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Eigenfunctions of continuous spectrum in the problem of the two zero range potentials

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Abstract. The paper deals with the application of the method of eigenfunctions of the S-matrix to the problem of two zero range potentials and continues our study of photodetachment, begun in a previous paper (Devdariani, Dadonova 2018). In the case under consideration the eigenfunctions of specific parity depend on two phases that lead to the explicit expressions for the characteristics of scattering and make it possible to construct the proper sets of wave functions for the problems of scattering and photodetachment. An interesting feature of the problem is that the two phases can coincide, which leads to a resonance in the transmission coefficient.

Keywords: zero range potentials, photodetachment, scattering, wafe function, S-matrix, diatomic molecules.

Introduction

The aim of the present work is to continue the study of the electron photodetachment process in diatomic molecules begun in (Devdariani, Dadonova 2018) modeled by two small radius potentials (ZRP). Another goal is to use the S-matrix eigenfunctions for this problem.

The idea of using small-radius potentials as the model of molecule is not new. For example, in (Lapidus 1970), such a model in a one-dimensional version is used to describe a positive molecular hydrogen ion. In (Devdariani, Dadonova 2015; 2018; Devdariani et al. 2014; 2017), the model is used to describe collisions of hydrogen atoms with a negative hydrogen atomic ion, which is much more realistic than using it to describe H_2^+.

The main difficulty in the description of processes involving states of molecular continua is related to the choice of wave functions of continuous spectrum. As a rule, plane waves are used for these purposes. In contrast, the approach based on the use of the exact wave functions of the model problem was proposed and developed in (Dadonova, Devdariani 2012; 2016).

In this paper, the approach based on the application of the S-matrix eigenfunctions (Demkov, Rudakov 1971) is used to construct the wave functions of the continuous spectrum in the one-dimensional and three-dimensional problem. The force centers are described in the framework of ZRP, so that in terms of physical applications we are talking about the process of photodetachment during the collision $H+H^-$. In this work, atomic units are used.

Basis based on the eigenfunctions of the S-matrix

For simplicity, we consider the scattering problem for a symmetric potential in the one-dimensional case. For each momentum value, two linearly independent functions of the continuous spectrum can be constructed. The behavior of an even function is described by the expressions:

$$\Psi_+ = \sin\left(k\left|x-x_1\right|+\delta_+\right)+\sin\left(k\left|x-x_2\right|+\delta_+\right),$$
$$x_{1.2} = \pm\frac{R}{2}.$$

For a behavior of an odd function we have:

$$\Psi_- = \sin\left(k\left|x-x_1\right|+\delta_-\right)-\sin\left(k\left|x-x_2\right|+\delta_-\right),$$

where

$$\Psi_+\left(-x\right) = \Psi_+\left(x\right) \ and \ \Psi_-\left(-x\right) = -\Psi_-\left(x\right).$$

A remarkable feature of these functions is that they diagonalize the S-matrix for an arbitrary symmetric potential $V\left(-x\right)=V\left(x\right)$ with eigenvalues $\exp\left(2i\delta_\pm\right)$. Of course, the functions allow us to write any function of the continuous spectrum of the problem as a linear combination of functions $\Psi_\pm$. For example, let us express the wave function that describes the scattering of an incident plane wave:

$$\Psi\left(x\to-\infty\right) = e^{ikx}+Re^{-ikx},$$
$$\Psi\left(x\to+\infty\right) = Te^{ikx},$$

where R, T are the reflection and transmission coefficients, respectively. For this case, the following equation is true:

$$\Psi\left(x\right) = \alpha\Psi_+\left(x\right)+\beta\Psi_-\left(x\right).$$

Using the asymptotic form of the functions $\Psi_\pm$ gives us:

$$\alpha = e^{i\delta_+},\ \beta = -e^{i\delta_-},$$
$$T = -ie^{i\left(\delta_++\delta_-\right)}\sin\left(\delta_+-\delta_-\right),$$
$$R = -e^{i\left(\delta_++\delta_-\right)}\cos\left(\delta_+-\delta_-\right).$$

