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LETTER TO THE EDITOR

Perturbative-variational calculations in two coupled harmonic oscillators

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Abstract. In this work, we shall show how the perturbative-variational approximation of eigenvalues and eigenvectors, that has provided very good results for one-dimensional problems, can be generalized to Hamiltonians with degenerate states. This generalization will be illustrated by applying it to a pair of coupled harmonic oscillators. The obtained results for the ground and first excited states have a very good precision when they are compared with the results of direct diagonalization of the Hamiltonian with 190 states in the same auxiliary basis used in the perturbative-variational approximation.

Nowadays, there exist a lot of techniques that provide very good approximations of the eigenvalues and eigenfunctions of every Hamiltonian, especially for one-dimensional Hamiltonians. Among these techniques the so-called perturbative-variational approximation has provided high precision results for some important cases [1, 2]. The basic idea of this approximation is to use the wavefunctions given by perturbation theory as trial functions for a variational calculation. Its effectiveness is principally due to the adaptability of the auxiliary basis in which we make the perturbative expansion to the eigenfunctions, and the possibility of using the successive perturbation orders to improve the trial wavefunctions. The adaptability of the auxiliary basis, which is not necessarily orthogonal [2], is optimized leaving some free parameters in the basis functions. In spite of the variational character of the perturbative-variational approximation that makes it especially useful for generating the ground state, it also provides very good results for the first excited states of the Hamiltonians studied [1, 2].

In this work, we shall extend the perturbative-variational approximation for non-one-dimensional problems. At first, this extension does not seem to show any formal problem at least for non-degenerate levels in the auxiliary basis. (We shall say that two functions in the basis are degenerate if their expectation values of the total Hamiltonian are equal.) In the case of non-degenerate levels, we can apply the obtained equations for the one-dimensional case. However, the extension is not so straightforward for degenerate states because the equations mentioned have singularities. Nevertheless, we shall find an easy solution for the problem that will allow us to use an approximation similar to the one-dimensional case.

As an example for studying the approximation, we have chosen the Hamiltonian of a pair of coupled harmonic oscillators which, in its simple form, can be written as

$$H(x, y) = p_x^2 + p_y^2 + x^2 + y^2 + \lambda x^2 y^2. \tag{1}$$

This Hamiltonian has received a lot of attention in the last years because it is related with several interesting physical problems [3–5]. Moreover, most of the techniques that provide good approximation for the eigenvalues have been applied to its

solution [6–8]. Except for the first excited states, which have been calculated by Killingbeck and Jones [7], all the calculations have been limited to the ground state energy and to the study of the behaviour of the approximations for different values of λ. In any case, it has been found that the convergence decreases when λ increases. We shall show that the perturbative-variational approximation improves the results compared with the previous methods for every value of λ, not only for the ground state energy but also for the first excited states, i.e. the first four oscillator shells. However, the method is not stable for higher excited states.

The organization of the letter will be as follows. First of all, we shall expound the general procedure and how we can avoid the problems with degenerate states. Then we shall apply it to the coupled harmonic oscillators. Thereafter we will show the results obtained, separating the non-degenerate states from the degenerate ones. The results will be compared not only with those in [6–8] but also with the direct diagonal-ization of the Hamiltonian in a truncated space of the functions of the auxiliary basis, as we shall discuss later.

As we have already mentioned, within the perturbative-variational approach, the trial wavefunctions are the ones provided by the successive perturbation orders as approximations to the exact eigenfunctions of our eigenvalue problem. The perturbation order may be considered as a free parameter, but the efficiency of the method is in the inclusion of one or more free parameters in the auxiliary basis in which we shall expand the function. Let us show the different elements that appear in the approxi-mation.

