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**THE ONE-DIMENSIONAL ANHARMONIC
OSCILLATOR**

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**Объединенный институт
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БИЯИИСТЕМА**

1. The problem of one-dimensional anharmonic oscillator (a.o.) is one of the oldest in quantum mechanics. It has been proved^{/1/} that a series of the usual perturbation theory diverges for any value of the anharmonic constant. There is a huge number of papers devoted to this problem. We mention only exact numerical calculations^{/2-5/}, a quasiclassical treatment^{/6/} and a modified perturbation theory (MPT)^{/7,8/}. An excellent review of the methods treating the one-dimensional a.o. is given in^{/9/}.

We feel that there is certain necessity in simple method which permits one to obtain, in a closed form, the energy levels of the a.o. with the accuracy of 1-2%. We prove that 1st order MPT meets these demands.

The consideration is organized as follows. In Sec.2 we apply MPT to the one-dimensional a.o. $\alpha x^2 + \beta x^4$ for $a > 0$. The comparison with exact results shows that accuracy obtained is not worse than 1-2% for all values of β and all the energies. In Sec.3 we consider the case of negative values of a and find that MPT breaks for negative energies. On the other hand, the WKB method adequately describes the energy levels and their splitting at the bottom of the potential well. So, these two methods complement each other. For $a = 0$ MPT gives a very simple formula

$$\epsilon_n = \left(\frac{81}{32} \frac{\hbar^4 \beta}{m^2} \right)^{1/3} (n + 1/2)^{2/3} \cdot \left(n^2 + n + \frac{1}{2} \right)^{1/3}.$$

It agrees with exact results within 1-2% accuracy.

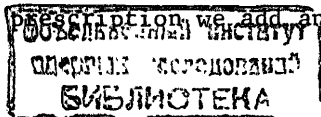
2. The Schroedinger equation for a one-dimensional a.o. is

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + \alpha x^2 \Psi + \beta x^4 \Psi = \epsilon \cdot \Psi. \quad (2.1)$$

Consider first the case $a > 0$. The transformation to the dimensionless variables being made ($y^2 = x^2 \cdot \sqrt{2\alpha m/\hbar}$) one obtains:

$$\frac{1}{2} \left(-\frac{\partial^2 \Psi}{\partial y^2} + y^2 \Psi \right) + \chi y^4 \Psi = \epsilon \Psi, \quad \chi = \frac{\hbar \beta}{2\omega_0 \alpha m}, \quad \epsilon = \frac{\epsilon}{\hbar \omega_0}, \quad \omega_0 = \sqrt{\frac{2\alpha}{m}}. \quad (2.2)$$

Following the MPT description, we add and subtract the quantity



$\frac{1}{2}\omega^2 y^2$ and present (2.2) as: $(H_0 + H_1)\Psi = \epsilon\Psi$,

$$H_0 = \frac{\omega}{2} \left(-\frac{\partial^2}{\partial z^2} + z^2 \right),$$

$$H_1 = \frac{1-\omega^2}{2\omega} z^2 + \chi \frac{z^4}{\omega^2}, \quad z^2 = \omega \cdot y^2.$$

Now treat H_1 in the 1st order of the usual PT. Then:

$$\epsilon_n = \langle n | H | n \rangle = \frac{1}{2} \cdot (n + \frac{1}{2}) \cdot (\omega + \omega^{-1} + C_n \cdot \omega^{-2}), \quad C_n = 3\chi \frac{n^2 + n + \frac{1}{2}}{h + \frac{1}{2}}. \quad (2.3)$$

Here $|n\rangle$ are eigenfunctions of H_0 : $|n\rangle = \frac{1}{\pi^{1/4}} \frac{1}{\sqrt{2^n n!}} \exp(-\frac{z^2}{2}) \cdot H_n(z)$.