It's important to note the resonant character of the coefficients for the following values:

$$\delta_+-\delta_- = 0,\frac{\pi}{2}.$$

We note that $R=f\left(\pi\right)$, where $f\left(\pi\right)$ is a backscattering amplitude and $T-1=f\left(0\right)$, where $f\left(0\right)$ is a forward scattering amplitude. This will be useful when comparing these expressions to the one-dimensional case with the scattering results in the three-dimensional case. The conservation of the normalization gives the optical theorem for the case under consideration:

$$\left|f\left(0\right)\right|^2+\left|f\left(\pi\right)\right|^2 = -2Ref\left(0\right).$$

The use of eigenfunctions of a certain symmetry is especially convenient when calculating processes associated with dipole transitions involving states of the continuous spectrum. Bremsstrahlung, photodetachment and photorecombination can be mentioned as examples of such processes. Bearing in mind the subsequent application to the processes of photorecombination and photodetachment, we write down the following wave function. The asymptotics of this wave function is a converging wave and an outgoing plane waves along or against the axis. For an outgoing wave we have:

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$$\alpha = e^{-i\delta_+},\ \beta = e^{-i\delta_-},$$

$$\Psi\left(x \to \infty\right) = e^{ikx} + f^*\left(0\right)e^{ikx},$$

$$\Psi\left(x \to -\infty\right) = e^{ikx} + f^*\left(\pi\right)e^{-ikx}.$$

The transition to the amplitudes of converging waves is associated with complex conjugation of the amplitudes of the diverging waves defined above, which corresponds to the general theory of scattering (Landau, Lifshitz 1974).

A zero range potential

Here, for the sake of completeness, we summarize some established results related to the zero potentials. The problem in one-dimension looks as follows. Details of the following formulae can be found in (Demkov, Ostrovskii 1988). We need to solve a Schrodinger equation (in atomic units):

$$-\frac{1}{2}\frac{d\Psi}{dx} = E\Psi$$

with a bounder condition

$$\frac{1}{\Psi}\frac{d\Psi}{dx}\bigg|_{x=0} = -\alpha_0 .$$

In the case of a bound state the solution is

$$\Psi^b\left(x\right) = \sqrt{\alpha_0}exp\left[-\alpha_0\left|x\right|\right],$$

$$E = \frac{\alpha_0^2}{2}.$$

For a continuum state we come to

$$\Psi^c\left(x\right) = \frac{1}{\sqrt{\pi}}sin\left[k\left|x\right| + \delta\right],$$

$$E = \frac{k^2}{2}.$$

Considering that

$$\int_{-\infty}^{+\infty}\Psi\left(k\right)\Psi\left(k'\right)dx = \delta\left(k - k'\right),$$

then

$$ctg\left[\delta\right] = -\frac{\alpha_0}{k}.$$

In the three-dimension case, the problem looks as follows:

$$-\frac{1}{2}\Delta\Psi = E\Psi$$

and a bounder condition

$$\frac{1}{r\Psi}\frac{d}{dr}\left[r\Psi\right]\bigg|_{r\to 0} = -\alpha_0$$

or equivalently

$$\Psi(r \to 0) = \frac{1}{4\pi}\left(\frac{1}{r} - \alpha_0\right)$$

with the solution for the bound state

$$\Psi^b = \frac{1}{\sqrt{4\pi\alpha_0}} \frac{exp\left[-\alpha_0 |\vec{r}|\right]}{|\vec{r}|}$$

for $E = -\alpha_0^2 / 2$ and for a continuum state

$$\Psi^c = \frac{1}{\sqrt{4\pi\alpha_0}} \frac{\sin\left[k|\vec{r}| + \delta\right]}{|\vec{r}|},$$

where

$$ctg\left[\delta\right] = -\frac{\alpha_0}{k}.$$

Two zero range potentials. One-dimensional problem

Now let us suppose that there are two equal zero range potentials placed at $x = \pm R / 2$. Then we seek the solution of the Schrodinger equation

$$\left(-\frac{1}{2}\frac{d^2}{dx^2} - \alpha_0\delta\left(x - \frac{R}{2}\right) - \alpha_0\delta\left(x + \frac{R}{2}\right)\right)\Psi = E\Psi.$$

