

Chapter 2

1/N-Expansion in Quantum Mechanics

The method of $1/N$ -expansion has been developed recently. It is used in different branches of theoretical physics. The idea of this method is the seeking of some parameter $N \gg 1$ for the considered system. The solution of the problem is achieved by the expansion in small parameter $1/N$. Sometimes the applicability of the solution is good even up to values of $N \sim 1$. For example, WKB-approximation produces often result with high accuracy and at the quantum numbers $n \sim 1$, though formally the condition of its applicability is $n \gg 1$. Choice of parameter N is usually connected with the increasing of number of states, or degrees of freedom of the considered system, dimension of space, and so on. Below we consider some simple examples of such approach for the solution of single-particle Schrödinger equation.

1/N Expansion for Deep One-Dimensional Potential Well

Let us consider the discrete states of a particle in one-dimensional potential well $U(x) = U_0 v(x/d)$ with the width d and with the one minimum in the point x_0 (see Fig. 1.2).

The function v determines the form of the potential well. The properties of such system depend on the value of the dimensionless parameter

$$N = \sqrt{\frac{md^2U_0}{\hbar^2}}. \quad (2.1)$$

The number of bound states increases with the growing of this parameter. In the case of $N \gg 1$ wave functions of low-lying levels are located nearly of the minimum of the potential, where $U'(x_0) = 0$. We can expand the potential in powers of $(x - x_0)/d$ (below we put in this Section $m = d = \hbar = 1$):

$$U(x) = U(x_0) + \frac{1}{2}\omega^2(x - x_0)^2 + \alpha(x - x_0)^3 + \beta(x - x_0)^4 + \dots \quad (2.2)$$

where

$$\omega = \sqrt{U''(x_0)}; \quad \alpha = \frac{1}{6}U'''(x_0); \quad \beta = \frac{1}{24}U^{(IV)}. \quad (2.3)$$

Here, the third and next terms of expansion are small perturbations of the harmonic oscillator with the frequency ω . The perturbation series for the energy E_n in powers of anharmonicity coefficients is (see [1], Sect. 38)

$$E_n = U(x_0) + \omega \left(n + \frac{1}{2} \right) - \frac{15}{4} \frac{\alpha^2}{\omega^4} \left(n^2 + n + \frac{11}{30} \right) + \frac{3}{2} \frac{\beta}{\omega^2} \left(n^2 + n + \frac{1}{2} \right) + \dots \quad (2.4)$$

This is typical example of 1/N-expansion for the energy levels in the considered problem. We have in this expansion:

$$U(x_0) \sim N^2; \quad \omega \sim N, \quad \frac{\alpha^2}{\omega^4} \sim \frac{\beta}{\omega^2} \sim 1 = N^0 \quad \text{and so on.}$$

Such expansion is asymptotically exact at $N \rightarrow \infty$. However it has high accuracy as well as at $N \sim 1$. In order to increase the accuracy we should take into account next terms in expansion (2.4). However, we should have in mind that this expansion is an asymptotic (divergent) series in $1/N$. Therefore, corrections of high orders increase, beginning with some number k , which depends on N . Usually, it occurs for sufficiently large values of k .

1/N Expansion for a Particle in Central Potential Well

In order to investigate binding states of a particle in the smooth central potential well $U(r) = U_0 v(r/R)$ we choose the expansion parameter

$$N \equiv n = l + n_r + 1. \quad (2.5)$$

In the case of Coulomb potential the quantity n is the principal quantum number. Radial quantum number n_r is supposed to be fixed, and orbital quantum number $l \rightarrow \infty$. Further, we substitute

$$U_0 \equiv \frac{n^2 g \hbar^2}{m R^2}. \quad (2.6)$$

Let us write the effective potential (1.32) as an expansion in $1/n$:

$$U_{\text{eff}}(r) = n^2 \left\{ g v(r) + \frac{1}{2r^2} - \frac{2n_r + 1}{2nr^2} + \frac{n_r(n_r + 1)}{2n^2 r^2} \right\}. \quad (2.7)$$

Here and below in this section we put $\hbar = m = R = 1$. Analogously, we write the energy of some level:

$$E_{nn_r} = n^2 \left\{ \varepsilon^{(0)} + \frac{1}{n} \varepsilon_{n_r}^{(1)} + \frac{1}{n^2} \varepsilon_{n_r}^{(2)} + \dots \right\}. \quad (2.8)$$

At $n \rightarrow \infty$ the particle is localized near to the minimum of the effective potential r_0 (this the point of classical equilibrium). Hence,

$$gr_0^3 v'(r_0) = 1, \quad \varepsilon^{(0)} = \frac{1}{2r_0^2} + gv(r_0). \quad (2.9)$$

Further, we restrict ourselves in Eq. (2.7) by the square term in powers of $(r - r_0)$. Then Eq. (1.31) for radial wave function $\chi(r)$ takes the form of Schrödinger equation for harmonic oscillator :

$$\chi_{nn_r}''(r) - \left[n^2 \omega^2 (r - r_0)^2 - \frac{n(2n_r + 1)}{r_0^2} - 2n\varepsilon_{n_r}^{(1)} \right] \chi_{nn_r}(r) = 0. \quad (2.10)$$