Clearly, exact eigenvalues of H should not depend upon ω . The MPT prescribes to use as ω one of the real roots of the equation $\partial\epsilon_n/\partial\omega = 0$. In our case this leads to

$$\omega^3 - \omega - 2 \cdot C_n = 0. \quad (2.4)$$

Combining (2.3) and (2.4) we obtain:

$$\epsilon_n = \frac{1}{4} (n + \frac{1}{2}) \cdot (3\omega + \omega^{-1}). \quad (2.5)$$

The form of solution depends on the sign of $Q = C_n^2 - \frac{1}{27}$. If $Q > 0$ then:

$$\omega = (C_n + \sqrt{Q})^{1/3} + (C_n - \sqrt{Q})^{1/3}. \quad (2.6)$$

For $Q < 0$;

$$\omega = \frac{2}{\sqrt{3}} \cos \frac{\phi}{3}, \quad y = \text{arctg} \left(\frac{1}{27 C_n^2} - 1 \right)^{1/2}. \quad (2.7)$$

It is useful to consider limiting cases of (2.7). If the anharmonicity is very strong ($\chi \gg 1$) then:

$$\epsilon_n = \left(\frac{81}{32} \right)^{1/3} \cdot \chi^{1/3} \cdot (n + \frac{1}{2})^{2/3} \cdot (n^2 + n + \frac{1}{2})^{1/3}. \quad (2.8)$$

In the opposite case (i.e., weak anharmonicity, $\chi \ll 1$, n is not very large, so that $C_n \ll 1$) one obtains

$$\epsilon_n = n + \frac{1}{2} + \frac{3}{2} \chi \cdot (n^2 + n + \frac{1}{2}). \quad (2.9)$$

The advantage of expressions (2.5)-(2.9) is in their simpli-

Table 1

Numerical results for the one-dimensional a.o.

X	n	ϵ_n^1	ϵ_n^2	Exact ^{/2/}	MPT
0.01	0	0.507255	0.507257	0.507256	0.50729
	1	1.53565	1.53565	1.53565	1.5358
	2	2.59083	2.59079	2.59085	2.5909
	3	3.6711	3.6709	3.6711	3.6708
	4	4.77486	4.77439	4.77491	4.7740
	5	5.90096	5.90001	5.90103	5.8993
	6	7.0482	7.0466	7.0483	7.0455
	7	8.2158	8.2132	8.2158	8.2116
	8	9.403	9.399	9.403	9.3968
0.3	0	0.63804	0.63816	0.63799	0.64163
	1	2.09431	2.09464	2.09464	2.105
	2	3.8392	3.8343	3.8448	3.8424
	3	5.796	5.773	5.797	5.7795
	4	7.91	7.87	7.91	7.8782
	5	10.161	10.111	10.167	10.115
	6	12.54	12.47	12.54	12.474
	7	15.03	14.94	15.03	14.942
	8	17.62	17.52	17.62	17.510
1.0	0	0.80405	0.80446	0.80377	0.8125
	1	2.73718	2.73779	2.73789	2.7599
	2	5.166	5.155	5.178	5.1724
	3	7.39	7.89	7.94	7.9079
	4	10.95	10.89	10.96	10.900
	5	14.192	14.097	14.203	14.109
	6	17.62	17.50	17.63	17.508
	7	21.23	21.07	21.24	21.076
	8	24.99	24.79	25.00	24.8
200	0	3.9357	3.9379	3.9309	4.0085
	1	14.0532	14.0583	14.0592	14.234
	2	27.44	27.35	27.55	27.484
	3	42.89	42.63	43.01	42.746
	4	59.94	59.48	60.03	59.582
	5	78.3	77.6	78.4	77.735
	6	97.8	96.9	97.9	97.034
	7	118.4	117.3	118.4	117.36
	8	139.9	138.5	139.9	138.61
20000	0	18.160	18.171	18.137	18.502
	1	64.958	64.982	64.987	65.803
	2	126.96	126.57	127.51	127.19
	3	198.6	197.4	199.2	197.93
	4	277.6	275.5	278.1	275.99
	5	362.8	359.7	363.2	360.16
	6	453.3	449.2	454	449.67
	7	548.7	543.5	548.9	543.93
	8	648.3	642.0	648.5	642.5

city which is preserved for 3-dimensional a.o. too. But are they accurate enough to use them in practice? In Table 1 we compare them both with exact calculations ^{/2/} and with the 2nd order of the same MPT ^{/8/}. In the latter case the ω satisfy the algebraic equation of the sixth degree, which may be solved only numerically. Two roots of this equation are real to which

