Shape resonances of Be$^-$ and Mg$^-$ investigated with method of analytic continuation

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The regularized method of analytic continuation is used to study the low-energy negative ion states of beryllium (configuration $2s^2\varepsilon p^2P$) and magnesium (configuration $3s^2\varepsilon p^2P$) atoms. The method applies an additional perturbation potential and it requires only routine bound-state multi-electron quantum calculations. Such computations are accessible by most of the free or commercial quantum chemistry software available for atoms and molecules. The perturbation potential is implemented as a spherical Gaussian function with a fixed width. Stability of the analytic continuation technique with respect to the width and with respect to the input range of electron affinities is studied in detail. The computed resonance parameters $E_r=0.282\text{ eV}, \Gamma=0.316\text{ eV}$ for the $2p$ state of Be$^-$ and $E_r=0.188\text{ eV}, \Gamma=0.167\text{ eV}$ for the $3p$ state of Mg$^-$, agree well with the best results obtained by much more elaborated and computationally demanding present-day methods.

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I. INTRODUCTION

Resonances in electron-atom or electron-molecule scattering, also addressed as transient negative ions, have attracted attention over the last decades. It is because these temporary states provide a pathway for electron-driven chemistry via dissociative electron attachment (DEA) and therefore, applications can be found in chemistry of the planetary atmospheres \[1\], nanolithography in microelectronic device fabrication \[2, 3\], and in cancer research where these states provide a mechanism for the DNA damage by low-energy electrons \[4, 5\].

Accurate calculation of energies and lifetimes of the resonances represents a challenging task that is more complicated than the determination of energies of the bound atomic or molecular states. Temporary negative ions differ from the bound states in two important respects: (i) they are not stable and decay into various continua, (ii) corresponding poles of the $S$-matrix are complex and they are expressed by $E = E_r - i\Gamma/2$. There have been numerous studies published using several methods for determination of the resonance energies and widths. Stabilization methods \[6–9\] search for a region of stability of the energies with respect to different confining parameters. Stieltjes imaging technique \[8\] allows to represent the resonant state by a square-integrable basis and the width is defined by the resonance-continuum coupling. Complex rotation methods \[10–12\] and the methods employing complex absorbing potential \[13, 14\] compute complex resonant energy as an eigenvalue of a complex, non-Hermitian Hamiltonian.

Recently the method of analytic continuation in coupling constant (ACCC) \[15–17\] has been applied to several molecular targets, such as $N_2$ \[18, 19\], ethylene \[20, 21\], and amino acids \[22\]. Furthermore, the known low-energy analytic structure of the resonance was incorporated into the inverse ACCC (IACCC) method providing so-called regularized analytic continuation (RAC) method. The RAC method was successfully employed for determination of $\pi^*$ resonances of acetylene \[23\] and diacetylene \[24\] anions, proving that the ACCC method can yield accurate resonance energies and widths for various molecular systems using data obtained with standard quantum chemistry codes.

Common feature of all methods of analytic continuation is an application of the perturbation potential $\lambda V$ to the multi-electron Hamiltonian $H$, i.e. $H \rightarrow H + \lambda V$. The role of this attractive perturbation is to transform the resonant state into a bound state. Although the RAC method was developed for strictly short-range perturbation $V$, authors were able to successfully use the Coulomb potential in its stead \[23, 24\]. This obvious inconsistency can yield reasonable results, because in practical applications the perturbation potential is often projected on a finite set of
short-range basis functions, e.g. Gaussian functions used by the quantum chemistry software. However, so obtained weakly-bound states need to be examined carefully because they may, in fact, be Rydberg states supported by the basis and the long-range tail of the Coulomb perturbation $V$ \[24\]. Such states need to be excluded from the continuation procedure as they do not represent a resonance transferred to a bound state. In order to avoid such complications, in the present study we adopt a short-range perturbation potential in a form the Gaussian function

\[
V(r) = -\lambda e^{-\alpha r^2}.
\]  

(1)

This choice of the perturbation was recently evaluated by White et al. \[19\] and applied to the well-known $^{2}\Pi_g$ resonance of $N_2^-$. Furthermore, Sommerfeld and Ehara \[25\] introduced another short-range potential, termed as Voronoi soft-core potential, which they successfully used to analyze the $^{2}\Pi_u$ resonance of $CO_2^-$. Present analysis of the Gaussian perturbation potential (1) will be carried out for expectedly simpler problems - atomic shape resonances of beryllium and magnesium. Both atoms are known to possess a $p$-wave shape resonance very close to the elastic threshold. While in the case of the $Mg^-$ the agreement between the available computed resonance parameters \[26–28\] and the experimental data \[29, 30\] is quite good, the situation is very different for the beryllium atom. There has been a great number of theoretical studies \[31–42\] aiming to numerically characterize $Be^-\ 2s^2\varepsilon p\ 2P$ resonance, with various levels of success. Table III in Ref. \[41\] clearly summarizes that the theory of the last four decades predicts the resonance position between 0.1 and 1.2 eV and the resonance width between 0.1 and 1.7 eV. Even the most recent calculations differ by about a factor of 3 for the two resonant parameters. Moreover, there are no experimental data available for the $Be^-$ resonance that could narrow the spread of all the available theoretical predictions.

