules [3]. Although processes like with neutral atoms have been studied in depth in the past, the novelty of the work is the use of the model approach which enables us to obtain an analytical solution. In the approach, the Zero-Range Potential Model [4, 5] is applied to describe the interaction of an electron with two identical atoms. The advantage of the model is that it can describe the bond states, the ones shown in Eq.1, as well as the states of the continuum. In order to simplify the discussion a one-dimensional model is considered.

2. Optical transitions
The theoretical analysis of optical transitions is based on the calculations of the transition dipole moment between two bound states involved or between a bound state and a state of continuum. It is obvious that the calculation can be simplified if one uses the wave functions of the opposite parity, that is \( \Psi(-x)\pm = \pm \Psi(x)\pm \).

2.1. Bond-to-bound transitions
Let’s start with radiative transitions produced by the reaction of charge exchange (1). In this case, the wave functions of the electron in the field of two delta potentials at a distance \( R \) from each other are as follows

\[ \Psi(x)\pm_b = C_b^\pm [B(\alpha_\pm - \frac{R}{2})_b \pm B(\alpha_\pm + \frac{R}{2})_b] \]

where \( B(\alpha_\pm \pm \frac{R}{2})_b = \exp(-\alpha_\pm |x \pm \frac{R}{2}|) \). (3)
\( C_b^\pm \) are the normalization constants and \( \alpha_\pm \) are the solutions of the equation \( \alpha_\pm = \alpha_0 \left( 1 + \exp(-\alpha_\pm R) \right) \). The proper molecular energies are \( U(R)^\pm = -\alpha_\pm^2 / 2 \), so that the binding energy of the electron in the atomic ion is \( -\alpha_0^2 / 2 \). The dipole moment for the bound-to-bound transitions is up to normalization constants

\[
D_{bb} = \sum (-1)^{j+1} f^b_i, \text{ where are } f^b_i(R) = \int_{-\infty}^{+\infty} B(\alpha_-, -\frac{R}{2})_b x B(\alpha_+, +\frac{R}{2})_b dx, \quad f^b_1(R) = -f^b_1(R), \quad f^b_2(R) = f^b_2(R) \tag{4}
\]

Then, \( f^b_1 - f^b_2 = \left( \frac{1}{\alpha_+} + \frac{1}{\alpha_-} \right) \frac{R}{2} \), but for \( \alpha R \gg 1 \) we get \( f^b_{3,4}(R) = 0 \) and \( C_b^{\pm} = \sqrt{\alpha_0 / 2} \), so that finally \( D_{bb} = R/2 \) is in agreement with the well-known result, e.g. [5].

2.2. Application of wave functions of definite parity for transitions to continuum

In calculating the dipole moment for the bound-to-bound transitions, functions of different parity have been used. But when calculating photodetachment or recombination one needs to calculate the dipole moment for the transitions between bound and continuum states. However, the correct wave function of the continuum, so called an ingoing wave \( \Psi^{in} \) in the case of photodetachment, do not have the definite parity what complicates the calculations. Thus, it is reasonable to express the ingoing wave functions through the functions of the definite parity \( \Psi(\pm x)^c_{\pm} \). Then, one obtains

\[
\Psi(k, x)^{in} = e^{-i\delta_+} \Psi^c_{\pm} + ie^{-i\delta_-} \Psi^c_{-} \tag{6}
\]

and the dipole moment for bound-to-continuum transitions is

\[
D(k)_{bc} = \int_{-\infty}^{+\infty} \Psi(x)^{\pm} x \Psi(k, x)^{in} dx = i e^{-i\delta_-} \int_{-\infty}^{+\infty} \Psi(x)^{\pm} x \Psi^c_{-}(k, x) dx \tag{7}
\]

2.3. Bond-to-continuum transitions

In the case of one delta potential \( \Psi^b_{\pm} = \sqrt{\alpha} \exp(-\alpha |x|) \) and \( \Psi^c_{-} = \frac{1}{\sqrt{\pi k}} \sin kx, \delta_- = 0 \), so we obtain the dipole moment for bound-to-continuum transitions according to (7)

\[
D(k)_{bc} = \pm i \sqrt{\frac{\alpha}{\pi k (\alpha^2 + k^2)^2}} \tag{8}
\]

The last formula leads to the correct expression for the detachment cross-section that is an alternate expression to the one obtained in Ref. [7].

In the case of two delta potentials, the even and odd continuum wave function are

\[
\Psi(x)^c_{\pm} = C_{\pm} \left[ B(k, -\frac{R}{2})_{c} \mp B(k, \frac{R}{2})_{c} \right] \text{ where } B(k, \pm \frac{R}{2}) = \cos \left( k \left| x \pm \frac{R}{2} \right| + \delta_{\pm} \right) \tag{9}
\]

and \( \delta_- = \frac{1 - \cos kr}{\pi k \sin kr} \). The corresponding expression of the dipole moment between the bound state \( \Psi^b_{\pm} \) and the continuum state \( \Psi^c_{-} \) is

\[
D_{bc} = \sum (-1)^{j+1} f^c_i, \text{ where are } f^c_i(R) = \int_{-\infty}^{+\infty} B(\alpha_+, -\frac{R}{2})_b x B(k, -\frac{R}{2})_{c} dx, \quad f^c_1(R) = -f^c_1(R) \tag{10}
\]

\[
f^c_2(R) = \int_{-\infty}^{+\infty} B(\alpha_+, -\frac{R}{2})_b x B(k, -\frac{R}{2})_{c} dx, \quad f^c_3(R) = -f^c_3(R) \tag{11}
\]

Then we get
\[ J_{1}^c - J_{2}^c = \frac{2R}{\sqrt{\alpha_{+}^2 + k^2}} \sin(\delta_0 - \delta_-) \], and for \( \alpha R \gg 1 \)
\[ J_{4}^c(R) = \frac{2\alpha R}{\alpha^2 + k^2} \cos(kR + \delta_-) \] (12)

As it follows from Eq.(12) the bound-to-continuum transitions lead to the formation of oscillating structures in the dipole moment and therefore, to oscillatory structures in the cross-sections of photodetachment in negative ion collisions (2). The structures are connected not only with the interference due to two possible ways of electron detachment. The reason for the oscillating structures production are two possible ways of electron detachment and resonances produced in scattering by two potential wells and described by the dependence of \( \delta_- \) on \( R \) and \( \alpha_0 \) [8].

3. Conclusions
The dipole moment for bound-to-bound and bound-to-continuum transitions have been obtained in the frame of the model of two delta potentials. The approach utilizing the wave functions with the definite parity simplifies the calculations in the case of transitions to the continuum. The results indicate the possibility of having oscillatory structures in the photodetachment cross-section, which depend on interatomic distance.

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