Resonance States of Atomic Anions

Alexei V. Sergeev and Sabre Kais
Department of Chemistry, Purdue University, 1393 Brown Building, West Lafayette, IN 47907
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Two methods are proposed to treat resonance states of an atom with a nuclear charge less than a "critical" value, which is the minimum charge necessary to bind N electrons. The first method represents a reformulated variational approach in order to consider resonance and bound states on an equal footing. The second method represents an extrapolating scheme which is based on a one-particle model. The energy of a two-electron atom was found in the entire range $0 \le Z < \infty$. In the region $0.877 < Z < 0.901$ near the critical charge $Z_c \approx 0.911$ our results agree with the numerical calculations of the complex energy by Dubau and Ivanov. Using the one-particle model, we estimated resonance energies of doubly charged negative ions of atoms with $Z \le 18$. Results for O^{--} and S^{--} are in good agreement with earlier estimates.

31.15.-p, 31.15.Pf, 32.10.Hq, 02.60.Gf

I. INTRODUCTION

There has long been an interest in the existence of long lived doubly charged negative atomic ions [1–3]. The possibility of doubly charged negative ion resonances has been raised in the case of oxygen by experiments of Peart et al. [4] who observed resonance like structures in electron-impact detachment cross section at energies of 19.5 and 26.5 eV. A Hartree Fock calculation of the closed-shell electronic configuration shows that the resonance energy of O^{--} is about 8 eV above O^-, which later was confirmed and modified by configuration interaction and other methods [2]. More recently, Sommerfeld et al. [5] performed a large scale multireference configuration interaction calculation using the complex rotation technique to investigate resonance states of H^{--}. Their results predict the existence of a $(2p^3)^4S$ resonance state of H^{--} with a resonance position of about 1.4 eV above the $(2p^2)^3P$ state of H^- and a lifetime of $3.8 \cdot 10^{-16}$ sec [6]. Until now, to the best of our knowledge, all observation of long lived resonances of doubly negative ions are associated exclusively with excited electronic configurations.

Considering resonance energy as an analytic continuation of bound state energy into an instability region, with the change of some parameters of the system, allows one to use essentially the same computational methods for both bound and the resonance states. For example, Rayleigh-Schrödinger perturbation theory originally designed to approximate bound states has been successfully used for resonance states together with methods of analytic continuation such as conformal mapping [7] and quadratic Padé approximants [8]. Applicability of variational methods was effectively extended to unstable quasistationary states by the method of complex coordinate rotation [9,10].

In this paper, we consider an atom in its ground electronic configuration state with the nuclear charge Z as a variable. Integer values of Z with $Z > N$ correspond to positive ions, with $Z < N$ to negative ions and with $Z = N$ to neutral atoms, where N is the number of electrons.

In Sec. II, we consider the ground state of the simplest two-electron system as a function of the nuclear charge. Here, we use precise variational calculations to determine the energy in the entire range of positive Z and to analyze its singularities. Exact results for this system are compared with approximation that is used later in Sec. III for multi-electron atoms.

In Sec. III, we find an approximate dependence of the energy on the nuclear charge by extrapolation from the known energies of a neutral atom and the corresponding negative ion. Energies and widths of doubly negative ions for isoelectronic series exhibiting a bound singly charged anion are estimated systematically for $N \le 18$. Results for O^{--} and S^{--} are in good agreement with a number of earlier theoretical predictions. Estimated positions and widths can be used to search for these resonances experimentally.

II. TWO-ELECTRON ATOMS

The variational method gives accurate results for bound states of He and H^-, but it fails when the nuclear charge is less than the critical value $Z_c \approx 0.911\,028\,225$ when the state turns to a resonance. In order to understand why the variational method becomes inadequate when $Z < Z_c$, let us perform the following numerical test. We use the Hylleraas trial wave function of the form

$$\psi_N = \sum_{i+j+k \le N} C_{i,j,k}[r_1^i r_2^j \exp(-ar_1 - br_2) + r_2^i r_1^j \exp(-ar_2 - br_1)] r_{12}^k \exp(-cr_{12}) \qquad (1)$$

Minimization of the energy functional with respect to the coefficients $C_{i,j,k}$ reduces the calculation to an eigenvalue problem for a finite matrix whose size increases as $\sim N^3/6$. We found several lowest eigenvalues for $N = 20$ with $a = 0.1$, $b = 0.8$, and $c = 0$.

The ionization energy $E_{\rm I} = -E - Z^2/2$ as a function of the nuclear charge is shown in Fig. 1 (solid lines). If $Z > Z_{\rm c}$ then the lowest level corresponding to maximum ionization energy, the upper curve in Fig. 1, gives the bound state energy. Fig. 1 shows that the upper curve rapidly bends to zero after going below Z_c. This means that the variational method gives a trivial result $E_{\rm I} = 0$ when the bound state ceases to exist. However, all the curves corresponding both to the minimum and to higher eigenvalues exhibit a typical avoided-crossing ladder pattern of proliferation of the bound state into continuum as a resonance. This situation which is similar to the two-electron problem in finite space [11] is the result of using of variational functions satisfying the boundary conditions of a bound state but not the boundary conditions of a resonance.

In order to calculate the resonance by variational method without encountering avoided-crossings, we make the boundary conditions more flexible by introducing a complex trial function. Until now, we considered the exponential parameters a, b, and c as real numbers independent of Z, and minimized the energy functional with respect to the linear coefficients $C_{i,j,k}$. Alternatively, we can minimize the energy with respect to both the linear and the non-linear parameters. In this way, we found that the optimized parameters a, b, and c are real for sufficiently large charges. If the charge is lower than some value (see Table I), then the minimum of the energy functional no longer exists. This situation is different from minimizing over the linear parameters only when the minimum of the energy functional *always* exists because a real symmetric matrix always has a minimum real eigenvalue. An analytic continuation of a minimum of some function, when this minimum ceases to exist, represents a complex stationary point. We found numerically the parameters a, b, and c as complex stationary points in the range $0 \le Z \le 1$ with up to $N = 5$. The result for $N = 5$ is shown in Fig. 1. The real part is a dashed line, and the imaginary part of the ionization energy is a dot-dashed line. By allowing the parameters of the trial function to be complex-valued, we eliminated the avoided-crossings and made the results to converge with increase of N. It is interesting that the traditional variational method, with real parameters a, b, and c, gives very accurate results at the inflection points, between adjacent avoided-crossings (see Fig. 1), but it never reproduces the imaginary part of the resonance.