Convergence patterns shown in Refs. \[41, 42\] demonstrate that the $Be^-$ resonance may be very sensitive to an accurate description of the electronic correlation energy. Therefore, in the present study we employ coupled-clusters (CCSD-T) and full configuration interaction (FCI) methods for the perturbed $Be^-$ electron affinities that will be then continued the complex plane by the RAC method. The basic ideas of the RAC method are given in the Sec. \[II\]. Quick summary of the quantum chemistry details is presented in Sec. \[III\]. In Sec. \[IV\] we analyze the stability and accuracy of the RAC method with the Gaussian perturbation potential \[1\]. Then conclusions follow.
II. RAC METHOD

The RAC method represents a very simple method for calculation of resonance energies and widths which embraces all known analytical features of coupling constant $\lambda(\kappa)$ near the zero energy \cite{24}. The method works as follows:

- The atom or molecule is perturbed by an attractive interaction $V$ multiplied by a real constant $\lambda$

$$H_{\text{neutral}} \rightarrow H_{\text{neutral}} + \lambda V,$$

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

- The same procedure is carried out for the corresponding negative ion

$$H_{\text{ion}} \rightarrow H_{\text{ion}} + \lambda V,$$

where the bound state energies $E_i^I$ are calculated for the same values of $\lambda_i$.

- Both energies are subtracted forming the electron affinity in the presence of the perturbation potential $V$

$$E_i^N - E_i^I = E_i = \kappa_i^2.$$

The new set of data points $\{\kappa_i, \lambda_i\}$ is then used to fit the function

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

It is represented as a Padé 3/1 function and it defines the level of complexity of the pole behavior at the low bound or continuum energies. We term it as RAC [3/1] method. The origin of its form and the fit formulae for [2/1], [3/2], and [4/2] methods can be found in Ref. \cite{23}. The parameters of the [3/1] fit, namely $\alpha$, $\beta$, $\delta$ and $\lambda_0$ are found by minimizing the $\chi^2$ functional

$$\chi^2 = \frac{1}{N} \sum_{i=1}^{N} \frac{1}{\varepsilon_i^2} \left| \lambda(\kappa_i) - \lambda_i \right|^2,$$

where $N$ denotes the number of the points used, while $\kappa_i$ and $\lambda_i$ are the input data. Once an accurate fit is found, only the parameters $\alpha$ and $\beta$ determine the resonance energy

$$E_r = \beta^2 - \alpha^4,$$

(7)
and the resonance width

\[ \Gamma = 4\beta \alpha^2. \]  

(8)

Role of the parameter \( \delta \) is to describe a virtual state with \( E_v = -1/\delta^4 \). Even in the case the studied system does not possess a virtual state this parameter represents a cumulative effect of the other resonances and other poles not explicitly included in the model. The weights \( \varepsilon_i \) (accuracy of the data) in Eq. (6) are generally unknown. The calculation can be routinely performed with constant \( \varepsilon_i = 1 \) or, if an importance of the data points closest to the origin needs to be stressed, increasing weights sequence (e.g. \( \varepsilon_i = i \)) can be used.

The RAC method has been recently critically evaluated by [White et al.][19]. Authors tested three types of the perturbation potential

\[
V(r) = -\frac{\lambda}{r},
\]

(9)

\[
V(r) = -\lambda e^{-\alpha r^2},
\]

(10)

\[
V(r) = -\lambda e^{-\alpha r^2},
\]

(11)

and they suggested that the attenuated Coulomb potential (10) is the best choice out of the three options and the Gaussian potential (11) does not represent a good choice for the RAC method. All these potentials are easily implemented into the standard quantum chemistry codes. The aim of the present contribution is twofold:

- to explore application of the Gaussian-type perturbation and to find its parameters that allow accurate extraction of the resonance data with the RAC method

- to demonstrate that the RAC method can be applied with success to low-lying atomic shape resonances

Before applying the RAC method one must consider two important issues.

