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Complex virial theorem and complex scaling

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We present the simple generalization to complex energies of the normal global real scaling used for bound-state calculations to produce a variational energy which satisfies the virial theorem. We show that in two limiting cases, one or the other of which is almost always satisfied in all calculations, the virially stabilized complex energy is sensitive to *only* the real part *or* the imaginary part of the complex virial expression. We then compute the virial expression for a number of wave functions for the $1s2s^2\,{}^2S$ He$^-$, $1s2s2p\,{}^2P^o$ He$^-$, and $1s^22s^2kp\,{}^2P^o$ Be$^-$ resonances and the corresponding virially stabilized resonance energies. In all calculations one of the limiting cases was applicable.

I. INTRODUCTION

The complex scaling[1] theorems stimulated considerable research to develop computation techniques using square-integrable basis functions for calculating resonance parameters (position and width) for many different resonant phenomena. Doolen[2] suggested a variational technique in which one constructs a variational wave function from a standard square-integrable basis such as Slater-type orbitals (STO's) or Hylleraas functions and then computes the eigenvalues of a scaled Hamiltonian $\mathscr{H}(r\exp(i\theta))\equiv\mathscr{H}(\theta)$ as a function of θ. One then assumes that the best approximate eigenvalue and eigenfunction are those for which the rate of change of the eigenvalue with respect to θ is smallest, i.e., for which the eigenvalue is most stable with respect to variation in θ. He used a theta trajectory[2] (a plot of the complex energy as a function of θ) to identify stabilization points. Subsequently, Froelich *et al.*,[3] Brändas and Froelich,[4] and Yaris and Winkler[5] showed that if a root of the secular equation satisfied the appropriate complex virial theorem, it would be invariant under a complex scaling of the form $\nu=\alpha\exp(i\theta)$. Techniques[4,5] were then suggested for fixing ν (or θ) by requiring that the root satisfy [or satisfy as well as possible if just $\exp(i\theta)$ is used] the appropriate complex virial theorem.

On the other hand, in bound-state variational calculations for atoms, the virial constraint has been used to determine a final global scaling. That is, scaling the wave-function radial coordinate by a real parameter α yields[6]

$$T(\alpha)=\alpha^2T(1) \tag{1}$$

and

$$V(\alpha)=\alpha V(1)\,, \tag{2}$$

where $T(1)$ and $V(1)$ are the unscaled expectation values for the kinetic and potential energy. Minimization of E, with respect to α, then yields

$$\alpha=-[V(1)/2T(1)]\,. \tag{3}$$

Direct substitution of Eq. (3) into Eqs. (1) and (2) shows

$$V(\alpha)/T(\alpha)=-2\,, \tag{4}$$

i.e., the virial theorem is satisfied and by construction, the energy is minimized with respect to α. The expression for the energy is then

$$E^v=-[V^2(1)/4T(1)]\,. \tag{5}$$

In Sec. II, we present the straightforward extension of the bound-state results to the resonance case, while pointing out various limiting cases. Section III contains the results of calculations of the virial expression using many different complex stabilization wave functions. Finally, Sec. IV contains concluding remarks.

TABLE I. Resonance energies (a.u.) and virial calculations for $1s2s^2\,{}^2S$ He$^-$ wave functions.

Wave function[a]	$-E_R^e$	$-E_I^e$ (10^{-3})	$-E_R^v$	$-E_I^v$ (10^{-3})	W_R	$W_{\rm I}$
Ψ_1 ($\chi_1=0.1$)	2.190758	0.22285	2.190758	0.22285	2.00135	2.02684
Ψ_1 ($\chi_1=0.2$)	2.190758	0.22282	2.190758	0.22282	2.00135	2.02271
Ψ_1 ($\chi_1=0.4$)	2.190758	0.22282	2.190758	0.22282	2.00135	2.02236
Ψ_1 ($\chi_1=0.6$)	2.190758	0.22282	2.190758	0.22282	2.00135	2.02235
Ψ_1 ($\chi_1=0.8$)	2.190758	0.22283	2.190758	0.22283	2.00135	2.02044
Ψ_2	2.190758	0.22282	2.190758	0.22282	2.00135	2.02292
Ψ_3	2.190758	0.22283	2.190755	0.21686	2.00136	1.99597
Ψ_4	2.190758	0.22270	2.190747	0.20636	2.00135	1.92306
Ψ_5	2.190758	0.22273	2.190759	0.22249	2.00135	1.98077

[a] χ_1 here is α in Ref. 8.