Let us consider the variational results from the point of view of analytic structure of the energy as a function of the nuclear charge. If the exponential parameters a, b, and c are real, then the energy (shown by solid lines in Fig. 1) is real and does not have singularities at the real axis. However, for sufficiently small charge there is a pair of complex conjugate square root branch points close to the real axis joining each branch of the energy function (shown as a continuous solid curve in Fig. 1) with the neighbor branch (the nearest curve that lies above or below). In contrast, if the exponential parameters a, b, and c are allowed to have complex values then the variational energy (shown by dashed and dot-dashed curves) has a single singularity at the real axis at the point where the minimum of the energy functional disappears and turns to a complex stationary point. This singularity models a singularity of the exact energy at the "critical" charge where the system goes from a bound state to a quasi-stationary state. Positions of this singularity $Z_*^{(N)}$ for different N are listed in Table I.

The numerical evidence is that most of the variational singularities $Z_*^{(N)}$ give lower bounds for the critical charge $Z_{\rm c} \approx 0.911\,028$ and converge with the increase of N although the convergence is not monotonous. Table I lists also variational "critical" charges $Z_{\rm c}^{(N)}$ defined as the zeroes of the ionization energy $-E^{(N)}(Z) - Z^2/2$. The "critical" charges $Z_{\rm c}^{(N)}$ could be calculated by solving a generalized eigenvalue problem by a variational method [12], they always give upper bounds for $Z_{\rm c}$. We found that convergence of $Z_{\rm c}^{(N)}$ to the critical charge is much faster than that of $Z_*^{(N)}$. By extending variational calculations of $Z_{\rm c}^{(N)}$ to higher N, the most accurate estimation of the critical charge was found earlier [12]. Calculations of $Z_*^{(N)}$ are generally more difficult than that of $Z_{\rm c}^{(N)}$ because they represent a singularity. They converge to the singularity Z_* of the function $E(Z)$, which is believed to limit the radius of convergence of the $1/Z$ expansion to $1/Z_*$. According to an earlier hypothesis based on the analysis of the $1/Z$ perturbation series [11], Z_* is slightly smaller than Z_c (see Table I) which means that $E(Z_*)$ lies above the continuum, but still corresponds to a localized wave function. More elaborate computations of the $1/Z$ series and its analysis by Baker et al. [13] show that Z_* and $Z_{\rm c}$ are equal.

We used the complex parameters a, b, and c calculated for the particular case of $N = 5$ in order to extend calculations to higher N by optimizing only the linear coefficients $C_{i,j,k}$. We found that "almost exact" variational energy calculated at $N = 25$ differs from the variational energy at $N = 5$ shown in Fig. 1 in the amount of less than $0.5 \cdot 10^{-4}$. Calculations show that the behavior of the parameters a, b, and c which are a stationary point of the energy functional is more unpredictable than that of the energy. Dependence of a, b, and c on N at $Z = Z_{\rm c}$ is shown in Fig. 2. It seems that the parameters oscillate as N increases. In our previous paper [12], we used near-average parameters $a/Z = 0.35$, $b/Z = 1.03$, and $c/Z = 0.03$ shown by dashed lines on Fig. 2 to perform large-N calculations of $Z_{\rm c}$.

Dependence of a, b, and c on Z for $N = 5$ is shown in Fig. 3. The parameters are continuous functions of Z with a square root singularity at $Z = Z_*$, below which they become complex-valued. Numerical results show many erratic swerves on the curves, this fact probably indicates the existence of many singularities close to the real axis.

Most of the above features are typical for any system

passing from a bound to a quasistationary state that is treated variationally, for example for Ne isoelectronic series with a nuclear charge below $Z_* = 8.74$ [14].

The above method is a more general version of the complex rotation or the complex stabilization method [10]. Instead of one non-linear complex variational parameter, the rotation angle, we are using three non-linear variational parameters a, b, and c.

Dubau and Ivanov [15] calculated the two-electron atom resonance in the vicinity of the critical charge using $1/Z$ expansion and the complex rotation method. Their results agree with our calculation, see Table II.

We extended calculations of the resonance to the range of $0 \le Z \le 1$. Results are shown in Fig. 4. The real part of the ionization energy is always negative at $0 < Z < Z_c$. It reaches its minimum at $Z \approx 0.45$, and the width reaches its maximum approximately at the same point. For small Z, convergence of the variational method becomes worse. It seems that both real and imaginary parts tend to zero when $Z \to 0$.

Our results for small Z apparently contradict that of Herrick and Stillinger [14]. They found that a small negative charge corresponds after suitable scaling to a tightly bound "di-electron" moving in a Coulomb field of the nucleus. The behavior of $E(Z)$ as $Z \to -0$ has the form

$$E(Z) = -1/4 - 4Z^2 + 256Z^4 + O(Z^5) \qquad (2)$$

Also by considering the simplest trial function

$$\phi_{\rm var}(\mathbf{r}_1, \mathbf{r}_2) = \exp\left[-\alpha(r_1 + r_2) - \beta r_{12}\right] \qquad (3)$$

they found that $E_{\rm var}(Z) = -1/4 - 4Z^2 + 448Z^4 + ...$ at $Z \to 0$ in a good agreement with (2).

We re-examined the variational calculations with the trial function (3) and found that Herrick and Stillinger actually dealt with two different branches of the variational energy which are displayed in Fig. 5. The first branch, the lower curve in Fig. 5, corresponds to a physical wave function with a positive exponential parameter α at sufficiently large Z. It goes almost to zero as the charge decreases and becomes complex below $Z_* = 0.084\,6$. The second branch corresponds to a divergent wave function with a negative α. It goes to $-1/4$ as the charge decreases and then turns to a physical branch with $\alpha > 1$ at negative Z. The second branch is also present in our calculations with the trial function (1), but we always disregard it. According to our numerical results, the energy goes to zero at $Z \to 0$ (see Fig. 4).

III. MANY-ELECTRON ATOMS

Applying the complex rotation method to systems of more than three charged particles faces slow convergence because of the difficulty to simulate the oscillatory character of the wave functions [10].

The present study deals with the ground state ionization energy of a multi-electron atom considered as a function of a nuclear charge. Since the size of the variational basis set grows exponentially with the increase of the number of electrons, we choose here to follow a simpler path. We use the reliable data for the ionization energy of a negative ion and a neutral atom, which were calculated or experimentally measured. We are going to use here an extrapolating technique in order to find a complex energy of a doubly charged negative ion. In contrast to simple extrapolating such as polynomial fits or analytic formulas with a few fitting parameters [16], we are solving here a one-particle Schrödinger equation with a potential that models the movement of a loosely bound valence electron that is going to dissociate when the charge approaches its critical value. This model is realistic in the vicinity of the critical charge and effectively reproduces the non-trivial singularity [17] of the ionization energy at the critical charge. Herric and Stillinger [14] used for Ne isoelectronic series a polynomial fitting formula plus a singular term $\sim (Z - Z_*)^{3/2}$. Their method correctly reproduces a similar singularity of a variational energy $\sim (Z - Z_*^{(N)})^{3/2}$, but it fails for the exact energy, which has a less trivial singularity as it was established by Dubau and Ivanov [15].

