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Improved variational method and wave functions for excited states

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The explicit construction of the approximate wave functions for excited states is performed in the framework of a perturbative-variational method with the help of a new minimization procedure for a integral discrepancy. The numerical verification of a new approach is performed by calculating the expectation values of powers of the quartic oscillator Hamiltonian. The detail graphical verification is fulfilled by means of a local discrepancy.

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1. Introduction

Two main difficulties arise when we attempt to solve the Schrödinger equation for the excited states within the framework of the variational method. The first of them is to construct the full set of the trial vectors $|\Psi_n(\omega)>$ or the trial wave functions $\Psi_n(\omega, x) =< x|\Psi_n(\omega)>$ with a variational parameter ω for the given initial Hamiltonian $\hat{H}$ and quantum numbers n. In the perturbative-variational approach, the trial vectors are constructed by means of perturbation theory (PT) with an unperturbed Hamiltonian $\hat{H}_0(\omega)$ depending on a variational parameter [1–3]. The next question is choosing the optimal value of a variational parameter. There are several ways to fix the parameter ω in the perturbative-variational approach. Some of them are connected with minimization of perturbative corrections of energy or eigenvectors. Such methods have a special character and are oriented for using PT for constructing the trial vectors, although, generally speaking, these vectors could be generated in another way. The prevalent way of fixing ω is the principle of minimal sensitivity or the fulfilment of usual requirement (see [4, 5])

$$\frac{\partial \bar{E}_n(\omega)}{\partial \omega} = 0 \tag{1}$$

for an expectation value of the origin Hamiltonian

$$\bar{E}_n(\omega) =< \Psi_n(\omega)|\hat{H}|\Psi_n(\omega) > \tag{2}$$

($< \Psi_n(\omega)|\Psi_n(\omega) >= 1$). There can be several stationary points, and there is no method to select one of them. We denote the point of absolute minimum as ω_e. Besides, energy in this sense is not a preferred quantity in comparison with the other expectation values. It is also well-known, that calculation of the energy with increased accuracy does not always lead to an improvement of the other characteristics. Thus, till present time the question how to find the

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universal criterion of choosing the optimal value of a varied parameter within the framework of the variational approach remains to be solved.

2. Local and integral discrepancies

In our opinion such criterion should be directly connected with the initial spectral problem

$$\hat{H}\Psi_n(x) - E_n\Psi_n(x) = 0. \tag{3}$$

Let us rewrite this Schrödinger equation in the following way

$$\frac{\hat{H}\Psi_n(x)}{<\Psi_n|\hat{H}|\Psi_n>} - \Psi_n(x) = 0 \tag{4}$$

for the normalized eigenfunctions ($<\Psi_n|\Psi_n>=1$). Now we introduce a discrepancy vector

$$|D_n(\omega)>=\frac{\hat{H}|\Psi_n(\omega)>}{<\Psi_n(\omega)|\hat{H}|\Psi_n(\omega)>} - |\Psi_n(\omega)> \tag{5}$$

and a local discrepancy

$$D_n(\omega,x) =<x|D_n(\omega)>=\frac{\hat{H}\Psi_n(\omega,x)}{<\Psi_n(\omega)|\hat{H}|\Psi_n(\omega)>} - \Psi_n(\omega,x) \tag{6}$$

for a normalized trial function $\Psi_n(\omega,x)$ which is not exact solutions of equation (3). In the case of an approximate wave function $\Psi_n(\omega,x)$ we have inequality $D_n(\omega,x)\neq 0$. In order to perform the complete estimation of approximation it is sufficient to compare two functions $\Psi_n(\omega,x)$ and $D_n(\omega,x)$. With such approach it is not necessary to find the exact solution of the Schrödinger equation for analysis of approximation exactness.

In addition to a local discrepancy we can determine an integral discrepancy

$$d_n(\omega) =< D_n(\omega)|D_n(\omega)>=\frac{<\Psi_n(\omega)|\hat{H}^2|\Psi_n(\omega)>}{<\Psi_n(\omega)|\hat{H}|\Psi_n(\omega)>^2} - 1 \tag{7}$$

which characterizes goodness of the approximation and is equal to zero for an exact solution of the Schrödinger equation.