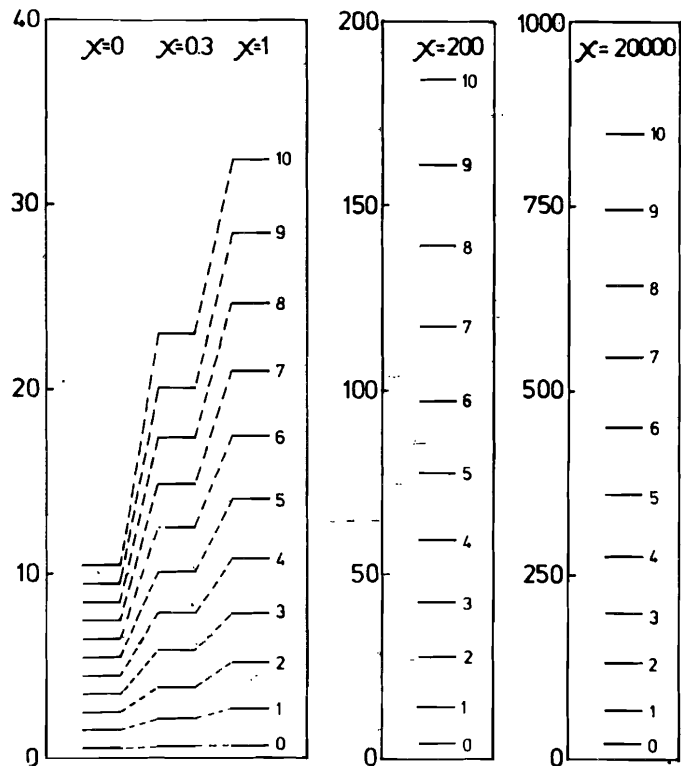


Fig.1. The energy levels of a one-dimensional anharmonic oscillator for different values of the dimensionless constant χ (see (2.2)). Numbers on the right of levels mean the quantum number n .

the energies ϵ_n^1 and ϵ_n^2 presented in Table 1 correspond. In the last column (see also fig.1) one finds the energy levels ϵ_n given by (2.5). We conclude that both ϵ_n and ϵ_n^2 agree with exact values with the 1-2% accuracy. For ϵ_n^1 the agreement is somewhat better.

It is useful to compare the 1st order MPT with other approximate methods. For instance the WKB method ^{/6/} gives the following expression for the a.o. energy levels:

$$\epsilon_n = \frac{a^2}{4\beta} \left\{ \left[1 + \left(\frac{2}{m\alpha^3} \right)^{1/2} 3\beta J \right]^{4/3} - 1 \right\}, \quad (2.10)$$

where J is obtained from the Bohr-Sommerfeld quantum condition which in the treated case is equivalent to the following transcendental equation

$$\frac{2}{\pi} K(k) \cdot J = \left(n + \frac{1}{2} \right) \hbar. \quad (2.11)$$

Here $K(k)$ is a complete elliptic integral of the 1st kind. Its modulus k is given by

$$k = \frac{1}{\sqrt{2}} \left\{ 1 - \left[1 + \frac{6\beta J}{(2m\alpha^3)^{1/2}} \right]^{-2/3} \right\}^{1/2}. \quad (2.12)$$

So, to obtain energy levels (2.10), one should first find J from (2.12). In the limiting cases the WKB method gives ^{/6/}:

$$\chi \ll 1; \quad \epsilon_n = n + \frac{1}{2} + 2\chi \left(n + \frac{1}{2} \right)^2$$

$$\chi \gg 1; \quad \epsilon_n \approx 1,3765 \cdot \left(n + \frac{1}{2} \right)^{4/3}.$$

We conclude:

- 1) the MPT final expressions (2.5)-(2.7) are much simpler;
- 2) contrary to the WKB method there is no need in preliminary solution of the transcendental equation;
- 3) the MPT works equally well both for large and small values of n , while WKB expressions are satisfactory only for large n .

