International Journal of Quantum Technologies ISSN: 3068-9090

PRIME OPEN ACCESS

Volume 2, Issue 4

Research Article

Date of Submission: 26 Oct, 2026
Date of Acceptance: 03 Nov, 2026
Date of Publication: 13 Nov, 2026

Practical Using the Resonant-Consistent Method for Optimizing A Exponents of Gaussian Basis Sets

Pavel Florián*

Central European Institute of Technology, Žerotínovo nám. 617/9, 601 77 Brno Czech Republic

***Corresponding Author:** Pavel Florián, Central European Institute of Technology, Žerotínovo nám, 617/9, 601 77 Brno Czech Republic.

Citataion: Florián, P. (2026). Practical Using the Resonant-Consistent Method for Optimizing A Exponents of Gaussian Basis Sets. *Int J Quantum Technol ,2*(4), 01-04.

Abstract

The resonant-consistent method, which was developed for Slater type orbitals (STOs), firstly introduced in [1] article and mathematically analyzed in article [2]. Is sustainable too for optimizing exponents of high-quality Gaussian basis sets with remained radial nodal structures. In this study is introduced plugin for Psi4 quantum chemistry package version 1.1.1, which replicate the resonant consistent method in article [1] (with half the default update rate for the exponents) for Gaussian basis sets and are shown the results of optimizing the exponents of aug-cc-pCVXZ basis for He, H2, LiH, BeH2 and H2O species.

Introduction

A new method of optimizing the basis sets named Resonant-consistent method, which was firstly successfully used in article was implemented too for using the Gaussian basis sets with Psi4 quantum chemistry package in form of Resonant-consistent Psi4 plugin version 2.0 for Psi4 version 1.1.1. This plugin was written in C++ and has a Python scripts. This implementation include a resonant-consistent basis optimizing mechanism, inner implementation of four ab-initio methods for expressing the correlation energies and atom orbitals occupancies (CISD, CCSD, DMRG and default MP2), non-orthogonality correction algorithm, implementation of ARO90 basis set for physicist (which is not suitable for a weak-correlated systems) and Python scripts for iterative optimizing [1].

In this work was too used the Python DEC Engine script for Divide-Expand-Consolidate scheme, which allow the using the ab-initio methods too for large chemical species, but small molecules in this study was not fragmented and was given directly to Psi4. This script was used for multi-iteration basis optimizing, which must be implemented outside Psi4 quantum chemistry package.

The Five Chemical Species Were Investigated for Comparison of a Plain Correlation-Consistent Basis Sets and Resonant-Consistent Method Optimized Basis Sets:

- He with aug-cc-pCVDZ, aug-cc-pCTDZ, aug-cc-pCVQZ, aug-cc-pCV5Z and aug-cc-pCV6Z,
- H2 with aug-cc-pCVDZ, aug-cc-pCTDZ, aug-cc-pCVQZ, aug-cc-pCV5Z,
- LiH, BeH2 and H2O with aug-cc-pCVQZ.

This optimalization of basis exponents was realized on scheme with additional 5 excited energy levels, and 8 iterations using the second-order Moller-Plesett perturbance theory - MP2 with the non-orthogonality correction and freezing the core electrons, if there are more shells on atoms.

The final computation was realized by Equation of motion coupled cluster singlets and doublets method (EOM-CCSD) and was computed a overall Hamiltonian spectroscopic data – five excited energy levels.
Etalon Computations of He and H2
The results of computation of He and H2 Hamiltonians (H) are in tables below (Table 1 and Table 2) with H without

Resonant-consistent method, H with Resonant-consistent method, its difference, difference to experimental values without Resonant-consistent method and difference to experimental values with Resonant-consistent method from left to right. With more basis function and more complete basis set are the results of correlation-consistent and resonant consistent method closer for both species (He and H2) and resonant-consistent method error is eliminated, which is in agreement with theory in articles [1,2].

Basis set	Number of basis	H plain [Ha]	H optimized [Ha]	H difference [Ha]	H plain to exp [Ha]	H optimized to exp [Ha]
aug-cc-pCVDZ	9	−2.88956790	−2.42334935	0.47000000	0.01000000	0.48003648
aug-cc-pCVTZ	23	−2.90023001	−2.87583071	0.02439930	0.00315582	0.02755512
aug-cc-pCVQZ	46	−2.90207659	−2.90008868	0.00198791	0.00130924	0.00329715
aug-cc-pCV5Z	80	−2.90238735	−2.90208916	0.00029819	0.00099848	0.00129667
aug-cc-pCV6Z	127	−2.90250817	−2.90224833	0.00025984	0.00087766	0.00113750