1. First is a choice of the perturbation potential, i.e. in the present context the choice of the exponent \( \alpha \) in Eq. (11). Presently there exist no general rule, no guide that helps us to choose the perturbation potential. Therefore, it is necessary to perform calculations for a set of values of the parameter \( \alpha \) to find an optimal choice. If the optimal range of values is found, it is reasonable to expect that the obtained resonance data should stabilize in such a range, because the exact function \( \lambda(\kappa) \) gives the same resonant data for every choice of the perturbation potential. Since the present [3/1] RAC function is only approximative, one
can only expect an existence of a plateau that gives approximative values of the resonance parameters.

2. The RAC method represents essentially a low-energy approximation to the exact function $\lambda(\kappa)$. It is therefore obvious that the method should be used in a range of energies (or momenta) limited by some maximal energy $E_M$. Our empirical experience shows that $E_m \sim 8E_r$ ($E_r$ is the sought resonance energy) gives a reasonable estimate for the range of energies.

### III. ELECTRON AFFINITIES

*Ab initio* calculations for the electron affinities $E_i(\lambda_i)$ in presence of the external Gaussian field (11) were carried out using the CCSD-T [43][44] and FCI methods as implemented in MOLPRO 10 package of quantum-chemistry programs [45]. Core of the basis set employs Dunning’s augmented correlation-consistent basis of quadruple-zeta quality aug-cc-pVQZ [46] for both atoms, Be and Mg. This basis set was additionally extended, in an even-tempered fashion, by 2 ($s, d, f, g$)-type functions and 6 $p$-type functions. Calculations for the neutral atoms and corresponding

![Figure 1](image_url)

**FIG. 1.** (Color online) Electron affinities of $\text{Be}^-$ and $\text{Mg}^-$ ions under the influence of the perturbation potential (11). Full lines are shown for the exponent $\alpha = 0.025$, while the broken lines are for $\alpha = 0.035$. Red color (light gray) describes the $\text{Be}^-$ ion and the black color is for the $\text{Mg}^-$. Negative ions used the same basis sets and the same correlation methods (CCSD-T or FCI). Typical
dependence of the electron affinities on external field (11) is shown in Fig. 1 for both negative ions, Be$^-\text{ and Mg}^-$, and in the range of energies used for the present analytic continuation. Fig. 1 yields the following observations:

- As expected, the weaker perturbation potential with $\alpha = 0.035$ requires a stronger scaling parameter $\lambda$ to achieve the same binding negative ion energies as the perturbation with $\alpha = 0.025$.

- Surprisingly, a larger scaling parameter (stronger perturbation) is necessary to bind the Mg$^-$ resonance that lies closer to the zero when compared to the Be$^-$ resonance (as will be seen below). Such behavior may be caused by the spatial extent of the Mg$^-$ $3p$ resonant wave function when compared to the reach of the $2p$ wave function of the Be$^-$ ion.

- The lowest binding energies are not included in the continuation input data because of the difficulties we encountered while using the quantum chemistry software. Hartree-Fock method is known to destabilize in very diffused basis sets, however low binding energies are inaccurate if a more compact basis is used.

Most of the present results were obtained with the CCSD-T method. However, once the the optimal exponent $\alpha$ (see the Sec. IV) was found for the beryllium atom, the affinity curve shown in Fig. 1 was also recomputed with the expensive FCI method and the basis as described above.

IV. RESULTS

As discussed in Sec. II our goal is to search for regions of stable results with respect to the two optimization parameters. First is the range of the input electron affinities defined by maximal affinity $E_M$. The second parameter, the exponent $\alpha$ in Eq. (11) defines the shape of the perturbation potential. Typical dependence of the resonance parameters on the maximal energy is shown in Fig. 2 for the fixed $\alpha$ parameters. It is clear that the stability is little worse for the Be$^-$ ion when compared to Mg$^-$ ion. However, it is possible to narrow the spread of the obtained resonance data by considering the value of $\chi^2$ defined by Eq. (6). Fig. 3 shows the dependence of $\chi^2$ quantity on the maximal energy $E_M$. A pronounced minimum at $E_M = 1.92$ eV is clearly visible. This allows an application of a condition of the best fit. Such a restriction leads to a well defined $E_M$ for each choice of the perturbation parameter $\alpha$ producing a data sets shown in Fig 4. For beryllium the resonance position and width stabilizes for $\alpha > 0.02$. The best fit is obtained for $\alpha = 0.035$.
resulting in $E_r = 0.323$ eV and $\Gamma = 0.317$ eV. In order to estimate accuracy of the correlation energy provided by the CCSD-T method we also recomputed this final results with the FCI method. The FCI affinities yield $E_r = 0.282$ eV and $\Gamma = 0.316$ eV. Detailed summary of the available theoretical results for the Be$^-$ resonance was presented in Tab. III of Ref. [41]. A comparison with the most recent computations will be given in Sec. V.