A. Description of the one-particle model

For a given atom with N electrons and a nuclear charge Z, let us consider a spherically-symmetric potential (also known as Hellmann potential [18]) of the form

$$V(r) = -\frac{1}{r} + \frac{\gamma}{r}\left(1 - e^{-\delta r}\right) \qquad (4)$$

with $\gamma = (N-1)/Z$.

Since in the neighborhood of the critical charge, particularly for the negative hydrogen ion [19], one of the electrons is held much farther from the nucleus than the others, we suggest a one-particle model of this electron in an effective potential of the atomic core comprising of the nucleus and $N-1$ electrons. In scaled coordinates $r \to Zr$, this potential is approximated by our model potential, Eq. (4). Our approximation is asymptotically correct both at small and at large distances from the nucleus where the scaled atomic core potential tends to $-1/r$ and to $-(Z-N+1)/(Zr)$ respectively. The transition between the two different asymptotic regimes occurs at distances roughly equal to $1/\delta$ that is about the atomic core radius.

The second parameter of the model potential, Eq. (4), δ, is chosen so that the ionization energy in the potential (4) is equal to the scaled ionization energy $Z^{-2}E_{\rm I}(Z)$ of the atom. Note that for atoms with more than two electrons, we consider here an excited state in the potential (4) with the same spherical quantum numbers (n, l) as quantum numbers of the loosely bound electron on an external atomic shell (in this aspect our approach differs from the method of pseudo-potentials [20] that deals

with the ground state in a potential with an additional repulsive term necessary to take into account orthogonality conditions). In this way, we map an arbitrary atom, which is characterized by a pair of numbers (N, Z) to the model one-particle system (4), which is characterized by a pair of parameters (γ, δ). Results of fitting the parameter δ for elements with $N \leq 10$ in our previous study [21] give evidence that δ depends on $1/Z$ almost linearly.

In summary, our model (4) effectively eliminates the singularity in the energy function $E_{\rm I}(Z)$ to be extrapolated by replacing it with a weakly varying function $\delta(Z)$ that can be accurately extrapolated by a linear dependence on $1/Z$ without taking into account a complex singularity at $Z = Z_*$. In our previous study [21], we fitted the parameter δ to meet the known binding energy of the neutral atom and its isoelectronic negative ion and then found δ as a function of $1/Z$ by a linear extrapolation. After that, we solved Schrödinger equation with the potential (4) and found some kind of extrapolation of the ionization energy of an atom to the range of $Z < N - 1$. Finally, by locating a zero of the ionization energy, we found critical charges for most of atoms with $N \leq 86$. In the present paper, we use the same technique to find resonances of doubly charged negative ions by calculating the ionization energy at $Z = N - 2$.

B. Results

For two-electron isoelectronic series, the parameter δ is 1.066 and 0.881 for He and H^- respectively. Decreasing of δ for H^- means increasing of the core radius that is induced by stronger repulsion between electrons. Results of extrapolating the ionization energy to the range $Z < 1$ with δ assumed as a linear function of $1/Z$ are shown in Fig. 4 together with more accurate variational results. As it was expected, the one-particle model gives fairly accurate results in the vicinity of the critical charge where it models the threshold singularity. Here, the real part is approximated more accurately than the imaginary part because the singularity manifests mostly in the imaginary part. Numerical results for the imaginary part are given in Table II. Since in the latter case the charge is close to the critical charge, we slightly corrected location of the singularity in our model by fitting δ at points $Z = Z_{\rm c} \approx 0.911$ and $Z = 2$ instead of fitting it at points $Z = 1$ and $Z = 2$.

For three-electron isoelectronic series, our model cannot be used in the same way because He^- does not exist and we don't know the behavior near the singular point $Z_{\rm c} = 2$. It is reasonable to expect that the resonance H^{--} is highly unstable because the isoelectronic ion He^- is already unstable. We tried to extrapolate the ionization energy by fitting δ at points $Z = 4$ (Be^+) and $Z = 3$ (Li) with subsequent extrapolation of δ to $Z = 1$ by a linear function in $1/Z$ and found a broad resonance with $E_{\rm I} = -0.109 - 0.089i$ for H^{--}.

For four-electron isoelectronic series, results of using our model for extrapolating the ionization energy are shown in Fig. 6. We found that the curve hits the border of continuum spectrum $E_{\rm I} = 0$ at $Z_{\rm c} = 2.864$ [21] and again at $Z'_{\rm c} = 2.17$. Very small imaginary part exists in the interval $Z'_{\rm c} < Z < Z_c$. The extrapolation gives *positive* ionization energy for He^{--}, $E_{\rm I} = 0.064$. Since a bound state of He^{--} does not exist, it means that we deal with a virtual state with an exponentially growing wave function. It may be also possible, that because of its limitations our method fails for He^{--} ion. We found positive ionization energies for another doubly charged negative ions of noble gases, for example Ne^{--} (see Table III).

The doubly charged negative ion of oxygen in the same electronic configuration as a closed-shell 10-electron configuration of a neutral atom of neon is the system that was studied theoretically using various methods, see Table III. However, this relatively stable ion was never observed experimentally. The extrapolated ionization energy as a function of Z is shown in Fig. 7.

Comparison of the ionization energy of O^{--} found by different methods is given in Table III. For critical discussion of some of these results, see [14]. Our result for resonance position is in agreement with most of the above results. However, our prediction of the resonance width is significantly lower than that of Herrick. It may be attributed to the fact that Herrick's 3/2-power term, which responsible for the width, is far from the actual singular behavior or to the fact that our model systematically underestimates the width as it happens for two-electron atoms.

We extended calculations of resonances of doubly charged negative ions to the first two rows of the Periodic Table. Here, we considered only that ions for which an isoelectronic singly charged negative ion is stable, for example we omitted C^{--} because N^- does not exist. Results are listed in Table IV. For the closed shell ion S^{--}, our ionization energy is slightly smaller than the previous estimates. The width for S^{--} is considerably smaller than for the ion O^{--} in agreement with an argument of Herrick and Stillinger [14].

IV. DISCUSSION

We have investigated the existence of resonance states for doubly charged atomic negative ions using two methods. The first method is a reformulated variational approach to treat resonance states. In Sec. II, we traced the position of the ground state energy level of two-electron atoms as the nuclear charge decreases. When the charge drops below the critical charge, the level goes into a complex plane and becomes a resonance. With only minor change of computer program, the Hylleraas-basis variational technique is used for accurate determination of position and width of the resonance inside instability re-

gion of small charges. These results are used to check the accuracy of the less accurate approximation developed in Sec. III necessary to study destabilization of the ground state of a multi-electron atom with decrease of its nuclear charge. The results of our second approach, the approximate one particle model, agree with earlier estimates of closed-shell resonances of O^{--} and S^{--}. In addition, the model predicts similar resonances of another di-anions which are isoelectronic to some bound singly-charged anion.