Table 1: Results Of Computation The Helium (He) Hamiltonians For Correlation-Consistent And Resonant-Consistent Optimized Basis Sets And Its Comparison To Experimental Value -2.90338583 Ha [3,4]

Basis set	Number of basis	H plain [Ha]	H optimized [Ha]	H difference [Ha]	H plain to exp [Ha]	H optimized to exp [Ha]
aug-cc-pCVDZ	18	-1.16000000	-1.14863834	0.01583979	0.00999188	0.02583166
aug-cc-pCVTZ	46	-1.17246693	-1.16978063	0.00268629	0.00200307	0.00468937
aug-cc-pCVQZ	92	-1.17337762	-1.17334275	0.00003487	0.00109238	0.00112725
aug-cc-pCV5Z	160	-1.17357272	-1.17357205	0.00000068	0.00089728	0.00089795

Table 2: Results of Computation the Hydrogen (H2) Hamiltonians For Correlation-Consistent and Resonant-Consistent Optimized Basis Sets and Its Comparison to Experimental Value -1.17447 Ha [5]

The results of computations the gaps are in tables below (Table 3 and Table 4) with gap without Resonant-consistent method, gap with Resonant-consistent method, its difference, difference to experimental value without Resonant-consistent method and difference to experimental value with Resonant-consistent method from left to right. The results of correlation-consistent and resonant consistent method are with more basis function and more complete basis set closer for both species (He and H2) and resonant-consistent method error is eliminated, which is in agreement with theory in articles [1,2].

Gap plain [eV]	Gap optimized [eV]	ΔE difference [eV]	E plain to exp [eV]	E optimized to experimantal [eV]
21.6500	24.7930	3.1460	1.8272	4.9732
20.9700	22.3550	1.3850	1.1502	2.5352
20.9030	22.8390	1.9360	1.0832	3.0192
20.8720	21.6350	0.7630	1.0522	1.8152
20.8250	21.2530	0.4280	1.0052	1.4332

Table 3: Results of Computation the Helium (He) Gaps (Differences of High Occupied Orbitals and Low Unoccupied Orbitals) And Its Comparison To Experimental Value 19.8198 eV [4]

Gap plain [eV]	Gap optimized [eV]	ΔE difference [eV]	E plain to exp [eV]	E optimized to experimantal [eV]
12.6700	12.5300	-0.1400	1.4700	1.3300
12.7560	12.7820	0.0260	1.5560	1.5820
12.7750	12.8120	0.0370	1.5750	1.6120
12.7870	12.8000	0.0130	1.5870	1.6000

Table 4: Results of Computation the Hydrogen (H2) gaps (Differences of High Occupied Orbitals and Low Unoccupied Orbitals) And Its Comparison to Experimental Value 11.2 eV [6]

Computations of Lih, Beh2 And H2o With Spectral Properties

Next were performed computations of electronic structures of LiH, BeH2 and H2O ground states (see Table 5) and its spectroscopic properties (see Table 6). The ground state energies were computed form sum of ionization energies of elements and molecular enthalpies obtained from NIST database similarly as the spectral lines. The ground state of water was obtained too from study and spectral lines from study [7-9].

The ground states are decreased and closest to experimental values with using the Resonant-consistent method. The correlation energies of LiH, BeH2 and H2O are -0.0367666, -0.0782518 and -0.291183 Ha, while the resonant-consistent decreases are -0.0000124, -0.0000053 and -0.0000220 Ha. The most correlated H2O has the deepest resonant-consistent decrease.

The spectral transitions of LiH, BeH2 was changed via resonant-consistent basis optimization negligible or imperceptibly. The first three spectral transitions of water were improved and set closer to the experimental data (spectral transitions at 7.41, 9.2 and 9.67 eV with 0.046, 0.00 and 0.051 oscillator strengths) [9].

Molecule	Number of basis	H plain [Ha]	H optimized [Ha]	H difference [Ha]	Converged	H [Ha] experiment
LiH	155	-8.0240060	-8.0240184	-0.0000124	True	-8.0621290
BeH2	201	-15.8512922	-15.8512975	-0.0000053	False	15.8902105
H2O	144	-76.3572392	-76.3572612	-0.0000220	False	-76.4095460

Table 5: Results of Computations of the Lithium Hydride (Lih), Beryllium Hydride (Beh2) And Water (H2o) Hamiltonians For Unoptimized And Resonant-Consistent Optimized Basis Sets and Its Comparison to Experimental Values