II. VIRIAL THEOREM FOR RESONANCE STATES

The virial theorem for complex resonant states for Coulomb potentials takes the form[7]

$$(2T_R^v+V_R^v)+i(2T_I^v+V_I^v)=0\ , \tag{6}$$

or

$$(V_R^v/T_R^v)=-2\ , \tag{7a}$$

$$(V_I^v/T_I^v)=-2\ . \tag{7b}$$

Just as is the case with bound-state variational calculations, there is no reason to expect a wave function determined by the stabilization of the energy with respect to variations in the nonlinear parameters to satisfy the complex virial theorem. One can, however, define a final complex global scaling of the wave-function radial coordinate such that the complex virial theorem is satisfied.

Let $\gamma\exp(i\chi)$ be a complex scale factor. Since it contains two parameters, one can, in general, adjust the two parameters to satisfy two constraints such as in Eqs. (7). That is, for

$$\eta=\eta_R+i\eta_I=\gamma^{-1}\exp(-i\chi) \tag{8}$$

and T_R and T_I (V_R and V_L) being the real and imaginary parts of the expectation values for the kinetic (potential) energy, respectively, one has the virially stabilized energy E_r^v,

$$\begin{aligned}E_r^v&=(T_R^v+V_R^v)+i(T_I^v+V_I^v)\\&=\eta^2T+\eta V\ ,\end{aligned} \tag{9}$$

where η is defined such that

$$2(\eta_RT_R-\eta_IT_I)+V_R=0 \tag{10a}$$

and

$$2(\eta_RT_I+\eta_IT_R)+V_I=0\ . \tag{10b}$$

The solutions of Eqs. (10) can be put in several forms. Two of these are

$$\begin{aligned}\eta_R&=-\tfrac{1}{2}(V_R/T_R)+\tfrac{1}{2}(T_I/T_R)^2[1+(T_I/T_R)^2]^{-1}\\&\quad\times[(V_R/T_R)-(V_I/T_I)]\\&=-(T_RV_R+T_IV_I)/[2(T_R^2+T_I^2)]\end{aligned} \tag{11a}$$

and

$$\begin{aligned}\eta_I&=\tfrac{1}{2}(T_I/T_R)[1+(T_I/T_R)^2]^{-1}\\&\quad\times[(V_R/T_R)-(V_I/T_I)]\\&=(T_IV_R-T_RV_I)/[2(T_R^2+T_I^2)]\ .\end{aligned} \tag{11b}$$

Alternately, γ and χ are given by

$$\begin{aligned}\gamma&=2\{(V_R/T_R)^2-(T_I/T_R)^2[1+(T_I/T_R)^2]^{-1}\\&\quad\times[(V_R/T_R)^2-(V_I/T_I)^2]\}^{-1/2}\\&=2[(T_R^2+T_I^2)/(V_R^2+V_I^2)]^{1/2}\end{aligned} \tag{12a}$$

TABLE II. Resonance energies (a.u.) and virial calculations for $1s2s2p\,{}^2P^o$ He$^-$ wave functions.

Wave function	$-E_R^e$	$-E_1^e$ (10^{-2})	$-E_R^v$	$-E_I^v$ (10^{-2})	W_R	W_I
Ψ_6(72)	2.157427	0.76154	2.157427	0.76154	2.00297	1.63697
Ψ_7(94)	2.156553	0.67781	2.156553	0.67781	2.00784	7.44531
Ψ_8(126)	2.156543	0.65256	2.156543	0.65256	2.00758	3.87884

TABLE III. Resonance energies (a.u.) and virial calculations for $1s^2 2s^2 kp\ {}^2P^o$ Be^- wave functions.

Wave function	$-E_R^e$	$-E_I^e$ (10^{-2})	$-E_R^w$	$-E_I^w$ (10^{-2})	W_R	W_I
Ψ_9	14.544 273	0.763 03	14.544 273	0.763 03	2.000 11	1.659 89
Ψ_{10} $(\chi_1=0.60)$	14.575 358	2.122 16	14.575 358	2.122 16	2.001 16	2.384 66
Ψ_{10} $(\chi_1=0.65)$	14.575 454	2.121 68	14.575 454	2.121 68	2.001 13	2.304 79
Ψ_{10} $(\chi_1=0.70)$	14.575 519	2.117 12	14.575 519	2.117 12	2.000 97	2.260 98

and

$$\chi=\tan^{-1}\left[\frac{(T_I/T_R)[(V_R/T_R)-(V_I/T_I)]}{(V_R/T_R)-(T_I/T_R)^2(V_I/T_I)}\right]$$

$$=\tan^{-1}\left[\frac{[(V_R/T_R)-(V_I/T_I)]}{[(V_R/T_I)+(V_I/T_R)]}\right] . \tag{12b}$$

Equations (11) and (12) then define the alternate forms of the complex global scale factors such that when they are substituted into Eq. (9), they yield a complex energy E_r^v which satisfies the complex virial theorem.