3. Let the harmonic constant $a < 0$ ^{*}. The potential energy

has a minimum value $(-V_0 = -\frac{a^2}{4\beta})$ at $x_0 = \pm \left(\frac{a}{2\beta} \right)^{1/2}$. Applying

the previous reasonings one obtains the following expressions for the energy levels:

$$\epsilon_n = \hbar \omega_0 \cdot \epsilon_n, \quad \omega_0 = \sqrt{\frac{2|a|}{m}}, \quad \epsilon_n = \frac{1}{4} \left(n + \frac{1}{2} \right) \cdot (3\omega - \omega^{-1}), \quad (3.1)$$

where ω is defined now as

$$\omega = \left(c_n + \sqrt{\frac{1}{27} + c_n^2} \right)^{1/3} - \left(\sqrt{\frac{1}{27} + c_n^2} - c_n \right)^{1/3}$$

$$c_n = 3\chi \frac{n^2 + n + 1/2}{n + 1/2}, \quad \chi = \frac{\hbar \beta}{2\omega_0 |a| m} = \frac{1}{16} \frac{\hbar \omega_0}{V_0}.$$

^{*} Expressions (2.10)-(2.12) obtained in ^{/6/} are valid for positive values of a only. The similar equations for $a < 0$ are given below (see (3.4)-(3.6)).

For $\chi \gg 1$ the anharmonic term dominates, and we arrive at (2.8). The case of weak anharmonicity ($\chi \ll 1$ and n is not very large) is more interesting. One obtains:

$$\mathcal{E}_n = -\frac{2}{3} V_0 \frac{(n + 1/2)^2}{n^2 + n + 1/2}. \quad (3.2)$$

So, the 1st order MPT predicts the lack of levels in the interval $-V_0 \leq \mathcal{E} \leq -\frac{2}{3} V_0$ and their definite grouping around the value $-\frac{2}{3} V_0$ (when $c_n \ll 1$).

On the other hand developing in the Schroedinger Eq. the potential-energy term near the minimum in $(x - x_0)^2$ one obtains:

$$\mathcal{E}_n = -V_0 + \sqrt{2} \hbar \omega_0 \cdot (n + \frac{1}{2}). \quad (3.3)$$

We conclude that expression (3.2) is incorrect, and MPT (at least its 1st order) does not work for negative energies.

Now solve the same problem using the WKB method. It leads to a transcendental equation which takes different forms for positive and negative energies. For $\mathcal{E} > 0$ one has:

$$\frac{\hbar \omega_0}{V_0} \cdot (n + \frac{1}{2}) = \frac{\epsilon}{(1 + \epsilon)^{1/4}} \frac{(1 - k^2) \cdot K + (2k^2 - 1) \cdot E}{k^2 (1 - k^2)} \cdot \frac{4}{3\pi} \quad (3.4)$$

Here $\epsilon = \frac{\mathcal{E}}{V_0}$, $\omega_0 = \sqrt{\frac{2|a|}{m}}$, $k^2 = \frac{1 + \sqrt{1 + \epsilon}}{2\sqrt{1 + \epsilon}}$,

From now K and E are complete elliptic integrals of the 1st and 2nd kind, respectively: $K = K(k) = F(\frac{\pi}{2}, k)$, $E = E(k) = F(\frac{\pi}{2}, k)$. If $\mathcal{E} < 0$ then:

$$\sqrt{2} \frac{\hbar \omega_0}{V_0} \cdot (n + \frac{1}{2}) = (1 + \sqrt{1 + \epsilon})^{3/2} \cdot [(2 - k^2) \cdot E - 2 \cdot (1 - k^2) \cdot K] \cdot \frac{4}{3\pi}. \quad (3.5)$$

Here $k^2 = \frac{2\sqrt{1 + \epsilon}}{1 + \sqrt{1 + \epsilon}}$. In the limiting cases one obtains either (2.8) (large positive energies) or (3.3) (at the bottom of the potential well). The case of zero energies is also interesting. We have the following Eq.

$$\gamma \cdot (n + \frac{1}{2}) = \begin{cases} \phi(\epsilon) & \text{for } \mathcal{E} < 0 \\ \frac{1}{2} \phi(\epsilon) & \text{for } \mathcal{E} > 0, \end{cases} \quad (3.6)$$

Here $\gamma = \frac{\pi \hbar \omega_0}{V_0}$, $\phi(\epsilon) = \frac{16}{3} - \epsilon \ln |\epsilon| - \epsilon (\ln 4 + 1)$.

