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Improved variational approach for radial wave functions

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The approximate radial wave functions for excited states corresponding to power-law potentials are constructed in the framework of a variational method with the help of a new minimization procedure for an integral discrepancy. The detailed graphical verification of approximate wave functions is fulfilled by means of local discrepancy. The approximate energy eigenvalues are in good agreement with exact numerical results.

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1. Introduction

The variational method is very efficient for solving the radial Schrödinger equation in the case of the ground states. However, difficulties arise when we describe excited states. The first of them is the construction of the trial functions $\Psi_{nl}(a_i, r)$ for the full set of excited states. The next question is choosing the optimal value of variational parameters a_i. There are several ways to fix parameters. The most popular of them is the principle of minimal sensitivity which requires that variational parameters $a_i = a_{i0}$ where a_{i0} are stationary points of perturbative or variational energy, as a function of a_i[1]. There can be several points of this kind, and there is no method to select one of them. 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 other characteristics. Thus, till present time the question how to find the universal criterion of choosing the optimal value of varied parameters within the framework of the variational approach remains to be solved.

In the present work we compared two methods of determining variational parameters - the method described in paper [2] and the method proposed in our paper [3].

2. Local and integral discrepancies

We study the Schrödinger equation for spherically symmetric potentials $V(r)$. The radial Schrödinger equation for power-low potentials can be written in the form

$$-\frac{d^2\psi(r)}{dr^2} + \left(r^k + \frac{l(l+1)}{r^2} - E\right)\psi(r) = 0 \qquad (1)$$

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As the trial functions, we used the functions [2]

$$\psi_{nl}(a,b,r) = Nr^{l+1}\exp(-(ar)^b)L_n^{\frac{2l+1}{b}}(2(ar)^b) \tag{2}$$

where $L_n^{\frac{2l+1}{b}}(2(ar)^b)$ is the Laguerre polynomial, a and b are variational parameters, N is a normalization factor ($< \psi_{nl}(a,b)|\psi_{nl}(a,b) >= 1$). In [2] the parameter a was determined from the condition of a minimum energy:

$$\frac{d}{da}\bar{E}_{nl}^{(1)}(a,b) = 0, \tag{3}$$

where

$$\bar{E}_{nl}^{(1)}(a,b) =< \psi_{nl}(a,b)|\hat{H}|\psi_{nl}(a,b) >, \tag{4}$$

and the special procedure was used for determining the parameter b:

$$b = \sqrt{(k+2)}(1 + 0.2075(k+1)(2-k)/(0.1381k^2 + 1.05k + 2.484)^{0.08104}$$

for all l and n at fixed k. To obtain the spectrum of eigenvalues of Eq. (1), we consider two criterium, to which the trial functions of problem should satisfy. First, we introduce virial characteristic

$$v_{nl}(a,b) =< \psi_{nl}(a,b)|(-\frac{d^2}{dr^2} + \frac{l(l+1)}{r^2} - \frac{1}{2}kr^k)|\psi_{nl}(a,b) >, \tag{5}$$

that is equal to zero for the exact solution of the Schrödinger equation. The condition

$$v_{nl}(a,b) = 0 \tag{6}$$

allows us to determinate the parameter $a = a_0(b)$. (This condition is equivalent to the condition (3) for polynomial potential). Thus, the considered problem is transformed into a one-parameter problem. As the second requirement imposed on the trial function, we select the requirement that integral discrepancy [3]:

$$d_{nl}(a,b) = \frac{< \psi_{nl}(a,b)|\hat{H}^2|\psi_{nl}(a,b) >}{(< \psi_{nl}(a,b)|\hat{H}|\psi_{nl}(a,b) >)^2} - 1, \tag{7}$$

is minimum. The corresponding criterium for selection of parameter b is:

$$\frac{d}{db}d_{nl}(a_0(b),b) = 0, \tag{8}$$

3. Verification of proposed approach

In addition to the energy, expectation values of the squared Hamiltoninan characterizing the goodness of the approximate eigenfunctions, are calculated:

