Resonance cross-section formula for low-energy elastic scattering

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A simple analytical formula for partial wave cross section describing low-energy elastic scattering in the presence of a shape resonance located near the elastic threshold is proposed. The formula is based on the extension of the regularized method of analytical continuation in the coupling constant (RAC) recently proposed by Horáček and co-workers. The RAC method provides the complex energies of resonances and virtual states requiring as input information a set of real bound state energies of a perturbed system for which standard highly sophisticated numerical codes may be employed. No scattering calculations are needed. These parameters define the low-energy partial wave resonance scattering cross section. Cross sections are calculated for the $2s^2 \varepsilon p\,^2P^0$ state of beryllium and $3s^2 \varepsilon p\,^2P^0$ of magnesium. The results compare well with recently published data.

I. INTRODUCTION

In many areas of physics, chemistry and biology low-energy resonances play important roles; see, for example, Refs. [1,2]. The cross sections and reaction rates in resonance regions change rapidly and may attain large values. Calculation of such resonance cross sections is a very difficult task. Resonances are defined as complex poles of the scattering *S*-matrix located on the unphysical sheet [3]. Determination of the resonance energy and in particular the resonance width is a difficult problem even for small systems [4]. In recent years we have developed a method of calculation of atomic and molecular resonances which is based on the so-called method of analytical continuation in the coupling constant (ACCC) and whose great advantage is that it requires the calculation of a set of real bound-state energies only. The ACCC method is based on the following idea [5,6]: to a Hamiltonian H that represents a system with no bound state but which supports a shape resonance near the threshold, an attractive short-range perturbation V multiplied by a real constant λ is added. At increasing $\lambda \geqslant \lambda_0$ the resonance transforms into a bound state. Bound-state energies $E = -\kappa^2/2$ are then determined for a set of values λ_i and the energies analytically continued back into the complex plane to the point $\lambda = 0$; for detail see Refs. [4–6]. This approach is quite successful and has been applied to the determination of resonance energies and widths of the $^2\Pi_g$ state of N_2^- [7], for the determination of resonance energies and widths for organic molecules: glycine, alanine, valine, and dimer of formic acid [8], and $^2B_{2g}$ shape resonance of ethylene [9]. The method of regularized analytical continuation (RAC) proposed by Horáček, Paidarová, and Čurík [10] uses the same idea but is based on the determination of zeros of the coupling function λ on the unphysical sheet [10]. This method has been applied recently to the determination of the $^2\Pi_g$ state of acetylene [11] and to atomic resonances [12].

These works clearly demonstrate that from the knowledge of the real coupling function $\lambda(\kappa)$ very precise values of resonance parameters may be obtained.

In the present work we take one step further. Instead of concentrating on the determination of resonance parameters we will ask whether other physically important quantities can be obtained from the knowledge of the real function $\lambda(\kappa)$. In the following we will show, in the framework of potential scattering theory, that the Jost function, partial phase shifts, and cross section also can be obtained with a good accuracy based on bound-state type physical parameters provided by the RAC method. Since for the calculation of the coupling function $\lambda(\kappa)$ highly accurate sophisticated numerical codes may be employed, which treat for example the correlation energy very accurately, it is expected that the proposed approach will provide the cross section with a high accuracy.

The resonance energy E_R and width Γ are not directly measurable. Experiments usually provide us with cross sections and the resonance parameters are determined indirectly by fitting some analytical expressions like the Breit-Wigner formula [3]. Formulas of this type work well for narrow resonances far from the threshold. However, for broad resonances ($\Gamma \geqslant E_R$) near the threshold, this approach fails. It is the purpose of this paper to find a model independent analytic expression for the partial wave cross section which describes correctly the low-energy resonance cross sections in terms of the RAC physically relevant quantities. The simplest such formula for *p*-wave scattering can be expressed solely in terms of E_R and Γ. In units of a_0^2 we get

$$\sigma_1(E) = \frac{12\pi E^2}{(E - E_R)^2 + \frac{\Gamma^2}{4}} \; \frac{\sqrt{E_R^2 + \frac{\Gamma^2}{4}} - E_R}{E_R^2 + \frac{\Gamma^2}{4} + 2E\left(\sqrt{E_R^2 + \frac{\Gamma^2}{4}} - E_R\right)}.$$ (1)

This formula contains the known Breit-Wigner resonance term multiplied by E^2 in accordance with the threshold law. The cross-section formula Eq. (1) is quite general and may

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represent a good description of any *p*-wave low-energy shape resonance scattering process. Details and more accurate forms are described in the text.

The proposed approach is applied to the $2s^2 \varepsilon p\, {}^2P^0$ state of beryllium and $3s^2 \varepsilon p\, {}^2P^0$ of magnesium. The obtained cross sections agree well with the recent published data.

It is important to mention that all calculated resonance parameters as well as the cross section have been obtained *ab initio*; no experimental data were used to fit the final results.

II. RAC METHOD

The RAC method [10] represents a very simple method for the calculation of resonance energies and widths. The method works as follows.

(1) An atom or molecule which does not form a stable anion is perturbed by an attractive short-range interaction V multiplied by a real constant λ

$$H_{\text{neutral}} \rightarrow H_{\text{neutral}} + \lambda V \tag{2}$$

and bound-state energies E_i^N of the neutral state are calculated for a set of values $\lambda_i \geqslant \lambda_0$.

(2) The same procedure is carried out for the ionic state

$$H_{\text{ion}} \rightarrow H_{\text{ion}} + \lambda V \tag{3}$$

and bound-state energies E_i^I are calculated for the same values of λ_i.