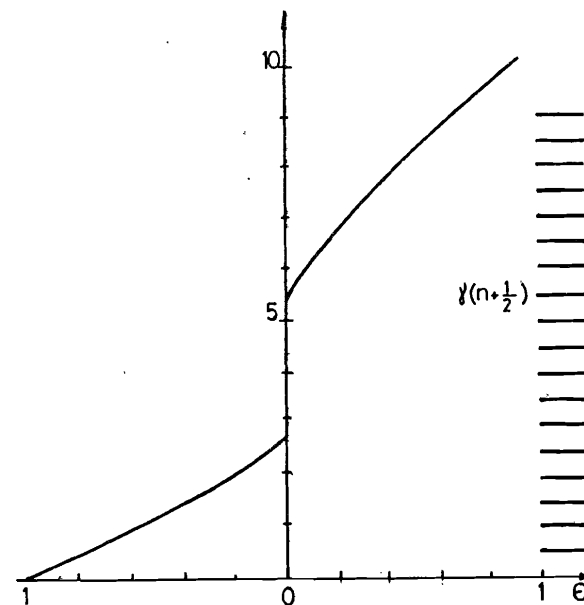
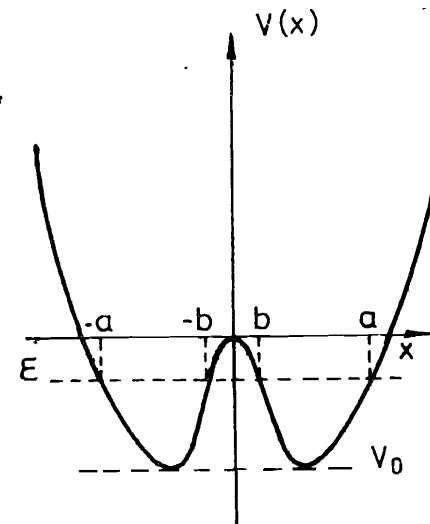


Fig. 2. The WKB method predicts the disappearance of the levels with quantum number n in the intervals $\frac{8}{3} < \gamma \cdot (n + \frac{1}{2}) < \frac{16}{3}$, $\gamma = \frac{\pi \hbar \omega_0}{V_0}$. The horizontal lines on the right side of the Fig. mean the left hand side of (3.6).

Fig. 3. The potential energy of the one-dimensional anharmonic oscillator ($a < 0$). The classical motion for $\mathcal{E} < 0$ takes place in one of the two potential wells (say, right). The oscillation amplitude grows as much as twice when one goes from $\mathcal{E} < 0$ to $\mathcal{E} > 0$.



Considering the r.h.s. of (3.6) (see Fig. 2) one observes that there are no solutions for $\frac{8}{3} < \gamma \cdot (n + \frac{1}{2}) < \frac{16}{3}$. This means that if one fixes anharmonicity β and traces a given energy level ($n = \text{const}$), attaching to the harmonic constant a still larger negative values, then for some value of a this level disap-

Table 2

Eigenvalues of the one-dimensional anharmonic oscillator
($H = -\Delta - z^2 x^2 + x^4$)^{4/}