$$E_{nl}^{(2)}(a,b) =< \psi_{nl}(a,b)|\hat{H}^2|\psi_{nl}(a,b) > \tag{9}$$

The results of calculations are presented in Table. An important characteristic of goodness of the approximate eigenvectors are the local discrepancies

$$D_{nl}(a,b,r) = \frac{\hat{H}\psi_{nl}(a,b,r)}{< \psi_{nl}(a,b,r)|\hat{H}|\psi_{nl}(a,b,r) >} - \psi_{nl}(a,b,r) \tag{10}$$

for the normalized trial function $\psi_{nl}(a,b,r)$ that is not exact solution of the Schrödinger equation.

Figures show the wave functions $\psi_{nl}(a,b,r)$ (solid lines) and local discrepancies $D_{nl}(a,b,r)$ for $k=4, n=3, l=1$ and $10 \cdot D_{nl}(a,b,r)$ for $k=0.5, n=3, l=1$ (dashed line). Fig. 1 and Fig. 3 correspond to the method proposed by us while Fig. 2 and Fig. 4 correspond to the method proposed in [2]. It is easy to see that the method proposed by us for selection of parameters makes it possible to obtain wave functions with substantially improved local characteristics. The fact that wave functions with improved global characteristics are determined by this method is illustrated by Table, where the values d_{nl}, $E_{nl}^{(1)}$ and $E_{nl}^{(2)}$ are presented for the potential $V(r) = r^4$. Two rows of the table correspond to each value of n and l . The first rows correspond to our variant of selection of parameters, and the second rows correspond to the variant proposed in [2]. Analysis of the data presented in Table show that the trial functions with the smallest integral discrepancy for excited states gives the best values for a set of characteristics $E_{nl}^{(1))}$ and $E_{n}^{(2)}$ at all the considered values of n and l.

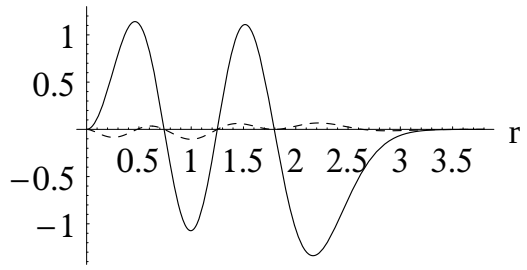

FIG. 1. The wave function and local discrepancy for $k=4, n=3, l=1$ (our variant).

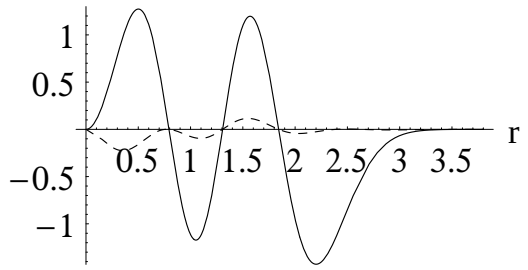

FIG. 2. The wave function and local discrepancy for $k=4, n=3, l=1$ (variant [2]).

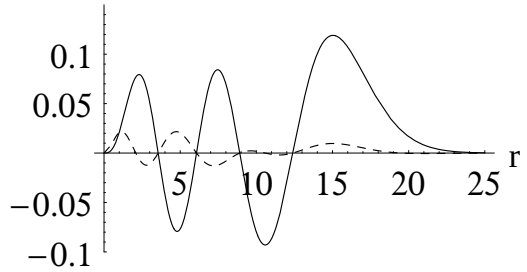

FIG. 3. The wave function and local discrepancy for $k=0.5, n=3, l=1$ (our variant).