Here the notation is introduced

$$\omega \equiv \sqrt{gv''(r_0) + \frac{3}{r_0^4}}. \quad (2.11)$$

In this approximation we obtain

$$\begin{aligned} \varepsilon_{n_r}^{(1)} &= \left(\omega - \frac{1}{r_0^2} \right) \left(n_r + \frac{1}{2} \right); \\ \chi_{nn_r}^{(0)}(r) &= \left\{ \frac{n\omega}{\pi 2^{2n_r} (n_r!)^2} \right\}^{1/4} H_{n_r}(\xi) \exp(-\xi^2/2). \end{aligned} \quad (2.12)$$

Here once more notation is introduced $\xi \equiv \sqrt{n\omega} (r - r_0)$.

According to Eq. (2.10), the unperturbed harmonic oscillator has the frequency $\omega_0 = n\omega$. In the region of localization of a particle the typical deviations of this particle from the equilibrium point are small:

$$(r - r_0) \sim \omega_0^{-1/2} \sim n^{-1/2} \ll 1.$$

Analogous estimates are valid for deviations of radial coordinate in anharmonic terms which can be considered as small perturbation of the harmonic oscillator. We write this perturbation in the form of sum of two terms: one term is even function of the variable $x \equiv r - r_0$ while the other term is odd function of this variable

$$\begin{aligned} V &= V^{(+)} + V^{(-)}; \\ V^{(+)}(x) &= \frac{1}{2r_0^2} n_r(n_r + 1) - \frac{3}{2} n(2n_r + 1) \frac{x^2}{r_0^4} + n^2 \beta x^4 + \dots; \\ V^{(-)}(x) &= (2n_r + 1) n \frac{x}{r_0^3} + n^2 \alpha x^3. \end{aligned} \quad (2.13)$$

Here the notations are introduced

$$\alpha = -\frac{2}{r_0^5} + \frac{1}{6}gv'''(r_0); \quad \beta = \frac{5}{2r_0^6} + \frac{1}{24}gv^{(IV)}(r_0). \quad (2.14)$$

The perturbation $V^{(+)}$ is a small quantity of the magnitude of $1/n$ compared to the $U_{\text{eff}}^{(0)}$, while the perturbation $V^{(-)}$ is a small quantity of the magnitude of $1/\sqrt{n}$. However, this distinction is essential in corrections to the wave functions only. Contributions to the energy shifts from even and odd parts of the perturbation are of the same order of magnitude. We obtain

$$\begin{aligned} \varepsilon_{n_r}^{(2)} = & \left\{ -\frac{15}{16} \left(s + \frac{22}{15} \right) A^2 + \frac{3}{8} (s+2) B \right. \\ & \left. - \frac{1}{4} (s+1) \left[6AC^{3/2} + 3C^2 + \frac{3}{2}C \right] + \frac{s}{8}C \right\} \omega. \end{aligned} \quad (2.15)$$

(compared with Eq. (2.4)). Here the notations are introduced $s = n_r(n_r + 1)$ and

$$A = \frac{\alpha}{\omega^{5/2}}; \quad B = \frac{\beta}{\omega^3}; \quad C = \frac{1}{\omega r_0^2}. \quad (2.16)$$

The further developments of $1/N$ -expansion method are considered in the problems of this chapter.

Parameter N as Dimension of the Space

Finally, we consider the case when the parameter N is the dimension of the space (i.e. $N = 3$ for real systems). The Laplacian for spherical symmetric functions in N -dimensional space is

$$\Delta f(r) = f'' + \frac{N-1}{r} f'; \quad r = \sum_{i=1}^N x_i^2.$$

This result can be obtained using the relation $\Delta = \text{div grad}$, and also $\text{grad} f(r) = f' \mathbf{r}/r$ and $\text{div } \mathbf{r} = N$. Therefore, the Schrödinger equation for s-state in the central

potential $U(r)$ is reduced to the usual one-dimensional wave equation by substitution $\Psi = r^{-(N-1)/2}\chi(r)$:

$$-\frac{1}{2}\chi'' + [U_{\text{eff}}(r) - E]\chi = 0; \quad U_{\text{eff}}(r) = U(r) + \frac{(N-1)(N-3)}{8r^2} \quad (2.17)$$

(here $\hbar = m = 1$). This effective potential differs from $U(r)$ by centrifugal potential for N -dimensional space (compare with the Eq. (1.32)). Therefore, 1/N-expansion can be made analogous to 1/n-expansion, see Problem 1.6.

It should be noted that the method of 1/N-expansion is applicable also for many-dimensional systems with non-separable variables, including many-body systems.