We shall write $|\phi_\eta\rangle$ for the functions which form the auxiliary basis where η belongs to an arbitrary countable set $\mathscr{A}$. Every one of these functions will depend on one or more free parameters that we shall not specify yet. We shall write H for our Hamiltonian and $E_\nu, |\psi_\nu\rangle$, $\nu \in \mathscr{A}$, for the exact eigenvalues and eigenvectors of H. So, the eigenvalue equation can be written as

$$H|\psi_\nu\rangle = E_\nu|\psi_\nu\rangle \qquad \nu \in \mathscr{A}. \tag{2}$$

In order to build the different perturbative approximations for every $|\psi_\nu\rangle$, we shall expand them in terms of our auxiliary basis

$$|\psi_\nu\rangle = \sum_{\eta \in \mathscr{A}} C_{\nu,\eta}|\phi_\eta\rangle. \tag{3}$$

Introducing (3) in (2) and projecting over $|\phi_\mu\rangle$ we shall get the eigenvalue equation (2) in our auxiliary basis $\{\phi_\eta\}_{\eta \in \mathscr{A}}$

$$\sum_{\eta \in \mathscr{A}} C_{\nu,\eta}(\langle \phi_\mu|H|\phi_\eta\rangle - E_\nu\delta_{\mu,\eta}) = 0 \qquad \forall \mu \in \mathscr{A} \tag{4}$$

where we have supposed that the elements in the auxiliary basis are orthogonal to each other. This condition is not necessary for the application of the method [2] but here we shall only use the orthogonal basis. It is important to note that up to here there is no approximation at all and (2) and (4) are equivalent.

The perturbative approximation to the state ν is generated by taking as a first approximation that $C^{(1)}_{\nu,\eta} = \delta_{\eta,\xi}$, where ξ is the state of the auxiliary basis closer to the ν state of H. This perturbative hypothesis applied to (4) gives the perturbative approxi-mation of first order to the eigenvalue and eigenfunction. This is

$$|\psi_\nu^{(1)}\rangle = |\phi_\xi\rangle \tag{5}$$

$$E_\nu^{(1)} = \langle \phi_\xi|H|\phi_\xi\rangle. \tag{6}$$

The perturbative approximations for the following orders, which form Brioullin–Wigner perturbation theory [9], are obtained from (4) imposing for every order l that $C^{(l)}_{\nu,\xi} = 1$. This allows us to obtain the approximation for the coefficients and the energy in order $l+1$ in terms of the corresponding elements in order l. Explicitly the equations are

$$C^{(l+1)}_{\nu,\mu} = \frac{\sum_{\eta \neq \mu} C^{(l)}_{\nu,\eta} \langle \phi_\mu | H | \phi_\eta \rangle}{E^{(l)}_\nu - \langle \phi_\mu | H | \phi_\mu \rangle} \qquad \mu \neq \xi \tag{7}$$

$$E^{(l+1)}_\nu = \sum_{\eta \in \mathscr{A}} C^{(l+1)}_{\nu,\eta} \langle \phi_\xi | H | \phi_\eta \rangle. \tag{8}$$

Using this, the perturbation approximation of order $l+1$ to the exact wavefunction can be written as

$$|\psi^{(l+1)}_\nu\rangle = |\phi_\xi\rangle + \sum_{\eta \in \mathscr{A}} C^{(l+1)}_{\nu,\eta} |\phi_\eta\rangle. \tag{9}$$

It must be noted that equation (7) will be applicable whenever the denominator is not equal to zero in any of the perturbative orders. This can happen even for one-dimensional Hamiltonians since the choice of the basis is independent of the Hamiltonian that we are solving and may be that two different states from the auxiliary basis have the same expectation value of the Hamiltonian. However, it is evident that this possibility is greater for the non-one-dimensional Hamiltonian, which may probably have real degenerate states.

A possible option for avoiding these singularities is to fix the coefficients that cause the trouble to some value for every order, as we did for $C^{(l)}_{\nu,\xi}$. An easy criterion for doing it, that takes into account the symmetries of the Hamiltonian, is to solve the eigenvalue equation of our Hamiltonian in the auxiliary basis restricted to the set of degenerate states. The coefficients of the states involved for any perturbative order will be the ones of the corresponding eigenfunction. It is evident that in this option exists an ambiguity, this is, for every degenerate state considered we have one equation of type (8), so we must decide which we must use for calculating the value of $E^{(l+1)}_\nu$. This answer is provided by the method because the final results are independent of this choice.

This practical option is not completely perturbative but this does not mean any restriction to the perturbative-variational approximation because this method only uses perturbation theory for building trial wavefunctions and the approximation of the eigenvalue will be the expectation value of the Hamiltonian in this state. Keeping this in mind, we can say that this choice is valid and only the results obtained will allow us to know how good this choice is.