In case of magnesium ion the resonance energy is very stable over the whole range of examined perturbation parameters $\alpha$. However, the width exhibits a weak dependence on the exponent $\alpha$. This feature may indicate that the low-order RAC method is inadequate for the Mg$^-$ resonance. Nonetheless, the best fit is obtained for $\alpha = 0.025$, giving $E_r = 0.188$ eV and $\Gamma = 0.167$ eV. The available data for the Mg$^-$ resonance are summarized in Tab. I. Presently computed resonance energy is about 40 meV higher that the experimental value of Burrow et al. [29, 50]. Such a discrepancy may have several possible reasons:

1. The experimental resolution is about 30–40 meV [29].

2. Discrepancy between the correlation energies of the CCSD-T and FCI methods and the present basis set is about 41 meV for the electron affinity of the beryllium atom. Similar difference can also be expected for the magnesium. Moreover, weaker stability of $\Gamma$ with re-
Exponent $\alpha$ is fixed at 0.035 and the increasing weights set $\varepsilon = i$ are used.

TABLE I. Comparison of the available data for the resonance energy $E_r$ and the resonance width $\Gamma$ for the $3s^2\varepsilon p\ 2p^2$ state of atomic magnesium.

| Method             | Resonance energy $E_r$(eV) | Resonance width $\Gamma$(eV) |
|--------------------|-----------------------------|------------------------------|
| Model potential    | 0.37                        | 0.10                         |
| Model potential    | 0.161                       | 0.160                        |
| Complex rotation   | 0.08                        | 0.17                         |
| Stabilization      | 0.14                        | 0.08                         |
| Complex SCF        | 0.50                        | 0.54                         |
| Finite elements    | 0.159                       | 0.12                         |
| Experiment         | 0.15±0.03                   | ~0.14                        |
| Recommended value  | 0.15                        | 0.16                         |
| Present RAC        | 0.19                        | 0.16                         |

The experimental resonance energy [29] was determined from the maximum of the measured cross section, whereas present method defines the resonance energy from a pole of the $S$-
FIG. 4. (Color online) Resonance energy $E_r$ (circles connected full lines) and the resonance width $\Gamma$ (diamonds connected with dashed lines) as functions of $\alpha$ parameter of the perturbation potential.

matrix. The two definitions give similar results for a narrow resonance ($\Gamma < E_r$), but for a broader resonance ($\Gamma \geq E_r$), as in the present case, the results may differ.

V. CONCLUSIONS

Present study confirms the observations of White et al. [19] in which the authors state that the Gaussian perturbation potential is more difficult to apply than potentials possessing the Coulomb singularity. It has been shown in the case of a model potential [19] that the trajectory of the resonant pole is more complicated for the Gaussian perturbation. In the present study we have shown that in order to obtain stable results, the RAC method must be restricted to fairly low electron affinities and a careful analysis of the results with respect to the width of the perturbation potential must be carried out.

Such procedure allowed us to apply the RAC method to one of the remaining enigmas among shape resonances of small atoms, the $2s^22p\,^2P$ resonance of $\text{Be}^-$. To the best of our knowledge there are no experimental data available for this resonance. Important role of the correlation energy in this system creates a challenging task for the theory, albeit the fact that $\text{Be}^-$ possess only 5 electrons. Consequently, about two dozens of theoretical predictions (found in Ref. [31–42]) do
not result in any kind of a consensus. Two methods with high level of correlation description, the CCSD-T and FCI methods, were applied in the present study. While the position of the resonance shifts to the lower energies by about 41 meV for the more accurate FCI method, the resonance width was found insensitive to the correlation treatment. Presently calculated FCI resonant energy $E_r = 0.282$ eV and width $\Gamma = 0.316$ eV are in a good agreement with the complex CI results of McNutt and McCurdy [35] that predict the $E_r = 0.323$ eV and $\Gamma = 0.296$ eV. Recent scattering calculations [42] determined the resonance with $E_r = 0.31 \pm 0.04$ eV and $\Gamma = 0.40 \pm 0.06$ eV again in a good agreement with the present results. However, another set of recent calculations by Tsenden et al. [41] place the resonance at $E_r = 0.756$ eV and $\Gamma = 0.874$ eV.

In case of the $2s^2\varepsilon p \ 2P$ resonance of Mg$^-$ a comparison with the experiment is available. Although, the present calculations determine the resonance about 40 meV higher than the experiment [29], they still exhibit the best agreement with the experimental data among the ab-initio methods.

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