2.1 1/N Expansion for Energy Levels of Binding States

Problems and Solutions

Problem 2.1

Find the energy spectrum of binding states using 1/ N expansion where N is given by Eq. (2.1). Consider the one-dimensional potentials:

$$\begin{aligned} (a) \quad U(x) &= -\frac{U_0}{\cosh^2(x/a)}; \\ (b) \quad U(x) &= U_0 \left(\frac{a}{x} - \frac{x}{a} \right)^2; \quad 0 < x < \infty; \\ (c) \quad U(x) &= U_0 \left[\exp\left(-\frac{2x}{a}\right) - b \exp\left(-\frac{x}{a}\right) \right]. \end{aligned}$$

Here the parameters U_0, a, b are positive numbers. Compare the obtained results with corresponding exact solutions.

Solution

All calculations are based on Eq. (2.4). Below we put $\hbar = m = a = 1$, $N = \sqrt{U_0}$.

(a) We have

$$\omega = \sqrt{2}N, \quad \alpha = 0, \quad \beta = -\frac{2}{3}N^2$$

Table 2.1 Energies of the ground term $n = 0$ at different values of N

$N = \sqrt{U_0}$	1	1.5	2	3	4
$-E_0(1/N)$	0.543	1.439	2.836	7.129	13.422
$-E_0^{\text{exact}}$	0.500	1.410	2.814	7.114	13.411
$-E_0^q$	0.418	1.314	2.711	7.004	13.297

Table 2.2 Energies of the first excited term $n = 1$ at different values of N

$N = \sqrt{U_0}$	1.5	2	3	4
$-E_1(1/N)$	0.318	1.007	3.886	8.765
$-E_1^{\text{exact}}$	0.231	0.942	3.842	8.732
$-E_1^q$	0.193	0.882	3.761	8.640

and

$$\begin{aligned}
 E_n(1/N) &= -N^2 + N\sqrt{2} \left(n + \frac{1}{2} \right) - \frac{1}{2} \left(n^2 + n + \frac{1}{2} \right) + O\left(\frac{1}{N}\right) \\
 &\approx -U_0 + \sqrt{2U_0} \left(n + \frac{1}{2} \right) - \frac{1}{2} \left(n^2 + n + \frac{1}{2} \right). \quad (2.18)
 \end{aligned}$$

Let us compare this spectrum with exact solution (see [1], Sect. 23):

$$E_n^{\text{exact}} = -\frac{1}{8} \left[\sqrt{1 + 8U_0} - (2n + 1) \right]^2, \quad (2.19)$$

and with the WKB-solution E_n^q which differs from Eq. (2.19) by change $1 + 8U_0 \rightarrow 8U_0$.

In the case of the ground term $n = 0$, we obtain at different values of N the results presented in Table 2.1:

It is seen that according to Eq. (2.19) the total number of levels in the considered potential is approximately $N\sqrt{2}$ at $N \gg 1$.

In the case of the first excited term $n = 1$ (this level appears at $N = 1$) analogous results are presented in Table 2.2:

These results allow to make a conclusion that $1/N$ expansion with terms up to the second order in $1/N$ is applicable even at $N \geq 1$. Bad accuracy occurs for shallow levels only.

(b) In this case we obtain

$$E_n(1/N) = \left(n + \frac{1}{2} \right) \sqrt{8U_0} + \frac{1}{8} + \dots$$

The exact expression for energy levels is

$$E_n^{\text{exact}} = \sqrt{8U_0} \left[n + \frac{1}{2} + \frac{1}{4} \left(\sqrt{8U_0 + 1} - \sqrt{8U_0} \right) \right].$$

The comparison of both expressions shows that 1/N-expansion has high accuracy also at $N \geq 1$; for example, we obtain for the ground level ($n = 0$) and $N = 1$ that $E_0(1/N)/E_0^{\text{exact}} = 1.026$.

(c) The first three terms of 1/N-expansion give the exact value of the energy spectrum (see [1], Sect. 23):

$$\begin{aligned} E_n(1/N) &= E_n^{\text{exact}} = -\frac{1}{4}U_0b^2 + \sqrt{\frac{1}{2}U_0b^2} \left(n + \frac{1}{2}\right) - \frac{1}{2} \left(n + \frac{1}{2}\right)^2 \\ &= -\frac{1}{8} \left[\sqrt{2U_0b} - (2n + 1) \right]^2. \end{aligned}$$

Obviously, the higher terms of 1/N-expansion vanish in the considered case.

We can conclude that in all considered cases 1/N-expansion has high numerical accuracy even on the boundary of its applicability. This method presents useful supplement to the WKB-approximation for low-lying energy levels.

Problem 2.2

Find the energy spectrum for power attractive potentials $U(r) \sim r^\nu$ using 1/n-expansion (see Eq. (2.6)). Compare with exact values of the energy E_{nn_r} .

