

Comment on "Improved many-body expansions from eigenvector continuation"

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(Dated: April 16, 2021)

In a recent paper [Phys. Rev. C 101, 041302(R) (2020)] Demol et al. published an interesting method to improve results from finite-order perturbation theory. Their applications on nuclear many-body problems show that the numerical results are very accurate, capable of converting divergent series to fast-converging sequences. We argue that one reason of this impressive accuracy is connected to those of related methods which proved to be useful in many-electron theory.

Owing to the complexity of the quantum many-body problem, perturbational theoretical (PT) approaches are extensively used even for strong interactions where the PT series is often divergent. This makes it important to develop methods which regularize divergences and predict accurate approximations to eigenenergies by resummation or similar techniques.

A successful theory was recently proposed by Demol et al.[1]. They noted that when treating a many-body Hamiltonian of form

$$H(c) = H_0 + c H_1$$

perturbatively (here H_0 is a zero order Hamiltonian, H_1 is the perturbation, $c \in [0, 1]$ is a continuously variable perturbation parameter), the many-body problem may be easier to solve for small values of parameter c even if the emerging many-body PT (MBPT) series at the physical value of c is divergent. The authors envision a basis set obtained by finding eigenvectors $\Psi(c_i)$ for several selected parameter values $c_i \leq R_e$, where R_e is the convergence radius of MBPT. Thereby, a low-dimensional manifold $\{\Psi(c_i)\}$ emerges, in the subspace of which exact eigenstates corresponding to the physical case $c = 1$ can be effectively approximated. They term this as eigenvector continuation. Further, to make the procedure more practical, they realize that the space $\{\Psi(c_i)\}$ is connected to the space of vectors $\{\Phi^{(k)}\}$ by a simple linear transformation, where $\Phi^{(k)}$ is the k -th order perturbational wave function, $k = 0, 1, \dots, P$. Finally, Demol et al. propose to solve the $(P+1) \times (P+1)$ dimensional matrix eigenvalue problem of $H = H(c = 1)$ in the overlapping metric of the perturbed functions:

$$\sum_{l=0}^P \langle \Phi^{(k)} | H | \Phi^{(l)} \rangle X_l^P = E^P \sum_{l=0}^P \langle \Phi^{(k)} | \Phi^{(l)} \rangle X_l^P \quad (1)$$

with increasing order P to get energies with increasing accuracy.

The results are impressive: the values of the ground state energies E^P converge fast with increasing P to the exact energies.

The aim of this Comment is to provide some explanation of this success and to relate the method proposed in [1] to other existing methods.

The perturbed wave functions $\Phi^{(k)}$, $k = 1, 2, \dots, P$ in Ref.[1] were computed from a recursive PT scheme which is worth recalling here:

$$\Phi^{(k)} = Q \left(H_1 - E_0^{(1)} \right) \Phi^{(k-1)} - Q \sum_{l=2}^{k-1} E_0^{(l)} \Phi^{(k-l)} \quad (2)$$

(see e.g. Ref.[2]), where $E_0^{(l)}$ are the ground state energies at order l , while Q is the reduced resolvent

$$Q = \left(1 - |\Phi^{(0)}\rangle \langle \Phi^{(0)}| \right) \left(E_0^{(0)} - H_0 \right)^{-1} \left(1 - |\Phi^{(0)}\rangle \langle \Phi^{(0)}| \right),$$

which in spectral resolution simplifies to

$$Q = \sum_{j \neq 0}^{\infty} \frac{|\Phi_j^{(0)}\rangle \langle \Phi_j^{(0)}|}{E_0^{(0)} - E_j^{(0)}},$$

if $\Phi_j^{(0)}$ is the j -th eigenvector of H_0 . (Though not explicitly stated there, we presume that in Ref.[1] the Rayleigh-Schrödinger PT is applied.)

As it is apparent from Eq.(2), the most dominant (and most expensive to compute) term in $\Phi^{(k)}$ is the first one, $Q H_1 \Phi^{(k-1)}$, which, apart from the reduced resolvent Q , essentially generate a Krylov basis, in which the exact wave function can be, in principle, expanded. This expansion, which goes via the nonorthogonal sequence of functions $H_1 \Phi^{(k-1)}$, is known to be slowly convergent. Much better expansion is provided by the Lanczos basis[3], which is generated by Schmidt-orthogonalizing the new vectors to the previous ones in each iteration step. Lanczos expansions were reported to be sometimes numerically unstable and/or slowly convergent[4–7].