It is obvious that there are two solutions for the bound states: the symmetric (Ψ_+) and antisymmetric (Ψ_-) one

$$\Psi_\pm^b(x) = C_\pm\left(exp\left[-\alpha_\pm\left|x - \frac{R}{2}\right|\right] \pm exp\left[-\alpha_\pm\left|x + \frac{R}{2}\right|\right]\right),$$

where $C_\pm$ are normalization constants; $\alpha_\pm$ are the solutions of the equations:

$$\alpha_\pm = \alpha_0\left(1 \pm exp\left[-\alpha_\pm R\right]\right),$$

which produce two molecular energy terms:

$$E_\pm = -\frac{\alpha_\pm}{2}$$

with

$$E_+(x = 0) = -2\alpha_0^2 \text{ and } E_-(x = 0) = 0.$$

For the free states the choice of solutions depended on the problem, e.g. scattering, photodetachment and so on. However, having in mind the application to the calculations of dipole moments for bound-continuum transition it is reasonable to choose the functions with defined symmetry $\Psi_\pm$

$$\Psi_\pm^c(x) = sin\left[-k\left|x - \frac{R}{2}\right| + \delta_\pm\right] \pm sin\left[-k\left|x + \frac{R}{2}\right| + \delta_\pm\right]$$

with $E = k^2 / 2$. The phase sifts $\delta_\pm$ can be calculated from

$$ctg\left[\delta_\pm\right] = -\frac{\alpha_0}{k}\frac{1 \pm cos\left[kR\right]}{1 \pm \frac{\alpha_0}{k} sin\left[kR\right]}.$$

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Two zero range potentials. Three-dimensional problem

Again, we construct symmetrical and antisymmetrical functions for the two zero range potentials at $\vec{r}_{01,02} = \pm R/2$:

$$\Psi^b_{\pm}(\vec{r}) = C_{\pm}\left(\frac{\exp\left[-\alpha_{\pm}\left|\vec{r}-\vec{r}_{01}\right|\right]}{\left|\vec{r}-\vec{r}_{01}\right|} \pm \frac{\exp\left[-\alpha_{\pm}\left|\vec{r}-\vec{r}_{02}\right|\right]}{\left|\vec{r}-\vec{r}_{02}\right|}\right),$$

which satisfy the boundary conditions

$$\Psi\left(\vec{r}\to\vec{r}_{01},\vec{r}_{02}\right) = C_{1,2}\left(\frac{1}{r_{01,02}} - \alpha_0\right).$$

$C_{1,2}$ are constants and

$$\alpha_{\pm} = \alpha_0 \pm \frac{exp\left[-\alpha_{\pm}\right]}{R}, E = -\frac{\alpha_{\pm}^2}{2}.$$

The continuum functions for the problem can be taken in the form

$$\Psi^c_{\pm} = \frac{sin\left[-k\left|\vec{r}-\vec{r}_{01}\right|+\delta_{\pm}\right]}{\left|\vec{r}-\vec{r}_{01}\right|} \pm \frac{sin\left[-k\left|\vec{r}-\vec{r}_{02}\right|+\delta_{\pm}\right]}{\left|\vec{r}-\vec{r}_{02}\right|}$$

with

$$ctg\left[\delta_{\pm}\right] = -\frac{\alpha_0}{k}\frac{1\pm\frac{cos\left[kR\right]}{\alpha_o R}}{1\pm\frac{sin\left[kR\right]}{kR}},$$

at $R = R_0 = \frac{1}{\alpha_0}$ the energy term the antisymmetric bound state interests the boundary of the continuum. It's interesting to note that if $R = R_0$ then equations for $ctg\left[\delta_{\pm}\right]$ for one- and three-dimensional cases coincide. Based on the two independent solutions $\Psi^b_{\pm}$ one can construct the wave functions for scattering and for detachment.

Conclusion

The use of the S-matrix eigenfunctions made it possible to construct the exact wave functions at all values of the electron coordinates. Since the constructed functions possess a certain symmetry with respect to the inversion, they are convenient for calculating the dipole moments of the transitions for the states of the continuous spectrum. The latter remark is fully valid for the ZRP-based models of multi atomic molecules (Demkov, Rudakov 1971) as well.

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