The corresponding Hamiltonian to a pair of coupled harmonic oscillators (1) is a good example to show the characteristics, the precision and the limitations of the perturbative-variational method. Obviously, the first step will be the choice of the auxiliary basis in which we shall apply the method. In this case, the structure of the Hamiltonian suggests to use the eigenfunctions of a pair of non-coupled harmonic oscillators with a common and free strength, α. Using cartesian coordinates, the functions of the basis will be

$$\phi_{n_1, n_2}(x, y; \alpha) = \sqrt{\frac{\alpha^2}{\pi 2^{n_1+n_2} n_1! n_2!}} \, H_{n_1}(\alpha x) H_{n_2}(\alpha y) \, e^{\alpha^2(x^2+y^2)/2}. \tag{10}$$

Where $H_n(z)$ is Hermite polynomial of order n [10]. It must be noted that in this case $\mathscr{A} = (\mathbb{N} \times \mathbb{N})$, with $\mathbb{N}$ the set of the natural numbers. We must emphasize that the

use of this basis, although it is suggested by the Hamiltonian, is independent of it and that it is not necessary to have any relation between the basis and the Hamiltonian for the application of the method. Of course, this simplifies the calculation.

Another possible choice of auxiliary basis would be to solve the Hamiltonian of a pair of non-coupled harmonic oscillators in polar coordinates. The functions in this case would be

$$\phi_{n,m}(r, \varphi; \alpha) = \sqrt{\frac{n!\, \alpha^{2(|m|+1)}}{\pi(n+|m|)!}}\; r^{|m|}\, e^{-\alpha^2 r^2}\, e^{im\varphi}\, L_n^{|m|}(\alpha^2 r^2) \tag{11}$$

where $L_n^k(z)$ are the generalized Laguerre polynomials. In this case $\mathscr{A} = (\mathbb{N} \times \mathbb{Z})$, with $\mathbb{Z}$ the set of the integer numbers. Although the best results obtained with both basis are equal, the general behaviour is not completely the same. For example, the order in which we get stability is different. This dependence on the basis used is evident and is caused by the different adaptability of the basis functions to the problem.

Once we have chosen the basis, we must establish the degeneration of the different states in the sense discussed above. This is, we must find out which states have the same expectation value of the Hamiltonian. In this case, this is quite simple because the natural degeneration of the non-coupled harmonic oscillator ($n_1 + n_2$ fixed for the cartesian case and $n + |m|$ fixed for the polar case) is reduced by the presence of the coupling term $H_1 = \lambda x^2 y^2$. In the case of the cartesian basis

$$\langle n_1 n_2|H_1|n_1 n_2\rangle = \frac{\lambda(2n_1 + 1)(2n_2 + 1)}{4\alpha^4}. \tag{12}$$

From this is clear that if $n_1 \neq n_2$ the states $n_1 n_2$ and $n_2 n_1$ will be degenerate. In the case of the polar basis we have a similar result. If $m \neq 0$ the states $n, +|m|$ and $n, -|m|$ will be also degenerate.

It is important to point out that this degeneration is not the degeneration of the exact eigenfunctions of the system. This degeneration may disappear if the Hamiltonian is able to connect the degenerate states in some perturbation order. This is, if

$$\langle n_1 n_2|H_1|n_{m_1} n_{k_1}\rangle\langle n_{m_1} n_{k_1}|H_1|n_{m_2} n_{k_2}\rangle \ldots \langle n_{m_i} n_{k_i}|H_1|n_2 n_1\rangle \tag{13}$$

is different from zero, where $n_{m_i} n_{k_i} l = 0, 1, \ldots$ can be any one of the states. For the particular structure of our Hamiltonian, and with the cartesian basis, it will occur only if $n_1 + n_2$ is even.

To conclude, and before discussing the results, we must mention that the criterion for fixing the coefficients in the case of degenerate levels, as they can only be doubly degenerate, leads to an even or odd combination of both states. So, in the following calculations and for degenerate states, we shall use these combinations.

Several aspects must be taken into account when we study the numerical results provided by the perturbative-variational method. There are differences for the ground state to the rest of the states. For the ground state, we are sure that the result will be upper bounds to the exact ground state energy. Therefore, this state is the best one to study the principal aspects of the method such as its convergency, the precision in the results and the dependence on the basis.