(3) Both energies are subtracted

$$E_i^I - E_i^N = E_i = -\frac{\kappa_i^2}{2} \tag{4}$$

forming the input data $\{\kappa_i, \lambda_i\}$. The set of data points $\{\kappa_i, \lambda_i\}$ is used to fit the function [10], which is appropriate for *p*-wave scattering:

$$\lambda(\kappa) = \lambda_0 \frac{(\kappa^2 + 2\alpha^2\kappa + \alpha^4 + \beta^2)(1 + \delta^2\kappa)}{\alpha^4 + \beta^2 + \kappa[2\alpha^2 + \delta^2(\alpha^4 + \beta^2)]}. \tag{5}$$

The parameters to be fitted, namely α, β, δ, and λ_0, are found by minimizing the χ^2 functional

$$\chi^2 = \frac{1}{N} \sum_{i=1}^{N} |\lambda(\kappa_i) - \lambda_i|^2. \tag{6}$$

Here N denotes the number of points used and κ_i and λ_i are the input data, $i = 1, \ldots, N$. As soon as a good fit is found and the parameters α, β, δ determined the resonance energy [i.e., the complex zero of the function $\lambda(\kappa)$] is given as

$$E_R = \frac{\beta^2 - \alpha^4}{2} \tag{7}$$

and the width Γ

$$\Gamma = 2\beta\alpha^2. \tag{8}$$

The parameter δ determines the energy of a virtual state $E_V = -\frac{1}{2\delta^4}$. The virtual state represents here a cumulative effect of other resonances and virtual states not explicitly included in the expression.

Higher RAC approximations can be constructed in a similar manner [10]. For example, to incorporate two resonances

in the fit we can write

$$\lambda^{[4/2]}(\kappa) = \lambda_0 \frac{(\kappa^2 + \alpha^2\kappa + \alpha^4 + \beta^2)(\kappa^2 + \gamma^2\kappa + \gamma^4 + \delta^2)}{(\alpha^4 + \beta^2)(\gamma^4 + \delta^2)(1 + \mu^2\kappa)(1 + \mu^2\varepsilon^2\kappa)}, \tag{9}$$

where

$$\mu^2 = \frac{1}{1 + \varepsilon^2} \left(\frac{\alpha^2}{\alpha^4 + \beta^2} + \frac{\gamma^2}{\gamma^4 + \delta^2} \right) \tag{10}$$

and fit the data. All the RAC coupling functions $\lambda(\kappa)$ take the form

$$\lambda^{[N,M]}(\kappa) = \lambda_0 h(\kappa), \tag{11}$$

where $h(0) = 1$. Our experience, however, shows that the [3/1] approximation, Eq. (5), usually represents the best compromise between accuracy and stability of the continuation process. Contrary to the parameters α, β, and δ, which have simple physical interpretation, the physical meaning of the parameter λ_0 is less obvious. For a given perturbation potential $V(r)$, λ_0 gives the strength of the perturbation which converts the resonance into the zero energy bound state. λ_0 depends on the strength of the perturbation V and, of course, on the atomic potential.

III. COUPLING CONSTANT FUNCTION FOR SEPARABLE INTERACTION

It is very difficult to obtain closed analytical expressions for the coupling function $\lambda(\kappa)$ even for the simplest realistic local potentials and $l = 0$ scattering. Many shape resonances in atomic and molecular physics are, however, generated by the centrifugal force ($l > 0$). To the best of our knowledge no analytical expressions of $\lambda(\kappa)$ are known for local realistic potentials and for partial waves with $l > 0$. In this work we will restrict ourselves to the *p*-wave problem $l = 1$ as a representative of states with nonzero angular momentum. Generalization to higher angular momenta is in principle straightforward.

For separable potentials, however, the calculation of $\lambda(\kappa)$ is quite simple [13]. Separable potentials have been used in nuclear and few-body physics with great success (see, for example, Refs. [14,15]). Very often separable approximations are used in atomic and molecular physics for the representation of nonlocal forces, for example, the exchange interaction [16–19]. The separable potentials can approximate any local potential and it is known that they represent very good approximation to local forces in the limit of low energy. The separable interactions are most easily studied in the momentum representation. The Lippmann-Schwinger equation for the T-matrix in momentum representation reads [14]

$$\begin{aligned} T_l(k, k', z) = V_l(k, k') \\ + \frac{1}{2\pi^2} \int_0^\infty dq\, q^2 V_l(k, q) \frac{1}{z - q^2} T_l(q, k', z) \end{aligned} \tag{12}$$

and for one term separable interaction

$$V_l(k, k') = -g_l(k)\tau g_l(k'), \tag{13}$$

where τ is the potential strength, can easily be solved [14]. For example, for negative energies $E = -\kappa^2$ we have

$$\langle k | T(-\kappa^2) | k' \rangle = \frac{\tau g_l(k) g_l(k')}{1 - \frac{2}{\pi}\tau \int_0^\infty \frac{p^2 g_l(p)^2}{p^2 + \kappa^2} dp} \qquad (14)$$

and for the positive energies the phase shifts in the l-partial wave are given as

$$\tan \delta_l(k) = -\frac{\tau k g_l^2(k)}{1 - \tau \frac{2}{\pi} \mathrm{P} \int \frac{p^2 g_l(p)^2 dp}{p^2 - k^2}}, \qquad (15)$$

where P means the principal value integration. The T-matrix has a pole at the bound-state energy, i.e., we can define a coupling function $\mu(\kappa)$ by the following equation:

$$1 - \frac{2}{\pi}\mu(\kappa) \int_0^\infty \frac{p^2 g_l(p)^2}{p^2 + \kappa^2} dp = 0, \qquad (16)$$

i.e.,

$$\mu^{-1}(\kappa) = \frac{2}{\pi} \int_0^\infty \frac{p^2 g_l(p)^2}{p^2 + \kappa^2} dp. \qquad (17)$$