Solution

Let us write the power potential in the form

$$U(r) = G \frac{1}{r^\nu} \equiv gn^2 \frac{\hbar^2}{mR^2} \frac{1}{\nu} \left(\frac{r}{R}\right)^\nu. \quad (2.20)$$

($G > 0$ for attractive potential). The notation is introduced here

$$R = \left(\frac{n^2 g \hbar^2}{mG} \right)^{\frac{1}{2+\nu}}.$$

We restore in Eq. (2.8) the dimensional factor \hbar^2/mR^2 and put $g = 1$ in the sakes of simplicity. Then we obtain 1/n-expansion for energy levels of a particle in the power potential:

$$\begin{aligned}
E_{nn_r} &= n^2 \frac{\hbar^2}{m R^2} \left\{ \varepsilon^{(0)} + \frac{1}{n} \varepsilon_{n_r}^{(1)} + \frac{1}{n^2} \varepsilon_{n_r}^{(2)} + \dots \right\} = \\
&= \left(\frac{n^2 \hbar^2}{m} G^{2/\nu} \right)^{\frac{\nu}{\nu+2}} \left\{ \varepsilon^{(0)} + \frac{1}{n} \varepsilon_{n_r}^{(1)} + \frac{1}{n^2} \varepsilon_{n_r}^{(2)} + \dots \right\}. \quad (2.21)
\end{aligned}$$

The expansion coefficients $\varepsilon_{n_r}^{(k)}$ are determined by Eqs. (2.9), (2.12) and (2.15). In the considered case we have $v(r) = r^\nu/\nu$ and $g = 1$.

Elementary derivations give the results $r_0 = 1$, $\omega = \sqrt{2 + \nu}$ and

$$\varepsilon^{(0)} = \frac{2 + \nu}{2\nu}; \quad \varepsilon_{n_r}^{(1)} = \left(n_r + \frac{1}{2} \right) (\sqrt{2 + \nu} - 1). \quad (2.22)$$

More cumbersome derivations result in the expression for the second order of expansion

$$\begin{aligned}
\varepsilon_{n_r}^{(2)} &= \frac{2 - \nu}{144(2 + \nu)} \left\{ \nu^2 - 15\nu - 52 + 36\sqrt{2 + \nu} + 6n_r(n_r + 1) \right. \\
&\quad \left. \times (\nu^2 - 9\nu - 34 + 24\sqrt{2 + \nu}) \right\} \quad (2.23)
\end{aligned}$$

It should be noted that in the case $\nu < -2$ the falling on the origin occurs (see Problem 1.6), and the frequency ω becomes imaginary quantity.

Below we illustrate the accuracy of the 1/n-expansion at $n \sim 1$ on the examples of some values of the power ν .

(1) Coulomb and oscillator potentials

First of all, we note that in the case of Coulomb potential ($\nu = -1$) and oscillator potential ($\nu = 2$) the first two terms (2.21) and (2.22) exactly reproduce the energy spectrum. The coefficient $\varepsilon_{n_r}^{(2)} = 0$ in both cases, as it should be.

(2) Linear potential

In the case of $\nu = 1$ we obtain according to Eqs. (2.22–2.23)

$$\begin{aligned}
\varepsilon^{(0)} &= \frac{3}{2}; \quad \varepsilon_{n_r}^{(1)} = \left(n_r + \frac{1}{2} \right) (\sqrt{3} - 1); \\
\varepsilon_{n_r}^{(2)} &= - \left[\frac{11 - 6\sqrt{3}}{72} + \frac{7 - 4\sqrt{3}}{12} n_r (n_r + 1) \right]. \quad (2.24)
\end{aligned}$$

Below we compare in several tables the results of derivation of energy levels according to Eqs. (2.21–2.24) with exact values of the energy

$$E_{nn_r}^{\text{exact}} \equiv \left(\frac{\hbar^2 G^2}{m} \right)^{1/3} \varepsilon_{nn_r}^{\text{exact}}$$

Table 2.3 Energies of levels with $n_r = 0$

l	0	1	2
$\varepsilon_{n0}^{\text{exact}}$	1.85576	2.66783	3.37178
$\delta_{n0}^{(0)}$	-0.19	-0.11	-0.075
$\delta_{n0}^{(1)}$	$5.5 \cdot 10^{-3}$	$1.4 \cdot 10^{-3}$	$6.3 \cdot 10^{-4}$
$\delta_{n0}^{(2)}$	$9.9 \cdot 10^{-4}$	$1.6 \cdot 10^{-4}$	$5.3 \cdot 10^{-5}$

Table 2.4 Energies of levels with $n_r = 1$

l	0	1	2
$\varepsilon_{n1}^{\text{exact}}$	3.24461	3.87679	4.46830
$\delta_{n1}^{(0)}$	-0.27	-0.20	-0.15
$\delta_{n1}^{(1)}$	$2.5 \cdot 10^{-3}$	$1.2 \cdot 10^{-3}$	$7.2 \cdot 10^{-4}$
$\delta_{n1}^{(2)}$	$-1.9 \cdot 10^{-5}$	$-4.9 \cdot 10^{-6}$	$-1.9 \cdot 10^{-6}$

which are derived from numerical solution of radial Schrödinger equation. In those tables the quantity

$$\delta_{nn_r}^{(0,1,2)} = \frac{E_{nn_r}(1/n)}{E_{nn_r}^{\text{exact}}} - 1 \quad (2.25)$$

is given for $n_r = 0$ and 1. The indexes 0, 1, and 2 in Eq. (2.25) correspond to the order of the terms taken into account in 1/n-expansion in Eq. (2.21). Besides of this, in these tables the exact values of $\varepsilon_{nn_r}^{\text{exact}}$ are given.