In table 1, we show the best results obtained for the ground state energy for different values of λ. The results have been obtained using the Gauss–Seidel method [11] in the iterative process of the equations (7) and (8). This Gauss–Seidel method reduces the number of iterations needed to achieve stability and improves the precision and stability especially for $\lambda > 1$. For example, with $\lambda = 10$ and using directly the equations

Table 1. Best perturbative-variational results for the ground state energy for different values of λ. α is the value of the strength of the oscillator and it is the only free parameter in the functions. We write n_c and n_p for the minimum perturbation order in which we get stability for the cartesian and polar basis, respectively. $2d$ is the maximum shell used in the calculation for the Gauss-Seidel iterative method [11, 2]. Remember that the ground state is only connected with shells with even number of quanta.

λ	α	n_c	n_p	d	E
0.1	1.05	3	4	8	2.024 138 321 415 73
0.5	1.20	6	7	14	2.108 213 779 698 54
1.0	1.30	8	10	16	2.195 918 085 200 09
2.0	1.40	10	13	19	2.339 566 210 159 25
3.0	1.50	12	18	20	2.458 376 906 236 76
4.0	1.60	13	21	23	2.561 626 575 640 04
5.0	1.70	16	25	27	2.653 909 777 953 22
10.0	1.90	19	37	31	3.019 177 714 771 97
100.0	2.70	38	70	48	5.460 970 397 923 37
1 000.0	3.90	43	81	55	11.232 439 267 209 9
10 000.0	5.70	48	93	59	23.945 989 627 819 0

(7) and (8) in the iterative process, we only get the seven first digits in the results and for $n_c = 26$.

When we use Gauss–Seidel method, it is necessary to limit the number of states that we shall use in the calculation. This number has been fixed in a way that does not affect the final result. The maximum shell of the pair of non-coupled oscillators used in the calculation is $2d$, where d is given in table 1, and it is almost independent of using a cartesian or polar basis. This is not the same for the order of stability. In this case, we can see that the order necessary to get stability with the cartesian basis, denoted in the table by n_c is smaller than the corresponding order for the polar basis, n_p. With respect to the expectation values of the Hamiltonian, they are independent of the basis used when we have reached stability and have a high precision. They are equal to the ones obtained by Fernandez and Castro [6], who use a renormalized perturbation series, but we need to use a lower order in the perturbation series to get stability and we know that our results are upper bounds to the exact energy.

In order to have a reference point for the energies obtained for the excited states we have performed a diagonalization of the Hamiltonian in the basis (10) moving the parameter α to improve the results. This procedure gives upper bounds not only for the ground state but also for the excited states [12]. It is important to compare the results provided by this method also from the ground state with the one from the perturbative-variational method. This can be seen for $\lambda = 1$ in table 2. The results are the same but to obtain this precision for direct diagonalization we need to use 190 states.

Let us now study the excited states. We shall use in this case only the cartesian basis because the convergency of the method is faster in this basis. It is important to note the symmetries of the Hamiltonian (1) in the cartesian basis. The total space is divided into four mutually orthogonal subspaces that cannot be connected by the Hamiltonian in any perturbative order. They are characterized by the numbers (n_1, n_2) to be (even, even), (even, odd), (odd, even) and (odd, odd) numbers. Note that the degeneration between the state (n_1, n_2) (even, odd) and (n_2, n_1) (odd, even) is intrinsic to the Hamiltonian and it cannot be broken by the perturbative-variational method. The orthogonality among the four subspaces has the important outcome that the states

Table 2. The first states for $\lambda = 1$. In the first column, we have written the initial state of the basis and with $\pi = +, -$ we represent the even, odd combination of the two degenerate states. E_{PV} are the results corresponding to the perturbative-variational approximation working with $\alpha = 1.3$ and $d = 30$ (see table 1). E_H are the results obtained from a direct diagonalization which the first 190 states with $\alpha = 1.30$ connected to the subspace considered.