Several special cases of Eqs. (11) and (12) are of interest. First, if T_R, V_R, T_I, and T_I do indeed satisfy the virial theorem, Eqs. (7), then

$$\eta_R=1 , \tag{13a}$$

$$\eta_I=0 , \tag{13b}$$

$$\gamma=1 , \tag{13c}$$

and

$$\chi=0 , \tag{13d}$$

as required. Alternately, if $|T_R| >> |T_I|$ and $|V_R| >> |V_I|$, then

$$\eta_R\approx-\tfrac{1}{2}(V_R/T_R) , \tag{14a}$$

$$\eta_I\approx\tfrac{1}{2}(T_I/T_R)[(V_R/T_R)-(V_I/T_I)] , \tag{14b}$$

$$\gamma\approx2\,|T_R/V_R| , \tag{14c}$$

and

$$\chi\approx\tan^{-1}\{(T_I/T_R)(V_R/T_R)^{-1}$$

$$\times[(V_R/T_R)-(V_I/T_I)]\} . \tag{14d}$$

Finally, if $|T_I| >> |T_R|$ and $|V_I| >> |V_R|$, then

$$\eta_R\approx-\tfrac{1}{2}(V_I/T_I) , \tag{15a}$$

$$\eta_I\approx\tfrac{1}{2}(T_R/T_I)[(V_R/T_R)-(V_I/T_I)] , \tag{15b}$$

$$\gamma\approx2\,|T_I/V_I| , \tag{15c}$$

and

$$\chi\approx\tan^{-1}\{(T_R/T_I)(V_I/T_I)^{-1}$$

$$\times[(V_R/T_R)-(V_I/T_I)]\} . \tag{15d}$$

TABLE IV. η and E_r^v.

Wave function	γ	χ^{a}	$-E_R^v$	$-E_I^{v\,\mathrm{a}}$
Ψ_1 $(\chi_1=0.1)$	0.999 32	−0.126 33(−5)	2.190 759	0.222 85(−3)
Ψ_1 $(\chi_1=0.2)$	0.999 33	−0.106 30(−5)	2.190 759	0.222 82(−3)
Ψ_1 $(\chi_1=0.4)$	0.999 33	−0.104 56(−5)	2.190 759	0.222 82(−3)
Ψ_1 $(\chi_1=0.6)$	0.999 32	−0.104 54(−5)	2.190 759	0.222 82(−3)
Ψ_1 $(\chi_1=0.8)$	0.999 33	−0.952 04(−6)	2.190 759	0.222 83(−3)
Ψ_2	0.999 33	−0.107 31(−5)	2.190 759	0.222 83(−3)
Ψ_3	0.999 32	0.268 07(−6)	2.190 756	0.216 86(−3)
Ψ_4	0.999 33	0.399 72(−5)	2.190 748	0.206 35(−3)
Ψ_5	0.999 33	0.106 58(−5)	2.190 760	0.222 48(−3)
$\Psi_6(72)$	0.998 52	0.101 56(−2)	2.157 430	0.760 89(−2)
$\Psi_7(94)$	0.996 09	−0.133 10(−2)	2.156 582	0.680 06(−2)
$\Psi_8(126)$	0.996 22	−0.987 16(−3)	2.156 752	0.654 18(−2)
Ψ_9	0.999 95	0.135 24(−3)	14.544 273	0.763 01(−2)
Ψ_{10} $(\chi_1=0.60)$	0.999 42	−0.201 75(−3)	14.575 363	0.212 25(−1)
Ψ_{10} $(\chi_1=0.65)$	0.999 44	−0.169 48(−3)	14.575 459	0.212 20(−1)
Ψ_{10} $(\chi_1=0.70)$	0.999 52	−0.149 83(−3)	14.575 522	0.211 73(−1)

[a] Number in parentheses is exponent of ten.

TABLE V. Real and imaginary parts of kinetic and potential energies and γ and χ from the limiting case given by Eqs. (14).