Our method is in fact some kind of refinements of Herrick and Stillinger method of analytic continuation [14]. We believe that our model reproduces the threshold singularity of the energy more realistically than 3/2-power singularity of Herrick and Stillinger. Generally, the method of analytic continuation from bound to resonance states appears very accurate when the threshold behavior of the energy is incorporated into continuation scheme, as it was demonstrated earlier for two-particle resonances in nuclear physics, see Chapter 5 of the book [29].

Although no multiple negative ions exist in a bound state [30,31,21], some long-lived resonances of doubly negative ions are observed experimentally [1]. Our results give evidence for some resonances that remain to be observed.

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FIG. 1. Variational results for the energy of the helium isoelectronic series. Non-linear parameters of the Hylleraas trial function (1) are $a = 0.1$, $b = 0.8$, and $c = 0$. The size of the basis set corresponds to $N = 20$. The restriction on the summation indexes $i + j^2 + k^2 \leq N$ is used instead of the more common restriction $i+j+k \leq N$ in order to decrease the number of terms in the sum (1) from $\sim \frac{1}{6}N^3$ to $\sim \frac{\pi}{8}N^2$ as it was suggested in [12]. These results are shown by solid lines. Variational results with parameters a, b, and c determined as a complex stationary point of the energy functional for $N = 5$ are shown by dashed and dot-dashed lines, real and imaginary parts respectively.

FIG. 2. Dependence of the optimal variational parameters a, b, and c calculated at $Z = Z_c$ on N.

FIG. 3. Optimal variational parameters a, b, and c for $N = 5$ as a function of the nuclear charge Z.

FIG. 4. Ionization energy for the helium isoelectronic series as a function of the nuclear charge including an instability region $0 \le Z < Z_c$. Bold lines are accurate results found by the variational method with a large basis set. Thin lines are results of the simplified one-particle model described in Sec. III A. Solid and dashed lines are real and imaginary parts respectively.

FIG. 5. Ionization energy for the helium isoelectronic series found using Stillinger's trial function (3). The lower curve approximates real ionization energy when $Z \ge Z_c$ and resonance energy when $Z < Z_c$ (for very small $Z < 0.085$ it has an imaginary part shown by a dashed line). The upper curve is an unphysical branch of the function which tends to $1/4$ at $Z = 0$ and after continuation to negative Z turns to ionization energy of a hypothetical system with Coulomb attraction between the particles.

FIG. 6. Ionization energy for the beryllium isoelectronic series extrapolated from bound systems Be and Li^- to a resonance state of He^{--}. A dashed line is an imaginary part of the energy times 100. The system He^{--} with a zero imaginary part is presumably in a virtual state.

FIG. 7. Ionization energy for neon isoelectronic series extrapolated from bound systems Ne and F^- to a resonance state of O^{--}. A dashed line is an imaginary part of the energy which is half-width of the level.

TABLE I. Singularities and critical charges for the helium isoelectronic series.

N	$Z_*^{(N)}$	$Z_c^{(N)}$
0	0.883 998	0.925 879
1	0.868 302	0.915 729
2	0.889 957	0.913 198
3	0.891 584	0.911 369
4	0.919 327	0.911 265
5	0.899 586	0.911 081
6		0.911 070
Stillinger [11]	0.894 1	0.911 2
Baker et al. [13]	0.911 028	

TABLE II. Resonances in the helium isoelectronic series for charges below the critical charge

$1/Z$	$-Z^{-2}\mathrm{Re}E$	$-Z^{-2}\mathrm{Im}E$	$-Z^{-2}\mathrm{Im}E$ (CRM [15])	$-Z^{-2}\mathrm{Im}E$ (model)
1.11	0.497 131	0.000 050	0.000 06	∼0.000 03
1.12	0.494 953	0.000 286	0.000 28	0.000 24
1.13	0.492 792	0.000 686	0.000 70	0.000 57
1.14	0.490 616	0.001 207	0.001 21	0.000 98

TABLE III. Energy of O^{--} resonance calculated by various methods

Reference	**Method**	$-E_\mathrm{I}$, eV
Clementi and McLean [22]	Hartree-Fock	8.30
Huzinaga and Hart-Davis [23]	Hartree-Fock-Roothaan[a]	7.68
Cantor [25]	Combining thermochemical data	7.94
Herrick and Stillinger [14]	Extrapolating formula including 3/2 power term	$5.38 - 0.65i$
	Eldén's [16] three-parameter formula	5.31
	Kaufman's [26] two-parameter formula	7.17
	Kaufman's [26] three-parameter formula	6.53
	Quadratic fit	7.09
Gadzuk and Clark [27]	Extrapolating of isoelectronic cases	8.8
Robicheaux et al. [28]	Polynomial fit	7.2[b]
Present paper	One-particle model	$7.65 - 0.22i$

[a]Huzinaga and Hart-Davis listed the total energy. We found ionization energy by subtracting Hartree-Fock total energy of the corresponding singly charged negative ion that is listed in papers of Clementi et al. [22,24]
[b]Estimated width is greater than 1 eV.

TABLE IV. Energies[a] of doubly charged negative ions[b]

Z	$-E_\mathrm{I}$, eV	Lifetime, 10^{-14} sec
2 He^{--}	-1.73	
4 Be^{--}	3.43	1.1
5 B^{--}	4.88	0.3
6 C^{--}	6.11[c]	
7 N^{--}	7.48	0.12
	7.97[d]	
	7.07[c]	
10 Ne^{--}	-0.92	
12 Mg^{--}	1.79	
13 Al^{--}	3.44	3.0
14 Si^{--}	4.76	0.5
	4.12[c]	
15 P^{--}	4.95	0.5
	4.47[c]	
16 S^{--}	4.91	0.7
	4.62[c]	
	4.7[e]	

[a]Tabulated energies are results of the present paper unless marked otherwise.
[b]For energy of O^{--} ion, see Table III.
[c]Hartree-Fock-Roothaan calculations of Huzinaga and Hart-Davis [23].
[d]Hartree-Fock calculations of Clementi and McLean [22].
[e]Polynomial fit of Robicheaux et al. [28].