It is seen that even at $l = 0$ 1/n-expansion for the energy E_{nn_r} has high accuracy already in the first order on $1/n$. If we take into account the term $\sim 1/n^2$ then accuracy of derivations increases strongly; errors of approximation decrease when l rises. Therefore, we restrict ourselves by the small values of the orbital quantum number l in order to illustrate applicability of 1/n-expansion in the most unfavorable case. We restricted ourselves also by small values of the radial quantum number n_r , but due to other reason. Small values of n_r are most favorable for applicability of 1/n-expansion. The localization region of a particle in the potential increases with growing of n_r (at the fixed value of l). Therefore effects of anharmonicity are more essential in such cases. Hence, the accuracy of 1/n-expansion diminishes (in particular, at $l \sim 1$). It is seen from the dependence of the coefficients of 1/n-expansion on n_r (see Eqs. (2.22) and (2.23)).

(3) High values of the power ν

Let us illustrate the accuracy of 1/n-expansion at larger values of the power ν . We restrict ourselves by terms on the order of $1/n$ in expansion (2.21). In Table 2.5 we give exact values of energies and errors of their calculations using 1/n-expansion for some values of the power ν and of the quantum numbers (l, n_r) .

Table 2.5 High values of the power ν

l	n_r	$\nu = 4$	$\nu = 6$	$\nu = 8$
0	0	1.50790; $-2.2 \cdot 10^{-2}$	1.64831; $-4.1 \cdot 10^{-2}$	1.80214; $-5.3 \cdot 10^{-2}$
0	1	4.62122; $1.7 \cdot 10^{-3}$	5.67414; $1.6 \cdot 10^{-2}$	6.57180; $3.5 \cdot 10^{-2}$
0	2	8.42845; $5.1 \cdot 10^{-3}$	11.1315; $2.2 \cdot 10^{-2}$	13.4512; $4.6 \cdot 10^{-2}$
1	0	2.82099; $-6.4 \cdot 10^{-3}$	3.21619; $-1.2 \cdot 10^{-2}$	3.58452; $-1.4 \cdot 10^{-2}$
1	1	6.36257; $2.9 \cdot 10^{-3}$	8.08082; $1.7 \cdot 10^{-2}$	9.54346; $3.7 \cdot 10^{-2}$
1	2	10.4570; $5.5 \cdot 10^{-3}$	14.1499; $2.3 \cdot 10^{-2}$	17.3455; $4.7 \cdot 10^{-2}$

The first number for each values of l, n_r is the exact value of $\varepsilon_{nn_r}^{\text{exact}}$, and the second number is the quantity $\delta_{nn_r}^{(1)}$ (see Eq. (2.25)). The energy of the level is given by relation

$$E_{nn_r}^{\text{exact}} = \left(\frac{\hbar^2}{m} G^{2/\nu} \right)^{\frac{\nu}{\nu+2}} \varepsilon_{nn_r}^{\text{exact}} \quad (2.26)$$

so that according to Eq. (2.21) the 1/n-expansion for the quantity ε_{nn_r} is of the form

$$\varepsilon_{nn_r} = n^{\frac{2\nu}{\nu+2}} \left\{ \varepsilon^{(0)} + \frac{1}{n} \varepsilon_{n_r}^{(1)} + \frac{1}{n^2} \varepsilon_{n_r}^{(2)} + \dots \right\}.$$

It is seen that the accuracy of 1/n-expansion decreases with growing of ν . This is explained by the fact that the considered potential is of the sharper form at large ν . Indeed, at $\nu \rightarrow \infty$ the power potential is transformed into the infinitely deep spherical potential well.

Problem 2.3

Apply 1/n-expansion for calculation of energy levels of a particle in short-range Hulthén potential

$$U(r) = -\frac{U_0}{\exp(r/R) - 1}.$$

Solution

We determine

$$v(r) = -\frac{1}{\exp(r) - 1}.$$

According to Eqs. (2.7, 2.9, 2.12) of 1/n-expansion we find the energy spectrum in parametric form:

$$g(r_0) \equiv \frac{mR^2U_0}{\hbar^2n^2} = \frac{(\exp(r_0) - 1)^2}{r_0^3 \exp(r_0)}; \quad (2.27)$$

$$E_{nn_r}^{(1/n)} = \frac{\hbar^2}{mR^2} n^2 \left\{ -\frac{1 - \exp(-r_0)}{r_0^3} + \frac{1}{2r_0^2} + \frac{1}{n} \left(n_r + \frac{1}{2} \right) \left[\omega(r_0) - \frac{1}{r_0^2} \right] + \dots \right\}, \quad (2.28)$$

where the notation is introduced

$$\omega(r_0) = \left[\frac{3}{r_0^4} - \frac{1}{r_0^3} \left(1 + \frac{2}{\exp(r_0) - 1} \right) \right]^{1/2}. \quad (2.29)$$

The parameter r_0 determines the point of stable classical equilibrium of a particle. According to Eq. (2.27) we have two values of r_0 for the given value of g (at $g < g_*$, see Fig. 2.1). We choose the smaller value of r_0 , since the larger values corresponds to unstable equilibrium: the maximum of the effective potential.