The coupling functions $\mu(\kappa)$ for separable potentials were studied in detail by Kok and van Haeringen [13] for $l = 0$ angular momentum. In the context of our problem it is necessary to consider higher partial waves. It is well known that the potentials $g_l(k)$ must satisfy the threshold law [3]

$$g_l(k) \approx k^l, \quad k \to 0. \qquad (18)$$

A typical potential commonly used in nuclear physics is [20]

$$g_l(p) = \frac{p^l}{(p^2 + a^2)^{\frac{l+n}{2}}}, \qquad (19)$$

where n is a positive integer. More complicated potentials can be easily constructed. For example,

$$g_l(p) = \frac{p^l}{\sqrt{(p^2 + a^2)(p^2 + b^2)}} \qquad (20)$$

was proposed for the s-wave case in [21] in order to study the relation between the short- and long-range properties of the

interaction. For the potential Eq. (19) with $n = 1$ and $l = 1$,

$$g_1(p) = \frac{p}{p^2 + a^2}, \qquad (21)$$

we get

$$\mu_1(\kappa) = 2 \frac{(a + \kappa)^2}{a + 2\kappa}, \qquad (22)$$

for $n = 2$,

$$g_1(p) = \frac{p}{(p^2 + a^2)^{3/2}}, \qquad (23)$$

$$\mu_1(\kappa) = 8a \frac{(a + \kappa)^3}{a + 3\kappa}, \qquad (24)$$

and, for $n = 3$,

$$g_1(p) = \frac{p}{(p^2 + a^2)^2}, \qquad (25)$$

$$\mu_1(\kappa) = 16a^3 \frac{(a + \kappa)^4}{a^2 + 4a\kappa + \kappa^2}, \qquad (26)$$

etc. The potential Eq. (20) for $l = 1$ gives the function $\mu_1(\kappa)$ in the form

$$\mu_1(\kappa) = (a + b) \frac{(a + \kappa)(b + \kappa)}{ab + \kappa(a + b)}. \qquad (27)$$

More complicated expressions for the function $\mu(\kappa)$ can be obtained for sums of separable terms. For example, for two separable terms

$$V = -|g_\alpha\rangle \mu_\alpha \langle g_\alpha| - |g_\beta\rangle \mu_\beta \langle g_\beta|, \qquad (28)$$

with

$$g_\alpha(p) = \frac{p}{p^2 + \alpha^2}, \quad g_\beta(p) = \frac{p}{p^2 + \beta^2}, \qquad (29)$$

we get

$$\mu_\alpha(\kappa) = \frac{4(\alpha + \beta)^2 (\alpha + \kappa)^2 [\mu_\beta \pi (\beta + 2\kappa) - 4(\beta + \kappa)^2]}{\pi [\mu_\beta \pi (\alpha - \beta)^2 (\alpha\beta + 2\alpha\kappa + 2\beta\kappa) - 4(\alpha + \beta)^2 (\beta + \kappa)^2 (\alpha + 2\kappa)]}. \qquad (30)$$

At this point it is important to mention that all the coupling functions obtained for the above-mentioned potentials (and many others not shown here) have exactly the same analytical forms (ratios of two polynomials in κ) as the λ functions of the RAC method used to describe scattering on local interactions. This similarity suggests that a separable approximation may be an excellent tool to describe the low-energy scattering even for more complicated forces (local or nonlocal).

IV. JOST FUNCTION AND CROSS SECTION

The Hilbert-Schmidt (HS) eigenvalue problem is defined as [3,4]

$$\left\{ H_0 + \frac{V}{\eta_i(\kappa)} \right\} |\psi_i\rangle = -\frac{\kappa^2}{2} |\psi_i\rangle \qquad (31)$$

or using the bound-state Green function $G_0(\kappa)$ as

$$G_0(\kappa) V |\psi_i\rangle = \eta_i(\kappa) |\psi_i\rangle. \qquad (32)$$

The HS eigenvalues and eigenfunctions (also called Sturmians) are of great physical significance. For example, the Jost function is given in terms of HS eigenvalues as [3,4]

$$f(k) = \Pi_i (1 - \eta_i(k)). \qquad (33)$$

Let us assume that the resonance is described by a separable potential of strength τ

$$V = -|g\rangle \tau \langle g|. \qquad (34)$$

The HS eigenvalue $\eta(\kappa)$ follows from

$$G_0(\kappa) |g\rangle \tau \langle g | \phi \rangle = \eta(\kappa) |\phi\rangle, \qquad (35)$$

where $G_0(\kappa)$ is the free particle Green function and the bound-state energy $E = -\frac{\kappa^2}{2}$. Let us formulate the one term separable RAC problem as follows:

$$G_0(\kappa)|g\rangle[\tau + \lambda(\kappa)]\langle g|\psi\rangle = |\psi\rangle. \tag{36}$$

Comparing Eqs. (35) and (36) we find that

$$\tau + \lambda(\kappa) = \frac{\tau}{\eta(\kappa)}, \tag{37}$$

i.e.,

$$\eta(\kappa) = \frac{\tau}{\tau + \lambda(\kappa)}. \tag{38}$$

In the case of separable potential with one term there exists only one eigenvalue. This allows us to write the Jost function in terms of $\eta(\kappa)$ as ($k = i\kappa$)

$$f(k) = 1 - \eta(-ik). \tag{39}$$

In terms of $\lambda(\kappa)$

$$f(k) = \frac{\lambda(-ik)}{\tau + \lambda(-ik)} \tag{40}$$

or in terms of the $h(\kappa)$ functions, Eq. (11),

$$f(k) = \frac{\xi h(-ik)}{1 + \xi h(-ik)}, \tag{41}$$

where $\xi = \frac{\lambda_0}{\tau}$ represents the strength of the perturbation relative to the strengths of the potential generating the resonance.