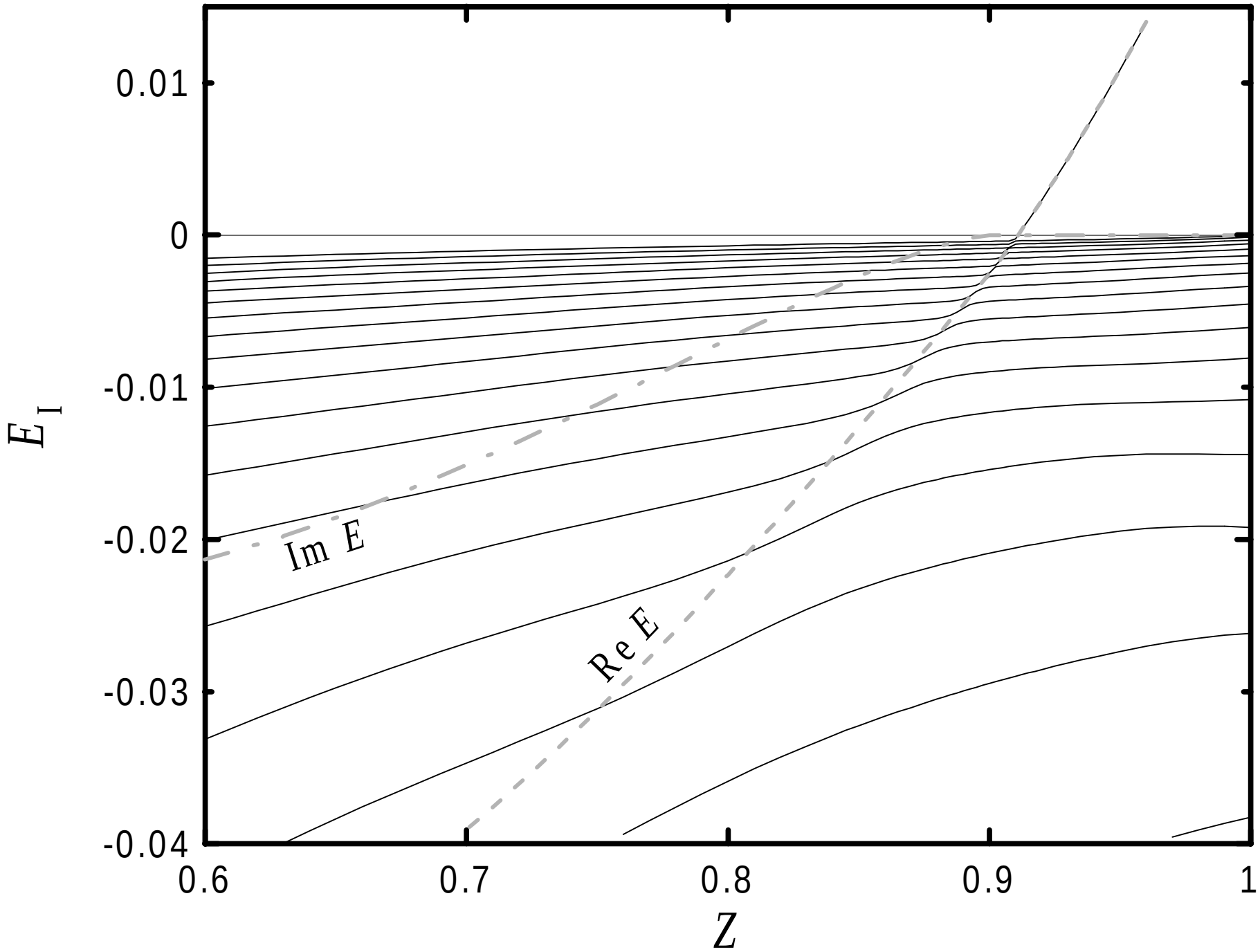


Fig. 1

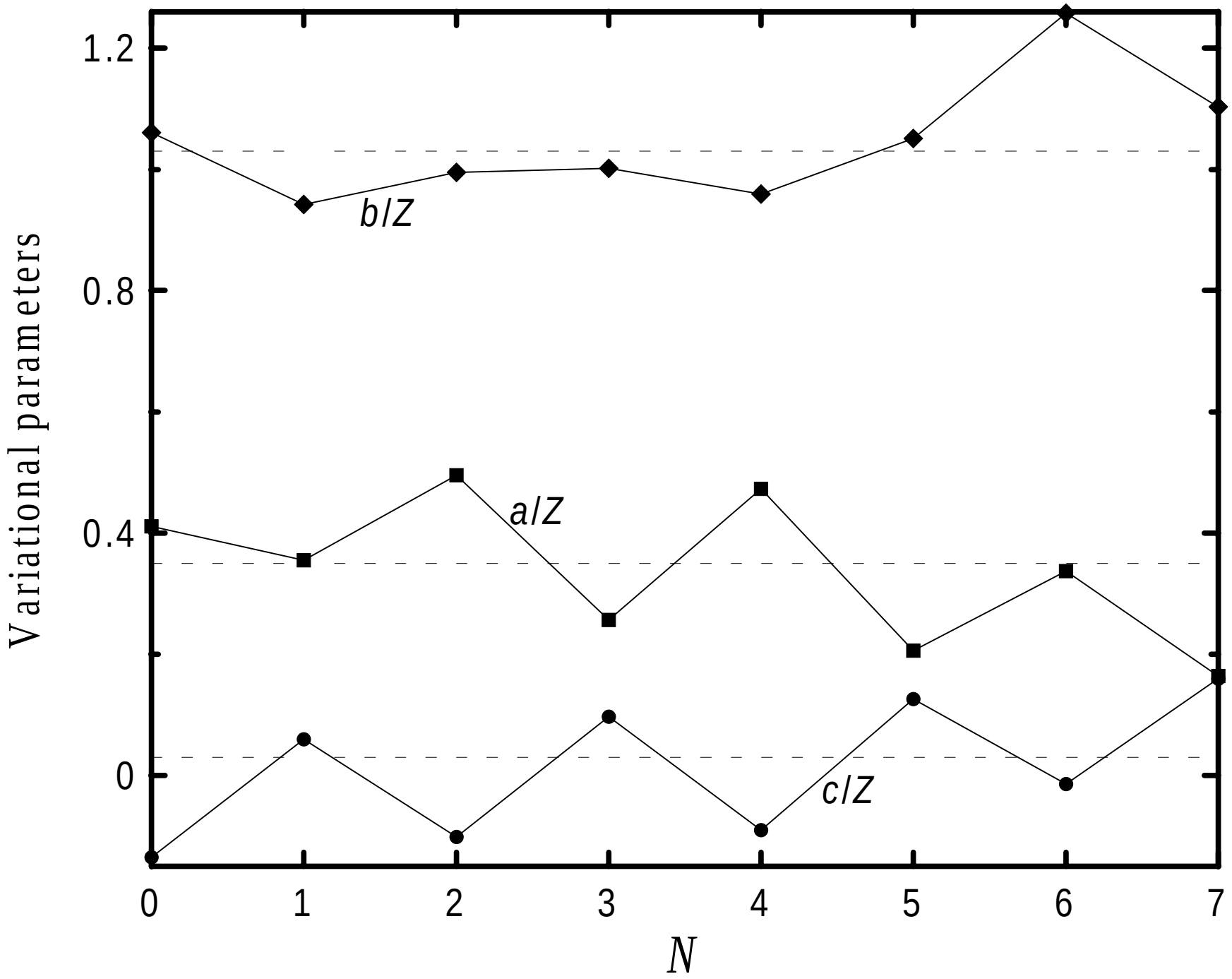
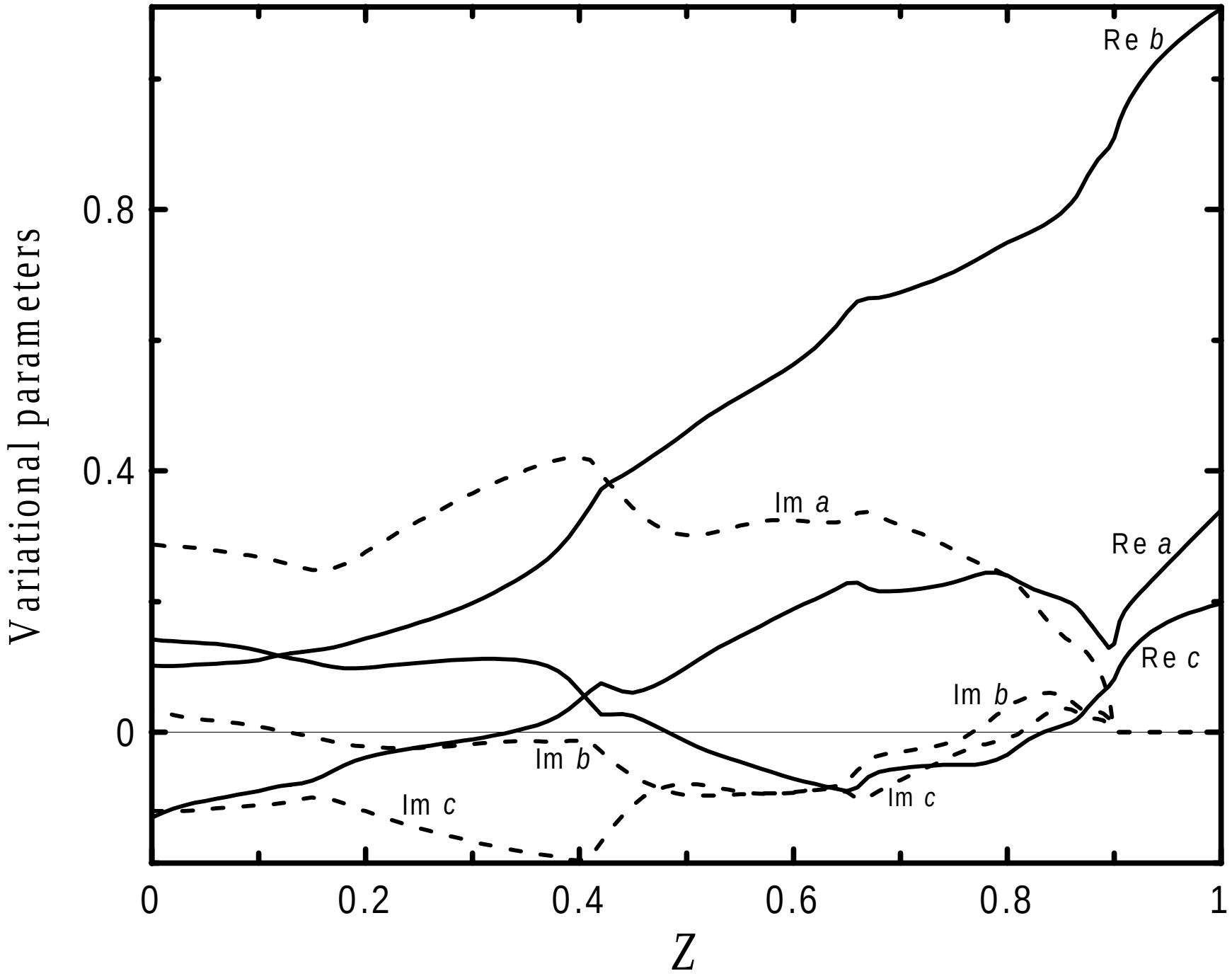


Fig. 2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Im a
Re a
Re c
Im b
Im b
Im c
Im c
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0.4
0
0
0.2
0.4
0.6
0.8
1
Z
Variational parameters