A significant breakthrough has been proposed by Davidson[5] in 1975 (for subsequent reviews with more details see[6, 8]). He, after obtaining P pieces of vectors in the iterative space, applied a PT-like formula to generate a new vector, which was immediately orthogonalized to the space of vectors obtained previously. Then, to

select the best approximation, the Hamiltonian is diagonalized in the space of thus obtained $P + 1$ vector, and the procedure is iterated until convergence. The latter is very fast in most cases. This algorithm has spread in many-electron configuration interaction codes[9–11].

It is apparent that the method of Demol et al[1]. is similar to Davidson’s technique with two small differences: 1) Demol et al[1]. use standard RSPT to generate an overlapping basis for representing the Hamiltonian, while Davidson’s matrices are diagonalized in an orthogonal metric at each step.

2) Stepping from P to $P + 1$ Demol generates a new basis vector by essentially acting on the P -th correction vector with the Hamiltonian, c.f. the first term on the rhs of Eq. (2). Compared to this, Davidson generates the new basis vector by acting with the Hamiltonian on the best estimate obtained by diagonalization at step P .

These differences are not too large to prevent sharing the good convergence properties of Davidson’s iteration and the eigenvalue continuation technique.

To illustrate the above, we tabulate the results of calculations of the correlation energy of a many-electron system, for which PT is divergent.

TABLE I. Convergence of the electron correlation energy (in atomic units) for the H_2 molecule described by triple zeta polarized basis[12] at 2.5 Å bond distance. The first order results are zero in the partitioning applied.

order	RSPT	BWPT	Eigenvalue continuation	Davidson iteration
2	-0.23167	-0.12650	-0.11857	-0.11857
3	-0.20390	-0.11544	-0.13109	-0.13474
4	0.07250	-0.13489	-0.13524	-0.13541
5	0.00406	-0.13110	-0.13538	-0.13543
6	-0.81974	-0.13562	-0.13543	-0.13543
exact	-0.13543			

Table I shows a comparison of RSPT, the Brillouin-Wigner[13, 14] PT (BWPT, *vide infra*), eigenvalue continuation as of Ref.[1], and a Davidson iteration scheme. The divergence of RSPT is apparent, while the BWPT results seem to have a convergent, although slow and oscillatory behavior. However, the numbers obtained from the two other iterative schemes are quite similar and converge nicely to the exact eigenenergy of the model Hamiltonian obtained from exact diagonalization.

A few further comments apply.

First, we fully agree with Demol et al[1]. that energy values obtained for smaller values of c , i.e., for $c_i \leq R_e$ contain much information and may be used to estimate the physical energy corresponding to $c = 1$. In fact, in our laboratory we have applied analytic continuation techniques based on these c values[15] and their complex generalizations[16, 17]. We note, however that, in order to apply these techniques, it was not necessary to resolve the problems $H(c_i)\Phi = E(c_i)\Phi$ for all points i , since energies $E(c_i)$ can be generated from the PT results at $c = 1$ by scaling the latter by c_i .

Second, Eq. (2) is based on a Rayleigh-Schrödinger PT scheme. This is of course preferred in a many-body theory if PT energies are directly used, since they are extensive with respect to the system size. However, if, via diagonalizations, the exact energies are approached, a simple Brillouin-Wigner PT method[13, 14] could be equally used to generate the wave function sequence $\{\Phi^{(k)}\}$, or the even simpler iterative form of the Schrödinger equation $H\Phi = E\Phi$ with $H = H_0 + H_1$:

$$\Phi^{(i+1)} = \Phi^{(0)} + \Delta E Q\Phi^{(i)} - QH_1\Phi^{(i)} \quad (3)$$

with $\Delta E = \langle \Phi^{(0)} | H_1 | \Phi \rangle$ being updated at each iteration step i . Note that this iteration procedure is simpler than the recursive RSPT formula (2), as the latter contains a non-Markovian part in its second term. We do not tabulate numbers obtained from (3) and subsequent diagonalizations (1), as the result is very similar to the 4th or 5th columns of Table I. The first 6 BWPT estimations are also shown there. At order 6, the estimation is correct to 3 digits, and we note that 5 digits accuracy is achieved only after 16 iterations by BWPT. It has to be added that BWPT iterations are more expensive than RSPT ones or those in eigenvalue continuation, since in BWPT the energy corrections are not expanded and one has to iterate for them at each order. For a detailed analysis of the mathematical structure of BWPT and RSPT, see e.g. Ref.[18]. A study on the convergence properties of BWPT can be found in Ref.[19].

ACKNOWLEDGMENTS

This work was completed in the ELTE Institutional Excellence Program (TKP20 20-IKA-05) financed by the Hungarian Ministry of Human Capacities.

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