Equation (2.28) is asymptotically exact at $n \rightarrow \infty$ and fixed values of r_0 and n_r . However, at $n \sim 1$ this expression also has a good accuracy. As an example, we consider the most unfavorable case $l = 0$ for 1/n-expansion. The exact energy spectrum of a particle in Hulthén potential with $l = 0$ is given by

$$E_{nn_r}^{\text{exact}} = -\frac{\hbar^2}{8mR^2} \frac{1}{(n_r + 1)^2} \left[\frac{2mR^2U_0}{\hbar^2} - (n_r + 1)^2 \right]^2, \quad l = 0. \quad (2.30)$$

Using Eq. (2.27), we obtain

$$E_{nn_r}^{\text{exact}} = -\frac{\hbar^2}{8mR^2} (n_r + 1)^2 \left[\frac{2(\exp(r_0) - 1)^2}{r_0^3 \exp(r_0)} - 1 \right]^2. \quad (2.31)$$

Here $n = n_r + 1$ for states with $l = 0$.

We compare in Table 2.6 the results of calculations of energies for ground $1s$ -state ($n_r = 0$) using Eqs. (2.28) and (2.31) at the various values of potential parameters. We present the values of the quantities

$$\delta^{(0,1)} = \frac{E_{nn_r}(1/n)}{E_{nn_r}} - 1, \quad (2.32)$$

where indexes 0 and 1 correspond to the order of 1/n-expansion in Eq. (2.28) (compare with results of the previous Problem).

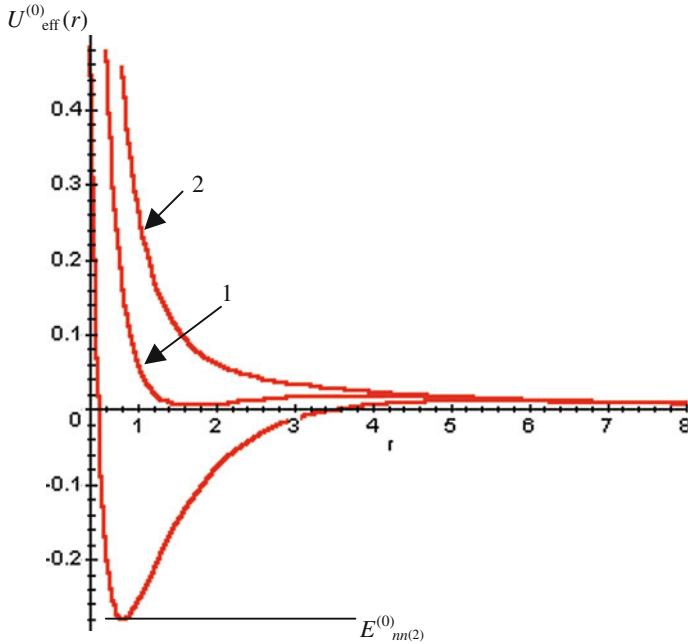


Fig. 2.1 Dependence of the effective potential $U_{\text{eff}}^{(0)} = n^2 (gv(r) + 1/2r^2)$ (see Eq. (2.7)) at the different values of the coupling constant g . Curve 1: $g = g_{cr}$ where the level with the energy $E_{nn_r} = 0$ appears; curve 2: $g = g_*$

Table 2.6 Energies of the ground 1s-state at the various values of potential parameters

r_0	0.1	0.2	0.5	0.8	1.0	1.3	1.5
g/g_{cr}	20	10	4.1	2.6	2.1	1.8	1.6
$\delta^{(0)}$	-10^{-3}	$-4 \cdot 10^{-3}$	$-3.5 \cdot 10^{-2}$	-0.12	-0.23	-0.52	-0.82
$\delta^{(1)}$	10^{-6}	$2 \cdot 10^{-5}$	$7 \cdot 10^{-4}$	$6 \cdot 10^{-3}$	$2 \cdot 10^{-2}$	$7 \cdot 10^{-2}$	0.16

It is seen that 1/n-expansion is applicable as well as at $n = 1$. Its convergency is slower with increase of r_0 , but essential errors appear only at $r_0 \sim 1.5$. The depth of the potential well diminishes with increase of r_0 ; the ratio g/g_{cr} illustrates this fact. The quantity g_{cr} is corresponding to the exact value of g when $E_{nn_r} = 0$, i.e., when a new level appears (see Fig. 2.1). According to Eq. (2.30) we have $g_{cr} = 0.5$ for the ground level. 1/n-expansion is inapplicable for shallow s-levels, since the wave function of s-level is localized far outside of the short-range potential at $E \rightarrow 0$. Indeed, at $r \rightarrow \infty$ we have $\chi \rightarrow \text{const} \neq 0$. However, the basics of 1/n-expansion is the assumption about localization of a particle nearly of the equilibrium point. Similar situation is realized for shallow levels in one-dimensional potentials (see Problem 2.1).