Fig. 3

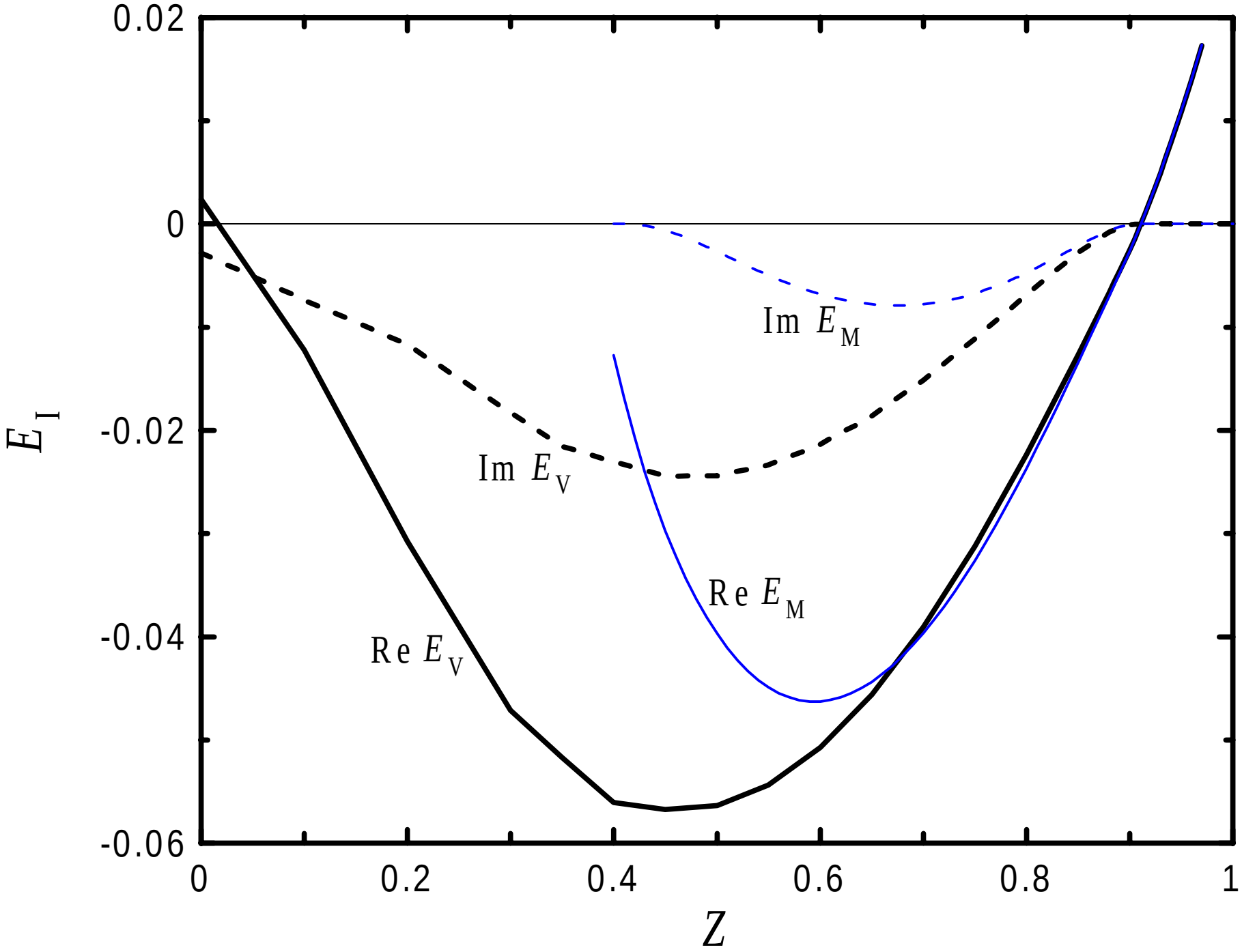

Fig. 4

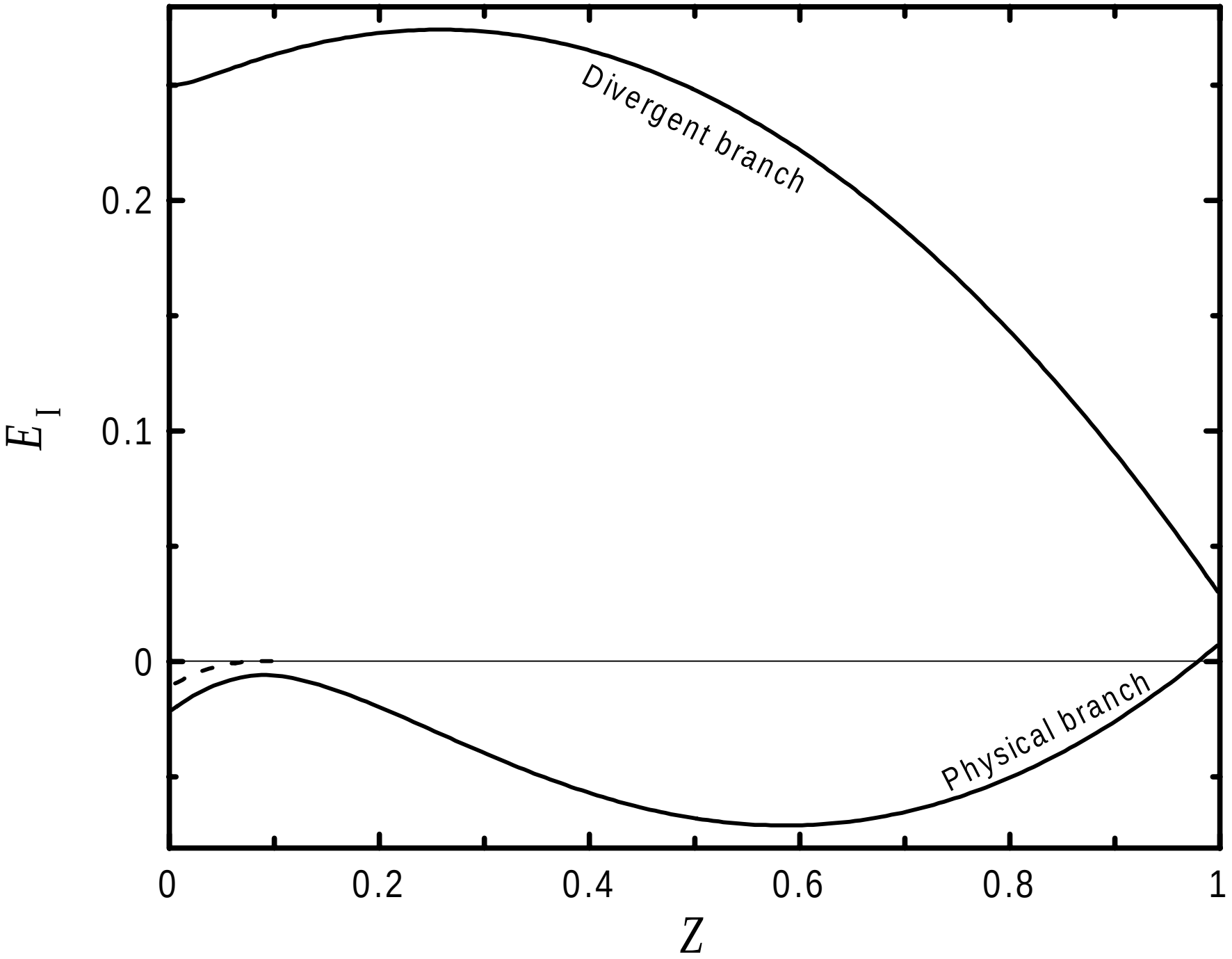