This is a very important relation putting in connecting the Jost function $f(k)$ with the coupling function $\lambda(\kappa)$ evaluated at complex $\kappa = -ik$. From the relation

$$f(k) = |f(k)|e^{-\delta(k)} \tag{42}$$

we can determine the phase shifts in terms of $\lambda(\kappa) = \lambda_0 h(\kappa)$

$$\tan \delta(k) = \frac{\text{Im}\{h(-ik)\}}{\xi \text{Re}\{h(-ik)\} + |h(-ik)|^2}. \tag{43}$$

Using $\lambda(\kappa)$ in the form Eq. (5) we get

$$\tan \delta(k) = \frac{2\alpha^2 k^3[1 + \delta^2(\omega\delta^2 + 2\alpha^2)]}{D(k) + \xi F(k)}, \tag{44}$$

where

$$D(k) = \omega^2 + k^2[4\alpha^4 + \omega^2\delta^4 + 2\alpha^2\delta^2\omega - \omega] - k^4\delta^2[2\alpha^2 + \omega\delta^2], \tag{45}$$

$$F(k) = \omega^2 + k^2[\omega^2\delta^4 + 4\alpha^4 - 2\omega] + k^4[1 + 4\alpha^4\delta^4 - 2\omega\delta^4] + k^6\delta^4, \tag{46}$$

$$\omega = \alpha^4 + \beta^2. \tag{47}$$

At the threshold $k \to 0$

$$\tan \delta(k) \approx \frac{2\alpha^2 k^3[1 + \delta^2(\omega\delta^2 + 2\alpha^2)]}{\omega^2(1 + \xi)} \tag{48}$$

in accordance with the threshold law for short-range potentials for $l = 1$

$$\delta(k) \approx k^3. \tag{49}$$

In the case of resonances close to the threshold ξ is very small and can be neglected in Eq. (44), yielding

$$\tan \delta_1(k) = \frac{2\alpha^2 k^3[1 + \delta^2(\omega\delta^2 + 2\alpha^2)]}{\omega^2 + k^2[4\alpha^4 + \omega^2\delta^4 + 2\alpha^2\delta^2\omega - \omega] - k^4\delta^2[2\alpha^2 + \omega\delta^2]}. \tag{50}$$

This formula contains only "physical" parameters α, β, and δ. These parameters define the location of the S-matrix poles on the unphysical sheet (the pair of resonance poles $k_r = \pm\beta - i\alpha^2$ and the virtual state pole $k_v = -\frac{i}{\delta^2}$) and determine the resonance energy $E_R = \frac{\beta^2 - \alpha^4}{2}$, the width $\Gamma = 2\beta\alpha^2$, and the energy of the virtual state $E_v = -\frac{1}{2\delta^4}$. Once the phase shifts are known [Eqs. (44) or (50)], based on the resonance parameters provided by the RAC method, the partial wave cross section

$$\sigma_l(k) = \frac{4\pi}{k^2}(2l + 1)\sin^2\delta_l(k) \tag{51}$$

can be calculated.

V. MODEL EXAMPLE

As a test we apply the proposed approach to potential scattering. We choose the potential in the Gauss form

$$V(r) = -V_0 e^{-qr^2}, \tag{52}$$

with the values $V_0 = -0.52$ a.u. and $q = 0.10$ a.u. This potential has a p-wave resonance state with the energy $E_R = 0.01078378$ a.u. and width $\Gamma = 0.01188189$ a.u. In electron

volts this corresponds to $E_R = 0.293$ eV and $\Gamma = 0.323$ eV. These parameters are very close to the recommended value of the $2s^2\varepsilon p\,^2P^0$ state of beryllium [22] ($E_R = 0.323$ eV and $\Gamma = 0.296$ eV). Now we can proceed in two ways.

(1) To calculate the function $\lambda(\kappa)$ for some suitably chosen perturbation potential and to get the resonance parameters as well as the cross section.

(2) To fit the RAC cross-section formulas Eq. (1), Eq. (44), or Eq. (50) to calculated or measured cross sections (phase shifts) in order to determine the resonance parameters.

Let us start with the first possibility. For a given Hamiltonian a suitable perturbation has to be chosen, a set of bound-state energies calculated, and the function $\lambda(\kappa)$ fitted. In the present calculation we used the function $\lambda(\kappa)$ in its simplest form, Eq. (5). Test bound-state data were calculated in the range (0.1–1.86) eV using the Gauss potential Eq. (52) with various values of the parameter q. As expected the results obtained in this approximation depend on the choice of the perturbation potential (here parameter q). This dependence decreases at higher approximations. The best fit was obtained with $q = 0.085$ yielding the resonance energy $E_R = 0.301$ eV and the width $\Gamma = 0.317$ eV in good agreement with the exact value. The cross section obtained from this calculation
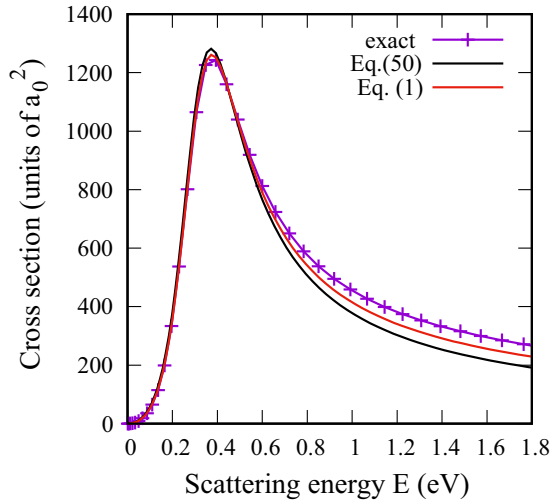
FIG. 1. Model cross section calculated from the RAC parameters. Black line: three-parameter formula Eq. (50); the red line: the two-parameter formula Eq. (1). The line with crosses—the exact cross section.
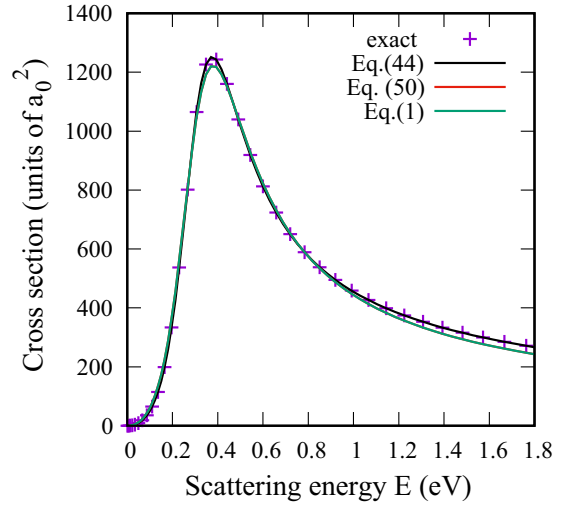