Above conclusions are confirmed by the fact that at $n \rightarrow \infty$ according to Eq. (2.28) we find the critical value $r_{0,cr}$ as a solution of the equation

$$\frac{2(1 - \exp(-r_0))}{r_0} = 1. \quad (2.33)$$

It is equal to $r_{0,cr} = 1.5936$. Hence, according to Eq. (2.27) we obtain the asymptotic value of $g_{cr}^{(0)}(1/n) = 0.7721$. More exact expressions of $1/n$ -expansion for calculation of the parameter g_{cr} at the finite values of n are given in the Problem 2.4.

Oppositely, at $g \rightarrow \infty$ and $r_0 \rightarrow 0$ the exactness of $1/n$ -expansion rises sharply. Indeed, Hulthén potential at small values of r is similar to Coulomb potential. But just small values of r are important only at $g \rightarrow \infty$. We have seen in the solution of the Problem 2.2 that zero approximation of $1/n$ -expansion gives exact values of Coulomb energies for any values of l and n_r .

In conclusion we consider shortly the case of $l \neq 0$. The wave function is localized even when a new level appears due to centrifugal potential barrier: $\chi_l \sim r^{-l}$ at $r \rightarrow \infty$. Therefore, no difficulties occur for application of $1/n$ -expansion even at $g \rightarrow g_{cr}$, when $E_{nn_r} \rightarrow 0$. Moreover, $1/n$ -expansion is applicable as well as at $g < g_{cr}$, when $E_{nn_r} > 0$ (but the effective potential still has the minimum at the point r_0). In this case the value of E_{nn_r} determines the energy of the quasi-stationary state. Its width Γ_{nn_r} is very small at $n \rightarrow \infty$. This width is determined by the penetrability of the potential barrier. However, when the quantity g diminishes further, points of stable and unstable equilibrium of a particle in the effective potential coincide with each other (see curve 2 in Fig. 2.1). The corresponding value of $g = g_*$ is determined from the equation

$$\omega(g_*) = 0. \quad (2.34)$$

In the case of Hulthén potential we find from this equation and Eq. (2.29) that $r_* = 2.576$ and $g_*^{(0)} = 0.6564$. Then the ratio $g_{cr}^{(0)}/g_*^{(0)} = 1.176$. Of course, the $1/n$ -expansion is inapplicable at $g \rightarrow g_*$. Indeed, according to Eq. (2.15) we have $\varepsilon_{n_r}^{(2)} \rightarrow -\infty$. The effective potential does not have a minimum at $g < g_*$, so that finite motion in the classical theory is impossible. Equilibrium points are moving to the complex plane in this case, and coefficients of expansion $\varepsilon_{n_r}^{(k)}$ are complex quantities. It is interesting that the formulas of $1/n$ -expansion are valid in this case when the value of g is far from g_* in quantum mechanics. They describe the quasi-stationary states, which present above-barrier resonance states (see Chap. 4). Imaginary part of the energy E_{nn_r} determines the width of such resonance states.

Finally, let us underline that the general peculiarities of application of $1/n$ -expansion for Hulthén potential are correct also for other smooth short-range potentials (Yukawa potential, exponential potential of the form $U(r) = -U_0 \exp(-r/R)$ and so on).

Problem 2.4

Obtain $1/n$ -expansion for a particle in the short-range central potential $U(r) = U_0 v(r/R)$ for *critical* value $\xi_{nn_r,cr}$ of the parameter

$$\xi \equiv \frac{mR^2 U_0}{\hbar^2}$$

which corresponds to appearing of the level with quantum numbers n, l . Illustrate the obtained result on some examples.

Solution

Above we have obtained Eqs. (2.9), (2.12) and (2.15) of $1/n$ -expansion for the energy of nl -level at the fixed value of the parameter $\xi \equiv n^2 g$. Critical values of this parameter are determined by $1/n$ -expansion of the form

$$\begin{aligned} \xi_{nn_r,cr} &= n^2 g_{nn_r,cr}; \\ g_{nn_r,cr}^{(1/n)} &= g_0 + \frac{g_1}{n} + \frac{g_2}{n^2} + \dots \end{aligned} \quad (2.35)$$

Coefficients of expansion are found from the condition that the energy $E_{nn_r} = 0$ when the level appears. Accordingly, we have $\varepsilon_{n_r}^{(k)} = 0$ in all orders of expansion. Using the expansion (2.35) for the parameter g in the effective potential (2.7), we obtain the next results.