Wave function	T_R	$-V_R$	T_I[a]	$-V_I$[a]	γ	χ[a]
Ψ_1 ($\chi_1=0.1$)	2.187 799	4.378 557	2.170 231(−4)	4.398 713(−4)	0.999 33	−0.126 34(−5)
Ψ_1 ($\chi_1=0.2$)	2.187 803	4.378 561	2.178 702(−4)	4.406 891(−4)	0.999 33	−0.106 28(−5)
Ψ_1 ($\chi_1=0.4$)	2.187 803	4.378 561	2.179 460(−4)	4.407 648(−4)	0.999 33	−0.104 58(−5)
Ψ_1 ($\chi_1=0.6$)	2.187 802	4.378 561	2.179 462(−4)	4.407 643(−4)	0.999 33	−0.104 53(−5)
Ψ_1 ($\chi_1=0.8$)	2.187 803	4.378 561	2.183 628(−4)	4.411 890(−4)	0.999 33	−0.952 04(−6)
Ψ_2	2.187 803	4.378 561	2.178 297(−4)	4.406 523(−4)	0.999 33	−0.107 31(−5)
Ψ_3	2.187 83	4.378 538	2.177 372(−4)	4.345 963(−4)	0.999 32	0.268 03(−6)
Ψ_4	2.187 794	4.378 541	2.235 577(−4)	4.299 151(−4)	0.999 33	0.399 73(−5)
Ψ_5	2.187 812	4.378 571	2.268 486(−4)	4.493 356(−4)	0.999 33	0.106 62(−5)
$\Psi_6(72)$	2.151 039	4.308 466	1.195 563(−2)	1.957 101(−2)	0.998 52	0.101 56(−2)
$\Psi_7(94)$	2.139 769	4.296 322	1.051 636(−3)	7.829 749(−3)	0.996 10	−0.133 10(−2)
$\Psi_8(126)$	2.140 314	4.296 857	2.266 759(−3)	8.792 393(−3)	0.996 22	−0.987 16(−3)
Ψ_9	14.542 703	29.086 975	1.156 292(−2)	1.919 323(−2)	0.999 95	0.135 25(−3)
Ψ_{10} ($\chi_1=0.60$)	14.558 509	29.133 868	1.532 618(−2)	3.654 775(−2)	0.999 42	−0.201 74(−3)
Ψ_{10} ($\chi_1=0.65$)	14.559 047	29.134 502	1.626 075(−2)	3.747 755(−2)	0.999 44	−0.169 48(−3)
Ψ_{10} ($\chi_1=0.70$)	14.561 410	29.136 929	1.678 944(−2)	3.796 065(−2)	0.999 52	−0.149 82(−3)

[a]Number in parentheses is exponent of ten.

Using Eqs. (11), one can put Eq. (9) into several useful forms:

$$E_r^v = -\tfrac{1}{4}V^2/T \tag{16a}$$

$$= -\tfrac{1}{4}(V_R+iV_I)^2/(T_R+iT_I) \tag{16b}$$

$$= -[\,(T_R V_R^2 + 2T_I V_I V_R - T_R V_I^2) + i(\,2T_R V_R V_I + T_I V_I^2 - T_I V_R^2)]/[4(T_R^2+T_I^2)]\ . \tag{16c}$$

Equation (16c) is particularly interesting for two limiting cases. If $|T_R| \gg |T_I|$, $|V_R| \gg |V_I|$, and $(V_R/T_R)\approx -2$,

$$E_r^v \approx (-1/4T_R^2)[(T_R V_R^2)+i(2T_R V_R V_I - T_I V_R^2)]$$

$$\approx \tfrac{1}{2}V_R + i(T_I+V_I) \approx E_R + iE_I = E_r\ . \tag{17a}$$

Also, if $|T_I| \gg |T_R|$, $|V_I| \gg |V_R|$, and $(V_I/T_I)\approx -2$,

$$E_r^v \approx (V_R+T_R)+i\tfrac{1}{2}V_I$$

$$\approx E_R + iE_I = E_r\ . \tag{17b}$$

Equations (17) show that for two very interesting cases E_r^v is approximately equal to the variational energy E_r regardless of how well T_I and V_I in the first case and T_R and V_R in the second case satisfy the virial theorem. That is, the complex energy E_r^v really only depends on how well the larger of E_R or E_I satisfies the virial theorem in these limiting cases.