The introduced characteristic $d_n(\omega)$ has a direct geometric sense. Let us set the normalized trial vector $|\Psi_n(\omega)>$ in Hilbert space. Under the action of the $\hat{H}$ operator, the vector $\hat{H}|\Psi_n(\omega)>$ is obtained. We can find the angle $\varphi_n(\omega)$ between the vectors $|\Psi_n(\omega)>$ and $\hat{H}|\Psi_n(\omega)>$ from the scalar product of these vectors:

$$\cos\varphi_n(\omega) = \frac{<\Psi_n(\omega)|\hat{H}|\Psi_n(\omega)>}{\sqrt{<\Psi_n(\omega)|\hat{H}^2|\Psi_n(\omega)>}}. \tag{8}$$

From here we obtain the relation

$$\tan^2\varphi_n(\omega) = d_n(\omega) \tag{9}$$

The Hamiltonian $\hat{H}$ rotates the approximate trial vector through an angle $\varphi_n(\omega)$ and dilates it, while under the action of the Hamiltonian the exact eigenvector is only dilated, but is not

rotated. The degree of closeness of the approximate eigenvector to the exact eigenvector is determined by the angle $\varphi_n(\omega)$ of rotation .

In [6] a new approach to the determination of ω from the integral discrepancy minimization condition was proposed. In this case, the PT first approximation was used, and quantitative estimate of the approximate eigenvectors was not complete enough. In the present paper, we go from the first to the third order of PT where the trial functions, becoming more precise, do not become too complicated.

So we propose to determine the parameter ω by minimization of $d_n(\omega)$ (minimal angle of rotation):

$$\frac{d}{d\omega} d_n(\omega) = 0. \tag{10}$$

Note that we find the absolute minimum of $d_n(\omega)$. We denote the point of this minimum as ω_d. The analogs of the quantity $d_n(\omega)$ have been used for a long time to estimate the degree of approximation, but not to choose the optimal values of the parameters of the trial functions.

3. Perturbative-variational approach

We illustrate our approach in the case of the quartic oscillator Hamiltonian :

$$\hat{H} = \frac{1}{2}(\hat{p}^2 + x^4) \tag{11}$$

which is often used as a test for different approximation methods.

In the present paper we use the operator method [1] in which the unperturbed Hamiltonian $\hat{H}_0(\omega)$ is a diagonal part

$$\hat{H}_0(\omega) = \sum_n E_n^0 |\Psi_n^0(\omega) >< \Psi_n^0(\omega)|, \tag{12}$$

$$E_n^0(\omega) =< \Psi_n^0(\omega)|\hat{H}|\Psi_n^0(\omega) >$$

of the initial Hamiltonian $\hat{H}$ in the basis of the eigenvectors $|\Psi_n^0(\omega) >$ of the harmonic oscillator Hamiltonian

$$\hat{H}_{osc}(\omega) = \frac{1}{2}\left(\frac{\hat{p}^2}{\omega} + \omega x^2\right). \tag{13}$$

The corresponding normalized eigenfunctions $\Psi_n^0(\omega, x) =< x|\Psi_n^0(\omega) >$ satisfy equation

$$\hat{H}_{osc}(\omega)\Psi_n^0(\omega, x) = \left(n + \frac{1}{2}\right)\Psi_n^0(\omega, x).$$

The trial wave functions are constructed according to the PT rules up to the third order ($p = 1, 2, 3$) in the following form

$$\Psi_n^{(p)}(\omega, x) = N\left(\Psi_n^0(\omega, x) + \sum_{m\neq n} C_{nm}^{(p)}\Psi_m^0(\omega, x)\right) \tag{14}$$

where the $C_{nm^{(p)}}$ values are defined by the relations

$$C_{nm}^{(p)} = \sum_{s=1}^{p} C_{nm}^{(s)},$$

$$C_{nm}^{(s)} = \left[E_m^0 - E_n^0\right]^{-1} \left[\sum_{k\neq n,m} H_{nk} C_{km}^{(s-1)} - \sum_{t=1}^{s-1} C_{nm}^{(t)} \sum_{k\neq m} H_{mk} C_{km}^{(s-t-1)}\right], \tag{15}$$

$$H_{mn} =< \Psi_m^0(\omega)|\hat{H}|\Psi_n^0(\omega) > .$$

In this case, equation

$$\hat{H}_0(\omega)|\Psi_n^0(\omega) >= E_n^0(\omega)|\Psi_n^0(\omega) > \tag{16}$$

has an exact solution. The normalization factor N for the trial function should be chosen so that the condition $< \Psi_n(\omega)|\Psi_n(\omega) >= 1$ is fulfilled. We denote the local and integral discrepancies corresponding to the p-th order of PT as $D_n^{(p)}(\omega, x)$ and $d_n^{(p)}(\omega)$.