Molecule	Spectra transition	ΔE plain [eV]	ΔE optimized [eV]	ΔE plain - optimized [eV]	Oscillator strength plain	Oscillator strength optimized
LiH	n->pi	3.684	3.680	0.004	0.0683884	0.0683989
	n->pi	4.658	4.658	0.000	0.1932060	0.1932094
	pi->sigma	5.937	5.938	-0.001	0.1932060	0.1932094
	pi->sigma	6.519	6.537	-0.018	0.0214792	0.0211027
	pi->sigma	6.795	6.796	-0.001	0.0011485	0.0008172
BeH2	pi->sigma	6.550	6.550	0.000	0.0000000	0.0000000
	sigma->sigma	8.685	8.685	0.000	0.0000000	0.0000000
	sigma->sigma	9.251	9.253	-0.002	0.4652135	0.4647348
	sigma->sigma	9.848	9.848	0.000	0.4652135	0.4647348
	sigma->sigma	9.975	9.960	0.015	0.0842933	0.0835439
H2O	$^1B_1$	7.690	7.690	0.000	0.0500000	0.0462000
	$^1A_2$	9.474	9.450	-0.026	0.0000000	0.0000000
	$^1A_1$ (3s)	10.039	10.030	0.009	0.0942000	0.0953000
	sigma->sigma	10.654	10.761	-0.107	0.0054373	0.0083240
	sigma->sigma	11.112	11.428	-0.316	0.0054373	0.0050288

Table 6: Results of Computations of The Lithium Hydride (Lih), Beryllium Hydride (Beh2) And Water (H2o) Gaps (Differences of High Occupied Orbitals and Low Unoccupied Orbitals), Spectral Transitions and Its Comparison to Its Experimental Values

Conclusion

In this study was confirmed the theory of resonant-consistent method described in articles and via Hamiltonians and spectral gaps of He and H2. With more complete and more similar to Slater type orbitals Gaussian basis sets were the resonant-consistent computational results more closest to results with plain correlation-consistent basis sets and experimental results. The correlation-consistent results were closest to experimental results, than resonant-consistent results, which is logical, due to incompleteness of the Gaussian basis sets and its difference from Slater type orbitals [1,2].

In series of computations of LiH, BeH2 and H2O was confirmed, that resonant-consistent optimization of basis sets is usable too in quantum chemistry computations, but for simple molecules with equilibrated geometries are the basis exponents of correlation-consistent basis sets near to his ideal values and using the resonant-consistent cause the ineffective additional computational resources consumption.

But for more correlated chemical species and edge cases become the exponents of correlation-consistent basis sets

wrong due to external influences and optimizing for atomic computations and there can be the resonant-consistent method with frozen core electrons good choice. Very interesting may by too combination of resonant-consistent method with ability to jump over the local energy landscape minima for optimizing a system Hamiltonians due to its self-consistent nature with gradient-descent method for fine tuning the basis exponents for all electrons together.

References

1. Florian P.; Optimization of basis sets by a resonant-consistent method for elements and basic compounds. International Journal of Quantum technology. vol .2, no. 1, 2026.
2. Florian P.; Partial derivarion of the sqrt(N) member in resonant-consistent method. International Journal of Quantum technology. vol .2, no. 3, 2026.
3. Kandula, Jize, Gohle, A., Pinkert, T. J., Ubachs, W., & Eikema, K. S. E. (2010). Deep-Ultraviolet Metrology and the Ionization Energy of the Helium Ground State. Laser Centre Vrije Universiteit, De Boelelaan 1081, 1081HV Amsterdam, Netherlands. 2010.
4. Martin, W. C. (1973). Energy levels of neutral helium (4He i).
5. Kolos, W., & Wolniewicz, L. (1968). Improved theoretical ground-state energy of the hydrogen molecule. The Journal of chemical physics, 49(1), 404-410.
6. Kol/os, W., & Wolniewicz, L. (1965). Potential-Energy Curves for the X 1Σ g+, b 3Σ u+, and C 1Π u States of the Hydrogen Molecule. The Journal of Chemical Physics, 43(7), 2429-2441.
7. Kramida, A., Ralchenko, Yu., Reader, J. (2024). NIST ASD Team. NIST Atomic Spectra Database (version 5.12). National Institute of Standards and Technology.
8. B. Ruscic, R. E. Pinzon, M. L. Morton, N. K. Srinivasan, M.-C. Su, J. W. Sutherland and J. V. Michael. (2006). Active Thermochemical Tables: Accurate Enthalpy of Formation of Hydroperoxyl Radical, HO_2. J. Phys. Chem. A. vol. 110, pp. 6592–6601.
9. W. C. Price. (1936). The Far Ultraviolet Absorption Spectra and Ionization Potentials of H_2O and H_2S. J. Chem. Phys. vol. 4, pp. 147–153.