FIG. 2. Fit to the model cross section by the RAC formula. Black line: fit with formula Eq. (44); red line: fit using the three parameter formula Eq. (50); green line: the two-parameter fit by Eq. (1). The exact cross section is shown as the line with crosses.

is shown in Fig. 1. The black line shows the cross section obtained with Eq. (50) and the red curve that with the two-parameter formula Eq. (1). The exact cross section is shown as the line with crosses. In the resonance region all cross sections nearly coincide. At higher energies they start to deviate as expected. The cross section is asymmetric extended to higher energies.

The formula Eq. (44) contains four parameters: parameters α and β which determine the resonance energy, the parameter δ which corresponds to a virtual state, and ξ which represents the background. It is seen in the present case that the last two parameters play a negligible role. This is demonstrated in Fig. 1 by the blue line which corresponds to the choices $\delta = 0$ and $\xi = 0$. The two parameter cross section deviates significantly from the four parameter one only at energies above 2 eV. By neglecting the parameter δ in Eq. (44) we can express the cross section in terms of resonance energy E_R and width Γ. In this way Eq. (1) has been obtained.

Let us discuss the second point—the inverse route. The goal is to test how accurate the obtained resonance parameters are when the cross section is known. By fitting the three parameter formula Eq. (50), i.e., using $\tan \delta_1$ in the form of Eq. (50) to 10 data points in the energy range (0.0–1.86) eV, we get $E_R = 0.292$ eV and width $\Gamma = 0.351$ eV. The obtained resonance energy differs by 1 meV from the exact one and the width by 26 meV from the exact value. More accurate values are obtained keeping all four parameters in the RAC formula, i.e., using Eqs. (44) for the phase shift. At this level of approximation we get $E_R = 0.294$ eV and $\Gamma = 0.324$ eV in excellent agreement with the exact data. The results both for the energy as well as for the width differ by less than 1 meV from the exact values. It is expected that higher RAC approximation will provide even better agreement with the exact values. These results demonstrate the power of the RAC method. Very precise resonance energies and widths may be obtained using the RAC cross-section formulas provided good cross-section data are available. The road from the cross

section to the resonance parameters is straightforward. The calculated cross sections are shown in Fig. 2. The black line denotes the four-parameter RAC cross section Eq. (44), the red line the three parameter cross section, Eq. (50), the green line the two-parameter cross section Eq. (1), and crosses the exact values. This approach provides us also with the phase shifts; this means that the process of phase shift analysis is simultaneously carried out. This allows us to test the RAC approach on another model free method which derives the resonance parameters from known phase shifts proposed by Krasnopolsky *et al.* [23] based on the use of Padé approximation (PA). This method is based on the representation of the partial wave S-matrix in the form [3]

$$S_l(k) = \frac{k^{2l+1} \cot \delta_l(k) + ik^{2l+1}}{k^{2l+1} \cot \delta_l(k) - ik^{2l+1}} \tag{53}$$

and on the fact that the function $k^{2l+1} \cot \delta_l(k)$ is, for short-range interaction, an analytical function of k^2. In this method the function $\gamma(k) = k^{2l+1} \cot \delta_l(k)$ is represented in the form of Padé approximation

$$\gamma(k) \approx \frac{P_N(k^2)}{Q_M(k^2)}, \tag{54}$$

where $P_N(k^2)$ and $Q_M(k^2)$ are polynomials in k^2. The resonances are then obtained by solving the polynomial equation

$$P_N(k^2) - ik^{2l+1} Q_M(k^2) = 0. \tag{55}$$

The calculated resonance parameters obtained in this way are collected in Table I. The results are in excellent agreement with the exact results as well as the RAC results. These results show that at least, for simple local interactions of Gauss type, the RAC method works excellently. The cross sections as well as the resonance parameters are obtained with a high accuracy. To check the performance of the RAC approach in realistic situations we apply it in the next section to real atomic resonances.

TABLE I. Calculation of the resonance energy and width from phase shifts generated by the Gauss potential, Eq. (52), by means of the Padé approach [23]. Left column—order of the Padé approximation.

Padé order	Resonance energy (eV)	Width (eV)
2/1	0.2848	0.3070
2/2	0.2958	0.3240
3/1	0.2934	0.3233
3/2	0.2935	0.3233
3/3	0.2935	0.3233
4/1	0.2935	0.3233
4/2	0.2935	0.3233
4/3	0.2935	0.3233
Exact	0.2934	0.3233

VI. APPLICATION TO $2s^2\varepsilon p\,^2P^0$ STATE OF BERYLLIUM

In this section we apply the formulas (1), (44), and (50) to atoms which form low-energy shape resonances. As it is well known, the direct scattering calculation at low energies is a very difficult problem. As a prototype we select the beryllium atom. The $2s^2\varepsilon p\,^2P^0$ state of beryllium has been studied by many authors: see, for example, Refs. [24–34]. The published data differ greatly in the resonance energy as well as in the width: $0.10\,\text{eV} < E_R < 1.20\,\text{eV}$ and $0.14\,\text{eV} < \Gamma < 2.60\,\text{eV}$; see Table III in [34]. The resonance energy and width recommended by Buckmann and Clark [22] is $E_R = 0.323\,\text{eV}$ and $\Gamma = 0.296\,\text{eV}$. Recently, Čurík *et al.* [12] have applied the RAC method to this state using the Gauss potential as the perturbing potential. At the CCSD-T level they have obtained the resonance energy $E_R = 0.323\,\text{eV}$ and $\Gamma = 0.316\,\text{eV}$ in excellent agreement with the recommended value [22]. More accurate full CI (FCI) data yielded the resonance energy $E_R = 0.282\,\text{eV}$ and $\Gamma = 0.316\,\text{eV}$. As already mentioned, the RAC parameters allow us to calculate the cross section. The CCSD-T cross section given by Eqs. (50) and (51) and the RAC parameters α, β, δ obtained in [12] are shown in Fig. 3 as the solid black line.