We will demonstrate our approach by calculating the following characteristics. First, we calculate the value of the integral discrepancy. Other natural characteristics of goodness of the approximate eigenvectors are expectation values of powers of the Hamiltoninan. The quantitative estimates of the approximation can be the following relative values

$$e_n^{(p)}(k,\omega) = \frac{< \Psi_n^{(p)}(\omega)|\hat{H}^k|\Psi_n^{(p)}(\omega) >^{1/k}}{E_n^{ex}} - 1, \tag{17}$$

where E_n^{ex} is the exact energy value. The exact energy values for Hamiltoninan (11) are known [7]. We emphasize that the characteristics $e_n^{(p)}(k,\omega)$ permit us to investigate the goodness of the trial vectors on the basis of the knowledge of only one physical quantity - energy.

4. Verification of proposed approach

We compare two variants of fixing a varied parameter. The first variant corresponds to the absolute minimum of the integral discrepancy ($\omega = \omega_d$). The second variant corresponds to the absolute minimum of energy ($\omega = \omega_e$). We also investigate the dependence of the approximate wave functions and local discrepancies on the order of PT.

Fig. 1 and Fig. 7 show the dependence of the integral discrepancies $d_n^{(p)}(\omega)$ on ω for $n = 15$ and $n = 20$ respectively. Fig. 3 and Fig. 9 show the dependence of the approximate wave functions $\Psi_n^{(p)}(\omega_d, x)$ for $n = 15$ and $n = 20$ respectively. Fig. 5 and Fig. 11 show the dependence of the local discrepancies $D_n^{(p)}(\omega_d, x)$ for $n = 15$ and $n = 20$ respectively. We see that increase of PT order leads to decrease of the integral discrepancies and improvement of the approximation when we choose the variational parameter by means of minimization of the integral discrepancy. Figures labeled by even numbers correspond to the energy minimization variant of the variational parameter choice. From comparison of figures it is evident that our proposed variant has the certain advantage. It is easily seen that $d_n^{(3)}(\omega)$ has one absolute minimum, while $e_n^{(3)}(1,\omega)$ has several local minima. The minimum of the function $d_n^{(3)}(\omega)$ corresponds to the flat part of the curve $e_n^{(3)}(1,\omega)$, i.e. this part of $e_n^{(3)}(1,\omega)$ is almost independent on ω. Besides, the value of ω_e, which determines the local minimum of $e_n^{(3)}(1,\omega)$ on this part coincides with the value of ω_d, realizing the minimum of $d_n^{(3)}(\omega)$, with an accuracy of 0.06%.

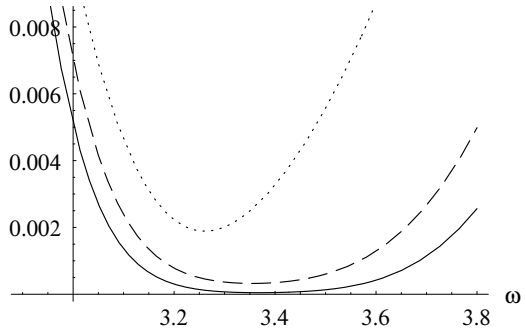

FIG. 1. The integral discrepancies for $n = 15$. (Dotted line for $d_{15}^{(1)}(\omega)$, dashed line for $d_{15}^{(2)}(\omega)$ and solid line for $d_{15}^{(3)}(\omega)$).

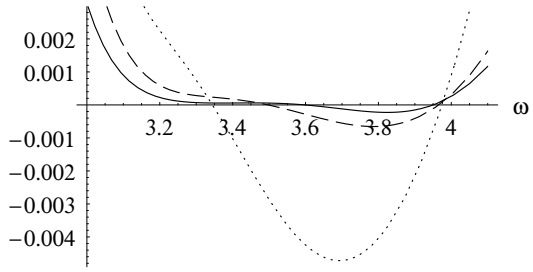

FIG. 2. The scaled energies for $n = 15$. (Dotted line for $e_{15}^{(1)}(1,\omega)$, dashed line for $e_{15}^{(2)}(1,\omega)$ and solid line for $e_{15}^{(3)}(1,\omega)$).