z^2	\mathcal{E}_0	\mathcal{E}_1	\mathcal{E}_{20}	\mathcal{E}_{38}	\mathcal{E}_{39}
0	1.06	3.8	122.6	284	293
	1.08	3.85	121.4	283.7	291.1
0.5	0.87	3.33	120	280	290
	0.9	3.4	118.8	277.3	287
1	0.657	2.83	117.5	276	286
	0.7	2.92	116.1	273.3	283
2	0.138	1.71	112	268	278
	0.25	1.85	111	265	275
4	-1.71	-0.125	102	252	262
	-0.98	-0.75	99.6	248	258
5	-3.41	-3.25	96.1	244	254
	-2.36	-1.79	94	240	250
7	-8.67	-8.66	84.8	228	237
	-6.31	-5.26	82	223	232
10	-20.6	-20.6	67.1	202	211
	-14.26	-14.13	63.1	196.1	204.5
15	-50.8	-50.8	36.1	157.6	165
	-34.8	-34.3	28	148.2	156
50	-615	-615	-42.2	-261	-261
	-411.7	-411.4	-391	-331.6	-327.3
100	-2486	-2486	-2210	-1960	-1960
	-1659.6	-1659.5	-1653.1	-1622.2	-1620

For each z^2 the 1st and 2nd lines present results of the ref. mentioned in the headline of the Table and the MPT results, resp. The authors of^{4/} present the energy levels with 12 significant numbers. For the lack of space we retain only 5 ones. This applies for Table 3, too.

For small negative energies ($\mathcal{E} = -\mathcal{E}_1$, $V_0 \gg \mathcal{E}_1 > 0$) one gets:

$$\omega = \sqrt{2} \pi \omega_0 \cdot \left(\ln \frac{84 V_0}{\mathcal{E}_1} \right)^{-1}$$

pears. It is clear that this disappearance is due to the twice increasing of the classical oscillation amplitude when one passes from $\mathcal{E} < 0$ to $\mathcal{E} > 0$ (see Fig.3).

There are few exact calculations of the energy levels for the negative values of a . In ref.^{3/} there was calculated the difference $\Delta \mathcal{E}$ between the energies of ground and first excited states. For the potential $V(x) = 1/2(x^2 - f^2)^2$ the authors obtained $\Delta \mathcal{E} = 1.37$; 0.79 and 0.23 for $f^2 = 0$; 1 and 2, respectively. The 1st order MPT gives; 1.38; 0.805 and 0.115. For the last value both energies \mathcal{E}_0 and \mathcal{E}_1 are negative. We mentioned above that the studied method does not work for this case. For $a < 0$ extensive calculations ($H = -\Delta - z^2 x^2 + x^4$) were made also in^{4/}. We collected them in Table 2 side by side with MPT results to see explicitly now MPT breaks for negative energies. On the other hand WKB method qualitatively right describes the energy levels at the bottom of potential well. It predicts the splitting of each level in two. Its magnitude is^{10/}

$$\Delta \mathcal{E} = \frac{\hbar \omega}{\pi} \exp(-\lambda), \quad \lambda = \frac{1}{\hbar} \int_{-b}^b |p| dx. \quad (3.7)$$

Here ω is the frequency of the classical particle motion in one of the two potential wells (Fig.3). To obtain ω and λ we integrate the equations of motion. As a result one has^{11/}

$$\omega = \frac{\pi}{\sqrt{2}} \frac{\omega_0 \sqrt{1+R}}{K(\sqrt{\frac{2R}{1+R}})}, \quad R = \sqrt{1 + \mathcal{E}/V_0}, \quad (3.8)$$

$$\lambda = \frac{8\sqrt{2}}{3} \frac{V_0}{\hbar \omega_0} \sqrt{1+R} \cdot [E(\sqrt{\frac{1-R}{1+R}}) - R \cdot K(\sqrt{\frac{1-R}{1+R}})]. \quad (3.9)$$

Now consider limiting cases of (3.7)-(3.9). At the bottom of the potential well

$$\mathcal{E} = -V_0 + \mathcal{E}_1 \quad (V_0 \gg \mathcal{E}_1 > 0), \quad \omega = \sqrt{2} \omega_0, \quad \lambda = \frac{8\sqrt{2}}{3} \frac{V_0}{\hbar \omega_0}$$

For $z^2 = 100$ this gives: $V_0 = z^4/4 = 2500$, $\hbar \omega_0 = 2z = 20$, $\lambda = 471.4$. So, the level splitting is negligible. The energy of levels is fairly well described by (3.3): $\mathcal{E}_n = -2500 + 20\sqrt{2(n+1/2)}$; This gives*: $\mathcal{E}_0 = -2485.86$ (-2485.87); $\mathcal{E}_{10} = -2203$ (-2210); $\mathcal{E}_{20} = -1920$ (-1960). The number in brackets are exact values taken from^{4/}.