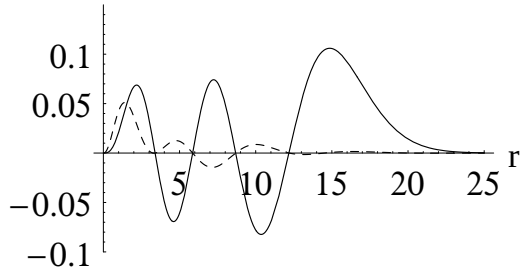

FIG. 4. The wave function and local discrepancy for $k=0.5, n=3, l=1$ (variant [2]).

Table 1: Numerical results in the case of potentials $V(r) = r^4$.

l	n	b	d	$E_{nl}^{(1)}$	$\sqrt{E_{nl}^{(2)}}$	E_{ex}[4]
0	0	2.40344	$5.7410 \cdot 10^{-3}$	3.80241	3.81331	3.79967
		2.39731	$5.7503 \cdot 10^{-3}$	3.80241	3.81332	
0	1	2.27218	$4.0607 \cdot 10^{-3}$	11.6579	11.6815	11.64474
		2.39731	$9.0944 \cdot 10^{-3}$	11.6700	11.7230	
0	2	2.23064	$5.1109 \cdot 10^{-3}$	21.2381	21.2923	21.23836
		2.39731	$1.5727 \cdot 10^{-2}$	21.2408	21.4072	
0	3	2.21239	$5.7842 \cdot 10^{-3}$	32.0777	32.1704	32.0985
		2.39731	$2.0173 \cdot 10^{-2}$	32.0451	32.3667	
1	0	2.41785	$1.5974 \cdot 10^{-3}$	7.11107	7.11669	7.10845
		2.39731	$1.6422 \cdot 10^{-3}$	7.11107	7.11690	
1	1	2.32847	$2.0455 \cdot 10^{-3}$	16.0439	16.0603	16.0327
		2.39731	$2.9214 \cdot 10^{-3}$	16.0589	16.0824	
1	2	2.28116	$2.9831 \cdot 10^{-3}$	26.3581	26.3974	26.3500
		2.39731	$6.3643 \cdot 10^{-3}$	26.3959	26.4798	
1	3	2.25590	$3.7131 \cdot 10^{-3}$	37.7718	37.8418	37.7742
		2.39731	$9.6523 \cdot 10^{-3}$	37.8204	38.0025	
2	0	2.42543	$6.5480 \cdot 10^{-4}$	10.8448	10.8483	10.8424
		2.39731	$7.0132 \cdot 10^{-4}$	10.8449	10.8487	
2	1	2.36126	$1.2148 \cdot 10^{-3}$	20.6534	20.6639	20.6435
		2.39731	$1.3723 \cdot 10^{-3}$	20.6626	20.6767	
2	2	2.31504	$1.9603 \cdot 10^{-3}$	31.6259	31.6569	31.6147
		2.39731	$3.1828 \cdot 10^{-3}$	31.6633	31.6714	

4. Conclusion

Thus, the considered examples demonstrate the efficiency of the method of optimization of variational parameters by fulfilment of the requirements of the virial theorem and condition that the integral discrepancy is minimum. It should be emphasized, that our criterion is not restricted to a particular realization of the trial functions in the form (2), but is general in character and can be used in case of arbitrary trial functions for description of different physical systems.

References

[1] I. D. Feranchuk et al. Operator method in the problem of quantum anharmonic ocsllator. Ann. of Phys. **238**, 370-440 (1995).

[2] H. Ciftci, E. Ateser and H. Koru. The power-law and logarithmic potentials. J.Phys.A: Math.Gen. **36**, 3621-3628 (2003).

[3] V. V. Kudryashov and V. I. Reshetnyak. Modification of the perturbative-variational approach. Proc. of 9-th Annual Seminar "Nonlinear Phenomena in Complex Systems", eds. L. Babichev and V. Kuvshinov (Institute of Physics, Minsk, 2000) p. 168-171.

[4] B.M.Karnakov, V.D. Mur, V.S.Popov. On the matching condition in the WKB method. Zh.Eks.Teor.Fiz. (JETP) **107**, no. 6, 1768-1779 (1995).