III. CALCULATION OF VIRIAL EXPRESSION

As noted in Sec. II one can define a final overall complex scaling of the wave-function radial coordinate relative to the radial coordinate of the Hamiltonian. Here we report the results for a number of wave functions which have previously been obtained in complex stabilization calculations. In Tables I–III we give the results for a number of wave functions for the $1s2s^2\,{}^2S$ He$^-$, $1s2s2p\,{}^2P^o$ He$^-$, and $1s^22s^2kp\,{}^2P^o$ Be$^-$ resonances. The wave functions are given in Refs. 8–11. Ψ_1 is the 51 configuration wave function[8] with the open shell single configuration target state. Ψ_2 is $\Psi_{\rm I}$ of Ref. 9, while Ψ_3 is $\Psi_{\rm II}$ of Ref. 9 with the complex basis function $r\exp(ikr)\exp(-\delta r)$ replaced by $\exp(ikr)\exp(-\delta r)$. Ψ_4 is identical to $\Psi_{\rm II}$ of Ref. 9. Ψ_5 is the same as Ψ_4 but with the configuration $[(1s1s')5s\ (\delta=0.5)]$ removed. Ψ_6, Ψ_7, and Ψ_8 are the 72, 94, and 126 configuration wave functions of Ref. 10, respectively. Finally, Ψ_9 and Ψ_{10} are two wave functions,[11] one with 32 configurations and one with 96 configurations, respectively, for the $1s^22s^2kp\,{}^2P^o$ shape resonance in Be$^-$. The difference between them is just the types of correlation of the $(2s)^2$ part of the wave function. In Ψ_9 only s orbitals are used for this correlation, while Ψ_{10} includes $npn'p\ {}^1S$ correlation effects. E_R^e and E_I^e are the real and imaginary parts of the complex resonant energy as obtained from the solution of the secular equation, while E_R^w and E_I^w are the same except they are computed as the expectation value of the Hamiltonian using the eigenvector obtained from the solution of the secular equation. A comparison of E_R^e with E_R^w and E_I^e with E_I^w provides an indication of the quality of the wave function. The potential difficulties in solving for the eigenfunctions are particularly evident for wave functions Ψ_3, Ψ_4, and Ψ_5.

Computing the eigenvalues of the overlap matrix for the configurations in Ψ_4, one finds some approximate linear dependence. The configuration removed from Ψ_4 to give Ψ_5 is the primary source of the problem as indicated by the considerable improvement. All other wave functions yield excellent results.

W_R and W_I are $-(V_R/T_R)$ and $-(V_I/T_I)$. The wave functions in Table I satisfy the real and imaginary parts of the virial expression quite well, while those in Table II only yield a good value of the real part of the virial expression. Those in Table III again yield excellent results for the real part of the virial theorem, but only moderately good results for the imaginary part.

The global complex scaling factors $\gamma\exp(i\chi)$ which yield wave functions which satisfy the real and imaginary parts of the virial theorem for each wave function along with the virially stabilized energies are given in Table IV. It is clear that even for those wave functions for which $-(V_I/T_I)$ was very different from two, E_r^v is approximately equal to E_r from the variational calculation. The reason for this can be seen in Table V. Here, we give the values of T_R, T_I, V_R, V_I, γ [from Eq. (14c)], and χ [from Eq. (14d)]. From Tables V and I—III it is obvious that these resonances and wave functions satisfy the limiting case in Sec. II, where $|T_R| \gg |T_I|$, $|V_R| \gg |V_I|$, and $-(V_R/T_R)\approx 2$. Thus, E_r^v is insensitive to the imaginary part of the virial expression. That is, while one can force the real and imaginary parts of the virial expression to be satisfied, E_r^v is insensitive to the imaginary part.

IV. DISCUSSION

We have discussed the extension of the virial scaling technique often used in bound-state calculations to the case of resonance calculations involving complex energies. Unlike the case for variational bound-state calculations where one obtains an upper bound so that the global real scaling to force satisfaction of the virial condition yields a necessarily improved energy, forcing satisfaction of the complex virial theorem does not guarantee an improved energy, but only that the complex energy is stabilized with respect to variations in the final global complex scaling parameter. In neither case, bound or resonant, is the energy guaranteed to be minimized or stabilized with respect to variations in any of the other nonlinear parameters in the wave function. Neither computing the virial expression nor constructing a virially stabilized energy E_r^v provides information on either stabilization of E_r^v with respect to other nonlinear parameters or convergence with respect of configuration interaction. This is particularly evident in Tables III and IV where the globally scaled wave functions Ψ_9 and Ψ_{10} yield very different real and imaginary resonant energies.

Finally, we have derived several limiting cases for the virially stabilized energy and the corresponding global-scaling parameter. This analysis shows that often the resonant energy is sensitive only to either the real or the imaginary part of the virial expression.

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