* The initial levels numeration^{4/} was changed to take into account their degeneration.

A particularly simple formula follows from (2.8) when harmonic constant $\alpha = 0$:

$$\epsilon_n = \left(\frac{81}{32} \frac{\hbar^4 \beta}{m^2} \right)^{1/3} \cdot \left(n + \frac{1}{2} \right)^{2/3} \cdot \left(n^2 + n + \frac{1}{2} \right)^{1/3}. \quad (3.10)$$

The comparison with exact results^{15/} (see Table 3) shows that inaccuracy of (3.10) is $\approx 1\%$.

We conclude that for $\alpha \leq 0$ the MPT and WKB methods complement each other. In fact, MPT works well for positive energies if c_n is sufficiently large. This includes the cases of large anharmonicity and arbitrary energy and vice versa. On the

other hand MPT method breaks for negative energies, while WKB one adequately describes the levels at the bottom of the potential well.

All this instils the hope that a combined use of the WKB and MPT methods gives good results for the three-dimensional anharmonic oscillator too.

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Table 3

Eigenvalues of the one-dimensional quartic oscillator
 $(-\Delta + x^4)^{1/5}$

n	ϵ_n	n	ϵ_n	n	ϵ_n	n	ϵ_n
0	1.06 1.08	8	37.9 37.6	21	130.64 129.4	37	274.27 271.6
1	3.8 3.85	9	43.98 43.57	23	147.1 145.6	39	293.95 291.03
2	7.46 7.44	10	50.26 49.78	25	164.01 162.4	41	313.96 310.85
3	11.64 11.57	11	56.73 56.19	27	181.4 179.6	43	334.29 331.
4	16.26 16.14	13	70.25 69.57	29	199.2 197.22	45	354.94 351.42
5	21.24 21.06	15	84.46 83.64	31	217.4 215.24	47	375.89 372.17
6	26.53 26.3	17	99.3 98.32	33	236 233.7	49	397.14 393.2
7	32.1 31.8	19	114.7 113.57	35	254.95 252.43		

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Одномерный ангармонический осциллятор

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Мы получили явные выражения для уровней энергии 1-мерного ангармонического осциллятора $\alpha x^2 + \beta x^4$, используя первый порядок, так называемой, модифицированной теории возмущений /МТВ/ и квазиклассический метод. Расчеты выполнены для широкого спектра значений ангармонической константы β и энергий. При положительной константе гармоничности α точность метода оказывается не хуже 1-2%. Результирующие формулы МТВ более просты и не требуют предварительного решения трансцендентного уравнения /как в случае ВКБ метода/. Особенно простые выражения получаются при $\alpha = 0$. Их неточность - около 1%. Мы обнаружили, что МТВ плохо работает при отрицательных энергиях /при этом $\alpha < 0$ /, в то время как ВКБ метод адекватно описывает уровни энергии и их расщепление вблизи дна потенциальной ямы. Таким образом, эти методы дополняют друг друга.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

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The One-Dimensional Anharmonic Oscillator

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We have obtained, in a closed form, the energy levels of a one-dimensional anharmonic oscillator (a.o.) $\alpha x^2 + \beta x^4$ using the 1st order of the so-called modified perturbation theory (MPT) as well as WKB method. The calculations were performed for a broad range of the anharmonic constant β and energies. We prove that inaccuracy of the 1st order MPT for positive harmonic constant is not worse than 1-2%. We note that MPT final expressions are much simpler. Contrary to the WKB method there is no need in the preliminary solution of the transcendental equation. A particularly simple formula is obtained for the energy levels of the pure quartic oscillator. It is found that for $\alpha < 0$ and negative energies MPT is not satisfactory. On the other hand WKB method reasonably describes the energy levels and their splitting at the bottom of the potential well. We conclude that these methods complement each other.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

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