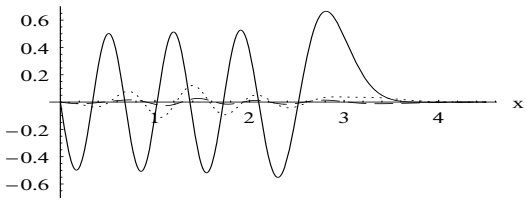

FIG. 3. The wave functions for $n = 15$. (Dotted line for $\Psi_{15}^{(3)}(\omega_d, x) - \Psi_{15}^{(1)}(\omega_d, x)$, dashed line for $\Psi_{15}^{(3)}(\omega_d, x) - \Psi_{15}^{(2)}(\omega_d, x)$ and solid line for $\Psi_{15}^{(3)}(\omega_d, x)$).

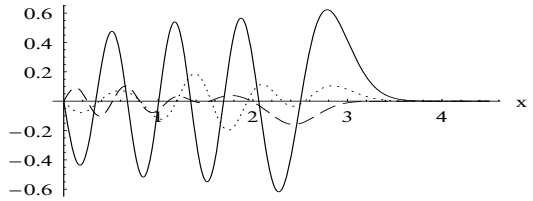

FIG. 4. The wave functions for $n = 15$. (Dotted line for $\Psi_{15}^{(3)}(\omega_e, x) - \Psi_{15}^{(1)}(\omega_e, x)$, dashed line for $\Psi_{15}^{(3)}(\omega_e, x) - \Psi_{15}^{(2)}(\omega_e, x)$ and solid line for $\Psi_{15}^{(3)}(\omega_e, x)$).

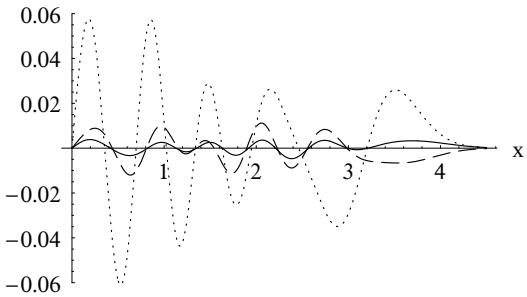

FIG. 5. The local discrepancies for $n = 15$. (Dotted line for $D_{15}^{(1)}(\omega_d, x)$, dashed line for $D_{15}^{(2)}(\omega_d, x)$ and solid line for $D_{15}^{(3)}(\omega_d, x)$)).

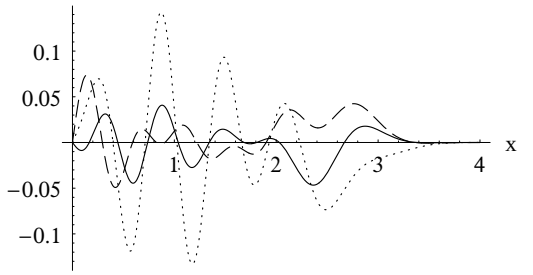

FIG. 6. The local discrepancies for $n = 15$. (Dotted line for $D_{15}^{(1)}(\omega_e, x)$, dashed line for $D_{15}^{(2)}(\omega_e, x)$ and solid line for $D_{15}^{(3)}(\omega_e, x)$).

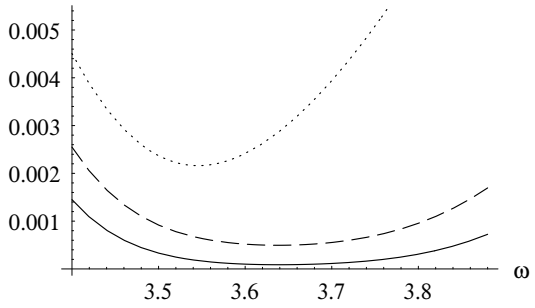

FIG. 7. The integral discrepancies for $n = 20$. (Dotted line for $d_{20}^{(1)}(\omega)$, dashed line for $d_{20}^{(2)}(\omega)$ and solid line for $d_{20}^{(3)}(\omega)$).