The cross-section peaks at the energy 0.382 eV with the full width at half maximum (FWHM) = 0.387 eV. The FWHM is broader than the resonance width by about 70 meV and the cross-section maximum is shifted from the resonance energy to higher energies by 64 meV due to near presence of the threshold. Sometimes the resonance energy is approximated by the value at which the phase shift equals $\delta(k) = \frac{\pi}{2}$. Using the phase shifts in the form Eq. (50) with the obtained RAC parameters we then arrive at the resonance energy $E_R = 0.432\,\text{eV}$ far away from the recommended energy.

To the best of our knowledge no experimental cross-section data have been published and hence no direct comparison of the theory with the experiment is currently possible. There are, however, calculations to which the present theory can be compared. For example, the e-Be scattering and electronic excitation was recently studied by Zatsarinny *et al.* [35]. They calculated partial wave phase shifts by using the converged coupled channel approach (CCC). The resonance energy of the $2s^2\varepsilon p\,^2P^0$ state is estimated to be in a broad energy range 0.269–0.354 eV and the width 0.341–0.461 eV, depending on
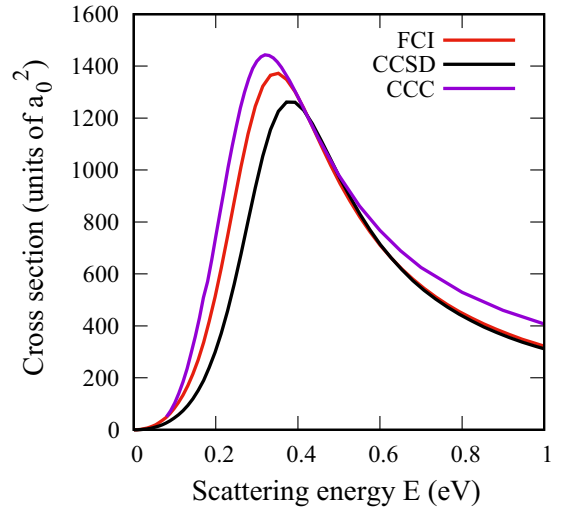

FIG. 3. P-wave cross sections for the $2s^2\varepsilon p\,^2P^0$ state of beryllium. The black line: the three-parameter RAC cross section calculated at the CCSD-T level; the red line: the three-parameter RAC cross section calculated at the full CI level; the violet line: the CCC calculation [35].

how the resonance parameters are obtained. From the maximum of the cross section they estimate the resonance energy $E_R = 0.320\,\text{eV}$ at the CCC level and $E_R = 0.354\,\text{eV}$ at the BSR level. The width $\Gamma = 0.461\,\text{eV}$ or 0.434 eV, respectively. From the phase shift analysis we obtain $E_R = 0.284\,\text{eV}$ at the CCC level and $E_R = 0.269\,\text{eV}$ at the BSR level and $\Gamma = 0.372\,\text{eV}$ and 0.431 eV respectively. The published data allow us to test the present approach. We have used their phase shifts to estimate the resonance energy and the width by fitting the RAC formulas.

The fits were performed again at four levels of approximation. (1) In Eq. (44) the parameters δ and ξ were set to zero and only a two parameter fit was performed. Levels (2) and (3) were two three-parameter fits. In the first, the fitting parameters were α, β, and ξ, whereas, in the second, we varied the parameters α, β, and δ. (4) The last fit was performed with all four parameters α, β, δ, and ξ. The results are shown in Table II. At all four levels of approximation we can estimate the resonance energy to be $\approx 0.24\,\text{eV}$ and width ≈ 0.30–$0.31\,\text{eV}$.

When the phase shifts are available we can calculate to resonance parameters by the PA approach [23]. The CCC

TABLE II. Calculation of the resonance energy and width of the $2s^2\varepsilon p\,^2P^0$ state of beryllium using the RAC formula for cross section based on the data by Zatsarinny *et al.* [35]. (1) Two-parameter fit; only the resonance parameters α and β are taken into account. (2) Three-parameter fit; the parameter ξ is added. (3) Three-parameter fit α, β, and δ. (4) All four parameters are included in the fit.

Parameters used	Resonance energy (eV)	Width (eV)
α and β	0.243	0.298
α, β, and ξ	0.244	0.310
α, β, and δ	0.244	0.310
α, β, δ, and ξ	0.243	0.298

TABLE III. Calculation of the resonance energy and width of the $2s^2\varepsilon p\,^2P^0$ state of beryllium from phase shifts [35] by means of the Padé approach [23]. Left column—order of the Padé approximation.

Padé order	Resonance energy (eV)	Width (eV)
2/1	0.2474	0.2955
2/2	0.2487	0.2906
3/1	0.2498	0.2882
3/2	0.2487	0.2934
3/3	0.2485	0.2984
4/1	0.2486	0.2964
4/2	0.2487	0.2936
4/3	0.2486	0.2940
4/4	0.2487	0.2935

resonance parameters obtained in this way are collected in Table III. The resonance is very stable at changing the order of Padé approximation and is remarkably close to the RAC results. Data in Tables I and II confirm that the resonance parameters obtained by the present RAC approach compare well with those obtained by the use of the Padé approximation—the difference is of the order of a few millielectronvolts.