State $(n_1, n_2)^\pi$	E_{PV}	E_H
(0, 0)	2.195 918 085 200 09	2.195 918 085 200 09
(0, 1), (1, 0)	4.526 743 874 391 03	4.526 743 874 391 03
$(2, 0)^-$	6.557 803 326 672 29	6.557 803 326 672 40
$(2, 0)^+$	7.031 272 340 129 99	7.031 272 340 130 03
(1, 1)	7.444 581 361 569 97	7.444 581 361 569 96
(3, 0), (0, 3)	8.928 061 054 225 64	8.928 061 054 226 28
(2, 1), (1, 2)	10.311 817 049 646 4	10.311 817 049 646 7
$(4, 0)^+$	11.103 253 537 431 5	11.103 253 537 438 6
$(4, 0)^-$	11.201 178 918 365 8	11.201 178 918 400 0
$(3, 1)^-$	12.332 331 271 118 5	12.332 331 271 118 8
$(3, 1)^+$	13.450 478 721 883 1	13.450 478 721 883 6
(2, 2)	13.580 556 252 436 3	13.580 556 252 446 6

generated by $(n_1, n_2) = (1, 0), (0, 1), (1, 1)$ are also upper bounds to the corresponding eigenvalues. However, this character of the upper bound disappears for the rest of the states. In spite of this limitation, the method keeps providing very good results for the lower excited states, upto $n_1 + n_2 \leqslant 4(3)$ for $\lambda = 1, (100)$. For higher exited states, the results worsen and the method is unstable.

In table 2, we show the energies of all the states with $n_1 + n_2 \leqslant 4$ for $\lambda = 1$. It can be seen that these results are very good and are almost equal to the ones obtained by direct diagonalization, which are all strict upper bounds to the corresponding eigenvalues. The high precision in the results of the states (0, 0), (1, 0) which is degenerated with (0, 1) and (1, 1) is not a surprise because in this case the perturbative-variational method also provides upper bounds. However, this property is lost for the rest of the states because the functions of the perturbative-variational method are not strictly orthogonal to all the states with lower energy but despite this, the results are still very good. This behaviour can be explained if we see that the functions obtained for the excited states are almost orthogonal to our approximation of the ground state wavefunction, which may be practically considered to be the exact wavefunction because the excellent results for the energy of this ground state. The different overlaps among the functions are shown in table 3. It must be emphasized that orthogonality among the states is an outcome of the method and it has not been imposed.

We have seen that the method becomes unstable for higher excited states. The reason of this instability is that the weight of the subspaces corresponding to lower states increases in the approximation of these higher excited states and reasonable values cannot be obtained. It is important to note that the perturbative-variational method has in this case only one free parameter (α) compared with the direct diagonalization, which is equivalent to make a variational calculation of a linear combination of functions in the basis [13] (in our case the trial wavefunction will have 190 free parameters).

Summing up, we have shown that the extension of the perturbative-variational method to degenerate systems does not imply any additional difficulty. The problem

Table 3. Overlap beween the perturbative-variational states related to the results shown in table 2. It must be noted that the subspaces with (n_1, n_2) (even, even), (even, odd) and (odd, odd) are mutually orthogonal.

(even, even)	$(2, 0)^+$	$(2, 0)^-$	$(4, 0)^+$	$(4, 0)^-$	$(2, 2)$
$(0, 0)$	-7.8×10^{-10}	2.1×10^{-10}	-6.0×10^{-10}	1.1×10^{-10}	-1.6×10^{-8}
$(2, 0)^+$		1.30×10^{-9}	-2.1×10^{-9}	8.9×10^{-10}	-7.1×10^{-8}
$(2, 0)^-$			3.5×10^{-9}	-2.8×10^{-9}	-3.7×10^{-8}
$(4, 0)^+$				4.3×10^{-9}	-7.8×10^{-8}
$(4, 0)^-$					-3.0×10^{-8}

(even, odd)	$(2, 1)$	$(0, 3)$	(odd, odd)	$(3, 1)^+$	$(3, 1)^-$
$(0, 1)$	6.8×10^{-8}	-4.9×10^{-12}	$(1, 1)$	2.2×10^{-12}	9.1×10^{-14}
$(2, 1)$		1.3×10^{-7}	$(3, 1)^+$		-2.5×10^{-13}

that we have found are the same as that in the non-degenerate case, that the instability of the method for high excited states. Obviously, the calculation of the matrix elements of the Hamiltonian in the auxiliary basis is necessary, and common to other similar techniques, and the need of making it analytically an important limitation to the method. However, the results are excellent and, in any case, comparable to the best results provided by the known methods. In this sense, it is important to emphasize again that we have only one free parameter in the calculation and that perturbation theory fixes the values of the coefficients in the expansion of the trial wavefunction. To conclude, that the character of upper bounds to the exact values of our results for the first states make them especially attractive when we compare with the results of other similar techniques.

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