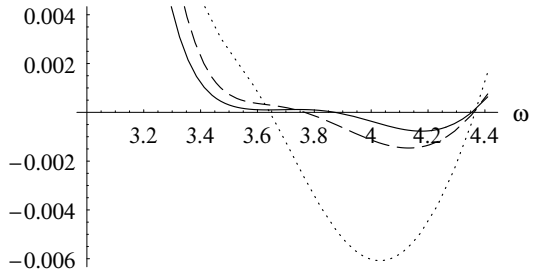

FIG. 8. The scaled energies for $n = 20$. (Dotted line for $e_{20}^{(1)}(1,\omega)$, dashed line for $e_{20}^{(2)}(1,\omega)$ and solid line for $e_{20}^{(3)}(1,\omega)$).

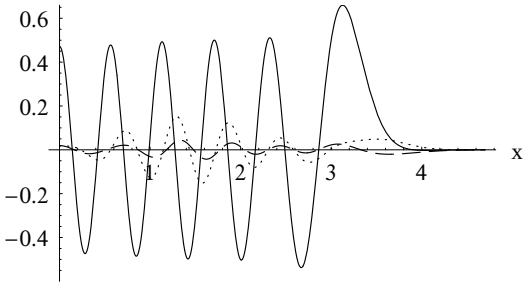

FIG. 9. The wave functions for $n = 20$. (Dotted line for $\Psi_{20}^{(3)}(\omega_d, x) - \Psi_{20}^{(1)}(\omega_d, x)$, dashed line for $\Psi_{20}^{(3)}(\omega_d, x) - \Psi_{20}^{(2)}(\omega_d, x)$ and solid line for $\Psi_{20}^{(3)}(\omega_d, x)$).

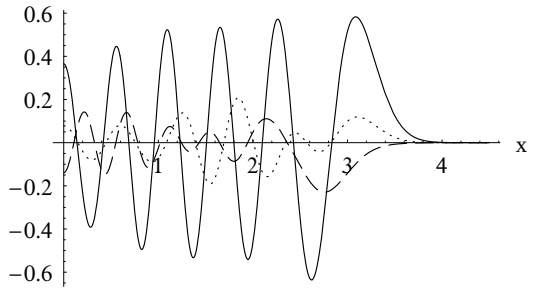

FIG. 10. The wave functions for $n = 20$. (Dotted line for $\Psi_{20}^{(3)}(\omega_e, x) - \Psi_{20}^{(1)}(\omega_e, x)$, dashed line for $\Psi_{20}^{(3)}(\omega_e, x) - \Psi_{20}^{(2)}(\omega_e, x)$ and solid line for $\Psi_{20}^{(3)}(\omega_e, x)$).

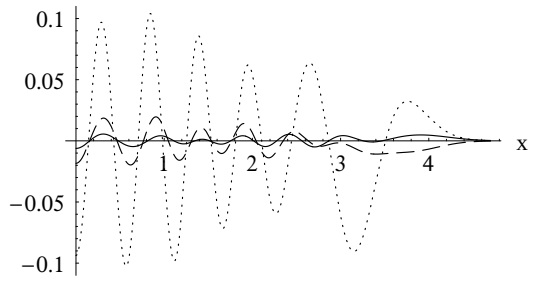

FIG. 11. The local discrepancies for $n = 20$. (Dotted line for $D_{20}^{(1)}(\omega_d, x)$, dashed line for $D_{20}^{(2)}(\omega_d, x)$ and solid line for $D_{20}^{(3)}(\omega_d, x)$).

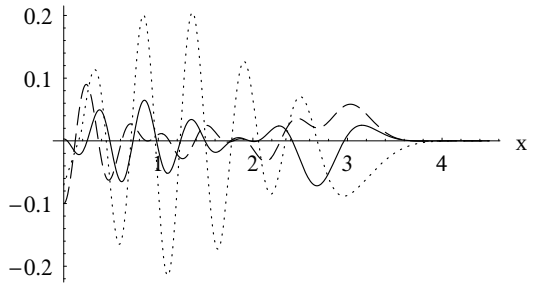

FIG. 12. The local discrepancies for $n = 20$. (Dotted line for $D_{20}^{(1)}(\omega_e, x)$, dashed line for $D_{20}^{(2)}(\omega_e, x)$ and solid line for $D_{20}^{(3)}(\omega_e, x)$).