The RAC predicted cross sections are shown in Fig. 3. The CCC cross section is depicted by the violet line and the CCSD-T cross section by the black line. In the case of beryllium also full CI calculation is possible (details of the bound state calculations are given in Ref. [12]). The resonance energy is lower by 40 meV from the CCSD-T result, while the resonance width does not change [12]. This is probably the most accurate calculation available nowadays. The cross section obtained at the FCI level is shown in Fig. 3 by the red line. The FCI cross-section peaks at $E = 359$ meV and is broader with FWHM = 459 meV than the CCSD-T cross section. Both the CCC and FCI cross sections are very close to each other. The resonance energy calculated at the FCI level decreased by 40 meV from the CCSD result.

VII. APPLICATION TO THE $3s^2\varepsilon p\,^2P^0$ STATE OF MAGNESIUM

In the case of the $3s^2\varepsilon p\,^2P^0$ state of magnesium the resonance is even closer to the threshold than that of beryllium. The resonance parameters recommended by Buckmann *et al.* [22] are $E_R = 0.15 \pm 0.03$ eV and $\Gamma \approx 0.16 \pm 0.03$ eV. Contrary to the previous case of beryllium, these data are based on measurement of Burrow *et al.* [25]. No cross-section data are, however, provided in [25]. Our RAC calculations at the CCSD-T level [12] yielded the resonance energy $E_R \approx 0.19$ eV and the width $\Gamma = 0.16$ eV. The cross RAC section calculated with three parameters (α, β, δ) is shown in Fig. 4 as the blue line. The cross section attains its maximum at $E = 0.221$ eV with the FWHM = 0.197 eV. In analogy with the Be case we can expect that a full CI calculation would lower the resonance energy by ≈ 40 meV, giving $E_R \approx 0.15$ eV in excellent agreement with the experimental result. This problem has been studied by Bartschat *et al.* [36]. Using their phase shifts we can apply the RAC formulas to calculate the
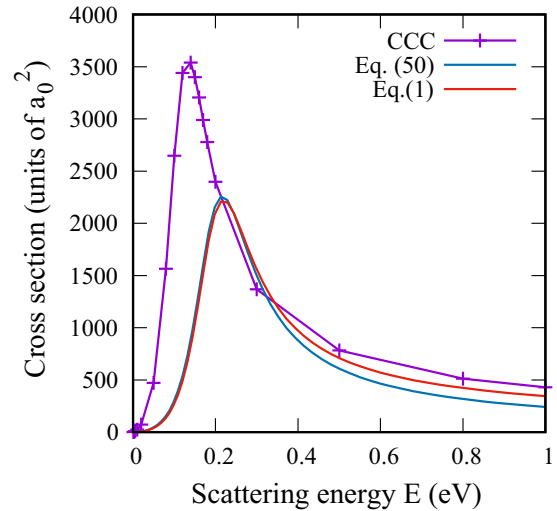

FIG. 4. P-wave cross sections for the $3s^2\varepsilon p\,^2P^0$ state of magnesium. The blue line: three-parameter RAC cross section; the red line: two-parameter cross section both calculated at the CCSD-T level; the line with crosses: the CCC calculation [36].

resonance parameters. The results are collected in Table IV. The resonance energy $E_R \approx 0.1$ eV seems to be too low as well as the width.

A comparison with the Padé method [23] gets similar result; see Table V. Both calculations indicate that the resonance energy 0.1 eV as well as the width resulting from the CCC calculation are too low in energy.

VIII. LIMITATIONS OF RAC METHOD

The RAC approach presented in this work is based on the assumption that all involved forces are of short range. In electron atom or electron molecule scattering, however, the long-range polarization force $-\frac{\alpha}{2r^4}$ is always present. Taking account of this long-range force greatly complicates the present approach and we postpone the detail study of this problem to our future work. Nevertheless, the agreement of the RAC results with the published data indicates that the influence of the polarization force on the resonance energy and width is not essential, even though the Be and Mg atoms have large polarizabilities.

TABLE IV. Calculation of resonance energy and width for the $3s^2\varepsilon p\,^2P^0$ state of magnesium using RAC formulas for cross section based on the data by Bartschat *et al.* [36]. (1) Two-parameter fit; only the resonance parameters α and β are taken into account. (2) Three-parameter fit; the parameter ξ is added. (3) Three-parameter fit with α, β, and δ. (4) All four parameters are included in the fit. This calculation yields the resonance energy $E_R \approx 0.10$ eV and $\Gamma \approx 0.12$ eV.

Parameters used	Resonance energy (eV)	Width (eV)
α and β	0.104	0.115
α, β, and ξ	0.104	0.118
α, β, and δ	0.104	0.118
α, β, δ, and ξ	0.105	0.122

TABLE V. Calculation of the resonance energy and width of the $3s^2 \varepsilon p \, ^2P^0$ state of magnesium from phase shifts [36] by means of the Padé approach [23]. Left column—order of the Padé approximation.

Padé order	Resonance energy (eV)	Width (eV)
2/1	0.0855	0.1010
2/2	0.0845	0.1197
3/1	0.0855	0.0955
3/2	0.1103	0.1235
3/3	0.1103	0.1235
4/1	0.1099	0.1219
4/2	0.1068	0.1179
4/3	0.1070	0.1180
4/4	0.1070	0.1180
5/1	0.1061	0.1201
5/2	0.1062	0.1188
5/3	0.1062	0.1188
5/4	0.1062	0.1188
5/5	0.1062	0.1188

The second limitation of the RAC is related to the fact that results are obtained in one partial wave only, whereas experiments provide us usually with the total cross section. The *s*-wave low-energy contribution to the total scattering cross section is usually small in the *p*-wave resonance energy region and probably can be approximated by simple expressions.