Fig. 5

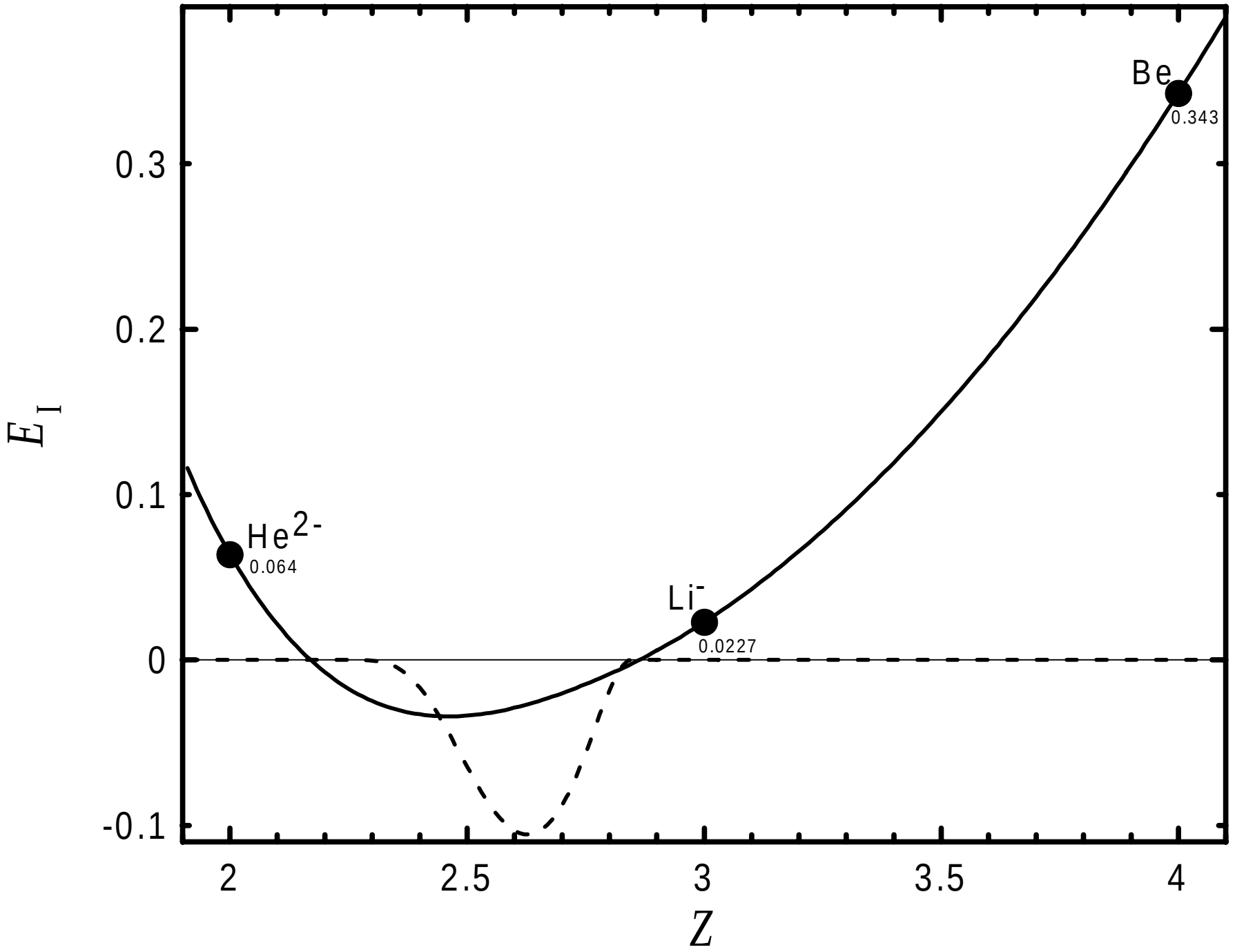

Fig. 6

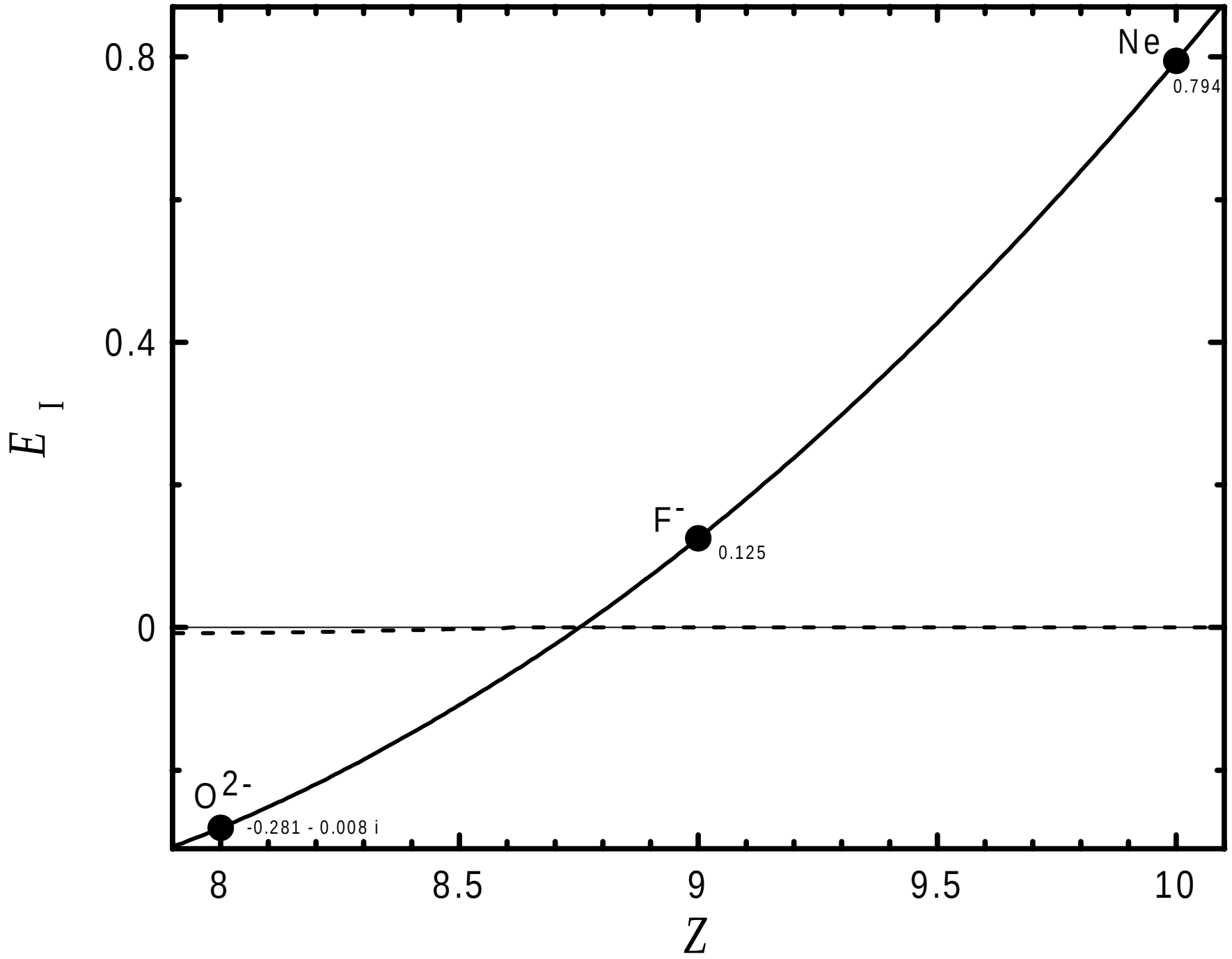

Fig. 7