Table 1: Numerical verification of the proposed approach.

n	p	ω	$d_n^{(p)}(\omega)$	$e_n^{(p)}(1,\omega)$	$e_n^{(p)}(2,\omega)$	$e_n^{(p)}(3,\omega)$	$e_n^{(p)}(4,\omega)$
15	1	3.261	$1.890\ 10^{-3}$	$1.360\ 10^{-3}$	$2.306\ 10^{-3}$	$3.426\ 10^{-3}$	$4.904\ 10^{-3}$
	1	3.693	$1.231\ 10^{-2}$	$-4.718\ 10^{-3}$	$1.391\ 10^{-3}$	$7.615\ 10^{-3}$	$1.444\ 10^{-2}$
	2	3.355	$3.240\ 10^{-4}$	$2.245\ 10^{-4}$	$3.865\ 10^{-4}$	$5.771\ 10^{-4}$	$8.275\ 10^{-4}$
	2	3.787	$4.617\ 10^{-2}$	$-6.543\ 10^{-4}$	$1.650\ 10^{-3}$	$4.067\ 10^{-3}$	$6.947\ 10^{-3}$
	3	3.368	$4.661\ 10^{-5}$	$5.643\ 10^{-5}$	$7.973\ 10^{-5}$	$1.116\ 10^{-4}$	$1.614\ 10^{-4}$
	3	3.824	$3.037\ 10^{-3}$	$-2.268\ 10^{-4}$	$1.290\ 10^{-3}$	$2.899\ 10^{-3}$	$4.805\ 10^{-3}$
20	1	3.546	$2.162\ 10^{-3}$	$1.787\ 10^{-3}$	$2.870\ 10^{-3}$	$4.108\ 10^{-3}$	$5.627\ 10^{-3}$
	1	4.031	$1.458\ 10^{-2}$	$-6.076\ 10^{-3}$	$1.144\ 10^{-3}$	$8.491\ 10^{-3}$	$1.626\ 10^{-2}$
	2	3.638	$4.950\ 10^{-4}$	$3.071\ 10^{-4}$	$5.546\ 10^{-4}$	$8.289\ 10^{-4}$	$1.155\ 10^{-3}$
	2	4.132	$8.146\ 10^{-3}$	$-1.462\ 10^{-3}$	$2.597\ 10^{-3}$	$6.872\ 10^{-3}$	$1.174\ 10^{-2}$
	3	3.639	$8.788\ 10^{-5}$	$9.943\ 10^{-5}$	$1.434\ 10^{-4}$	$1.980\ 10^{-4}$	$2.732\ 10^{-4}$
	3	4.177	$6.884\ 10^{-3}$	$-7.707\ 10^{-4}$	$2.663\ 10^{-3}$	$6.255\ 10^{-3}$	$1.029\ 10^{-2}$

Each cell in Table 1 contains six lines. The first pair of lines corresponds to the first order of PT, the second pair of lines corresponds to the second order of PT and the last pair of lines corresponds to the the third order of PT. Each odd line corresponds to the discrepancy minimization variant and each even line corresponds to the energy minimization variant. From the analysis of Table 1 it is clearly seen that the improvement of the integral discrepancy $d_n(\omega)$ leads to the systematic improvement of all the characteristics $e_n(k,\omega)$.

5. Conclusion

Thus, the considered example demonstrates the efficiency of the minimization of the absolute discrepancy as a method of optimization of a variational parameter. It should be emphasized, that our criterion is not restricted to a particular realization of the trial functions such as PT-series, but is general in character and can be used in the case of arbitrary trial functions for description of different physical systems within the variational approach. Finally, we stress that the proposed estimate of the approximation validity by means of the local discrepancy can be applied to all approximate methods, not only to the particular variational method.

References

[1] I. D. Feranchuk et al, Ann. of Phys. **238**, 370 (1995)

[2] F. Arias de Saavedra and E. Buendia, J. Phys. A **22**, 1933 (1989)

[3] K. L. Chan et al, Phys. Lett. A **162**, 227 (1992)

[4] H. Ciftci, E. Ateser and H. Koru, J. Phys. A **36**, 3621 (2003)

[5] H. Ciftci, R. H. Hall and Q. D. Katatbeh, J. Phys. A **36**, 7001 (2003)

[6] V. V. Kudryashov and V. I. Reshetnyak, Nonlinear Phenomena in Complex Systems, eds. L. Babichev and V. Kuvshinov (Institute of Physics, Minsk, 2000) p. 168.

[7] K. Banerjee et al, Proc. R. Soc. Lond. A **360**, 575 (1978)