IX. CONCLUSIONS

A cross-section formula that accurately describes partial wave low-energy elastic scattering suitable for systems dominated by a shape resonance located close to the elastic threshold was proposed based on very accurate bound-state energy data. This formula establishes one to one relation between the cross section and the resonance parameters, thus making the resonance energy and resonance width directly obtainable. The cross-section formula can be used in two ways. Once the RAC resonance parameters are known, from the bound-state data of the perturbed system, the cross section can be calculated. On the other hand, if the experimental cross section is given, the resonance parameters as well as the phase shifts can be inferred.

Based on the RAC calculations the low-energy *p*-wave cross sections for the scattering of electrons with beryllium and magnesium atoms were proposed. Since to the best of our knowledge there are no direct experimental measurements of these cross sections, we compared our data with the CCC calculations by Zatsarinny *et al.* [35] and Bartschatt [36]. The comparison is shown in Figs. 3 and 4.

The cross sections discussed here are quite narrow but present day experimental techniques with electron beams with meV resolution may be capable of confirming our predictions.

[1] B. Boudaiffa, P. Cloutier, D. J. Hunting, M. A. Huels, and L. Sanche, Science **287**, 1658 (2000).

[2] E. Alizadeh, T. M. Orlando, and L. sanche, Annu. Rev. Phys. Chem. **66**, 379 (2015).

[3] R. G. Newton, *Scattering Theory of Waves and Particles* (McGraw-Hill, New York, 1966), Sec. 17.2.

[4] V. I. Kukulin, V. M. Krasnopolsky, and J. Horáček, *Theory of Resonances: Principles and Applications* (Kluwer Academic Publishers, Dordrecht/Boston/London, 1988).

[5] V. I. Kukulin and V. M. Krasnopolsky, J. Phys. A: Math. Gen. **10**, L33 (1977).

[6] V. M. Krasnopolsky and V. I. Kukulin, Phys. Lett. **69A**, 251 (1978).

[7] J. Horáček, P. Mach, and J. Urban, Phys. Rev. A **82**, 032713 (2010).

[8] P. Papp, Š. Matejčik, P. Mach, J. Urban, I. Paidarová, and J. Horáček, Chem. Phys. **418**, 8 (2013).

[9] J. Horáček, I. Paidarová, and R. Čurik, J. Phys. Chem. **118**, 6536 (2014).

[10] J. Horáček, I. Paidarová, and R. Čurík, J. Chem. Phys. **143**, 184102 (2015).

[11] R. Čurik, I. Paidarová, and J. Horáček, Eur. Phys. J. D **70**, 146 (2016).

[12] R. Čurík, I. Paidarová, and J. Horáček, Phys. Rev. A **97**, 052704 (2018).

[13] L. P. Kok and H. van Haeringen, Ann. Phys. (NY) **131**, 426 (1981).

[14] G. E. Brown and A. D. Jackosn, *The Nucleon-Nucleon Interaction* (North-Holland, Amsterdam, 1976).

[15] N. V. Shevchenko and J. Haidenbauer, Phys. Rev. C **92**, 044001 (2015).

[16] T. N. Rescigno and A. E. Orel, Phys. Rev. A **23**, 1134 (1981).

[17] T. N. Rescigno and A. E. Orel, Phys. Rev. A **24**, 1267 (1981).

[18] H-D. Meyer, J. Phys. B: At. Mol. Phys. **21**, 3777 (1988).

[19] W. Domcke, M. Berman, C. Mündel, and H.-D. Meyer, Phys. Rev. A **33**, 222 (1986).

[20] T. R. Mongan, Phys. Rev. **175**, 1260 (1968).

[21] W. van Dijk, M. W. Kermode, and S. A. Moszkowski, J. Phys. A: Math. Gen. **31**, 9571 (1998).

[22] S. J. Buckman and C. W. Clark, Rev. Mod. Phys. **66**, 539 (1994).

[23] V. M. Krasnopolsky, V. I. Kukulin, and J. Horáček, Czech. J. Phys. B **35**, 805 (1985).

[24] J. Hunt and B. L. Moiseiwitsch, J. Phys. B: At. Mol. Phys. **3**, 892 (1970).

[25] P. D. Burrow and J. Comer, J. Phys. B: At. Mol. Phys. **8**, L92 (1975).

[26] P. D. Burrow, J. A. Michejda, and J. Comer, J. Phys. B: At. Mol. Phys. **9**, 3225 (1976).

[27] C. W. McCurdy, T. N. Rescigno, E. R. Davidson, and J. G. Lauderdale, J. Chem. Phys. **73**, 3268 (1980).

[28] J. F. McNutt and C. W. McCurdy, Phys. Rev. A **27**, 132 (1983).

[29] P. Krylstedt, M. Rittby, N. Elander, and E. Brändas, J. Phys. B: At. Mol. Phys. **20**, 1295 (1987).

[30] L. Kim and Ch. H. Greene, J. Phys. B: At., Mol., Opt. Phys. **22**, L175 (1989).

[31] P. Krylstedt, N. Elander, and E. Brändas, J. Phys. B: At., Mol., Opt. Phys. **22**, 1623 (1989).

[32] J-J. Hsu and K. T. Chung, Phys. Rev. A **52**, R898 (1995).

[33] J. P. Sullivan, P. D. Burrow, D. S. Newman, K. Bartschat, J. A. Michejda, R. Panajotovic, M. Moghbelalhossein, R. P. McEachran, and S. J. Buckman, New J. Phys. **5**, 158 (2003).

[34] T. Tsednee, L. Liang, and D. L. Yeager, Phys. Rev. A **91**, 022506 (2015).

[35] O. Zatsarinny, K. Bartschat, D. V. Fursa, and I. Bray, J. Phys. B: At. Mol. Phys. **49**, 235701 (2016).

[36] K. Bartschat, O. Zatsarinny, I. Bray, D. V. Fursa, and A. T. Stelbovics, J. Phys. B: At. Mol. Phys. **37**, 2617 (2004).