Equation (2.9) is applicable in zero order of $1/n$ -expansion. However, we should substitute g by g_0 and put $\varepsilon^{(0)} = 0$. Hence, we obtain

$$g_0 = -\frac{1}{2r_0^2 v(r_0)}; \quad r_0 v'(r_0) = -2v(r_0). \quad (2.36)$$

The first approximation can be found from Eq. (2.12) by formal substitution $\varepsilon_{n_r}^{(1)} \rightarrow -g_1 v(r_0)$. Taking into account Eq. (2.36), we obtain

$$g_1 = -\frac{2n_r + 1}{2v(r_0)} \left(\omega - \frac{1}{r_0^2} \right) = (2n_r + 1) (\omega r_0^2 - 1) g_0. \quad (2.37)$$

Here, the frequency ω is given by Eq. (2.11), but with substitution $g \rightarrow g_0$.

It should be noted in the derivations of second-order terms in $1/n$ that besides substitution $\varepsilon_{n_r}^{(2)} \rightarrow -g_1 v(r_0)$, additional terms occur in the perturbative potential:

$$\delta V = n g_1 \left\{ v'(r_0) (r - r_0) + \frac{1}{2} v''(r_0) (r - r_0)^2 \right\},$$

(compare with (2.13)). Taking it into account, we obtain

$$g_2 = \frac{\omega}{v(r_0)} \left\{ \frac{15}{16} \left(\frac{22}{15} + s \right) A^2 - \frac{3}{8} (2 + s) B - \frac{s}{8} C + \frac{1+s}{4} \left(6A\sqrt{C} + 5C + 1 - \frac{1}{C} \right) \right\}. \quad (2.38)$$

Here the coefficients A , B , C , and s are determined by Eq. (2.16) with substitution g by g_0 .

Equations (2.36–2.38) present solutions of the problem for calculation of $\xi_{nn_r,cr}$ with accuracy up to terms of the order of $1/n^2$. Now we consider some applications of these expressions.

We begin with the Tietz potential

$$U(r) = -U_0 \frac{R^3}{r(r+R)^2}.$$

In this case we have $v(r) = -r^{-1}(r+1)^{-2}$. According to above formulas we obtain:

$$\begin{aligned} r_0 &= 1, \quad \omega = \frac{1}{2}, \quad \alpha = -\frac{3}{8}, \quad \beta = \frac{23}{32}, \\ g_0 &= 2, \quad g_1 = -(2n_r + 1), \quad g_2 = \frac{1}{2}n_r(n_r + 1). \end{aligned}$$

It follows from Eq. (2.35) that

$$\xi_{nn_r,cr} = \frac{1}{2} (2n - n_r - 1) (2n - n_r). \quad (2.39)$$

This result of $1/n$ -expansion coincides with exact solution at all values of quantum numbers l and n_r . It should be noted that in the case of $n_r = 0$ the wave function with zero energy is of a simple form

$$\chi_{n0}^{(0)}(r) = N \frac{r^{l+1}}{(r+R)^{2l+1}}.$$

Next we consider the Yukawa potential

$$U(r) = -U_0 \frac{R}{r} \exp\left(-\frac{r}{R}\right).$$

Table 2.7 Accuracy of calculation of energies with $n_r = 0$

l	0	1	2	5
$\xi_{nn_r,cr}^{\text{exact}}$	0.8399	4.5410	10.947	46.459
$\delta^{(0)}$	0.62	0.20	0.12	0.053
$\delta^{(1)}$	0.14	0.022	$8.3 \cdot 10^{-3}$	$1.8 \cdot 10^{-3}$
$\delta^{(2)}$	0.055	$5.4 \cdot 10^{-3}$	$1.5 \cdot 10^{-3}$	$1.5 \cdot 10^{-4}$

Table 2.8 Accuracy of calculation of energies with $n_r = 1$

l	0	1	2	5
$\xi_{nn_r,cr}^{\text{exact}}$	3.2236	8.8723	17.210	58.496
$\delta^{(0)}$	0.69	0.38	0.26	0.14
$\delta^{(1)}$	-0.054	-0.025	-0.014	$-5.6 \cdot 10^{-3}$
$\delta^{(2)}$	0.030	$5.5 \cdot 10^{-3}$	$1.8 \cdot 10^{-3}$	$2.4 \cdot 10^{-4}$

In this case we have $v(r) = -\frac{1}{r} \exp(-r)$, and parameters of $1/n$ -expansion are:

$$r_0 = 1, \quad \omega = \frac{1}{\sqrt{2}}, \quad \alpha = -\frac{2}{3}, \quad \beta = \frac{55}{48}, \quad g_0 = \frac{e}{2},$$

$$g_1 = -\frac{e(\sqrt{2}-1)(2n_r+1)}{2\sqrt{2}}, \quad g_2 = \frac{e}{\sqrt{2}} \left[\frac{43\sqrt{2}-72}{288} + \frac{37\sqrt{2}-48}{48} n_r(n_r+1) \right].$$

Here $e = 2.718\dots$. Two Tables 2.7 and 2.8 illustrate the accuracy of calculation of the parameter $\xi_{nn_r,cr}$ with the help of $1/n$ -expansion.

In above tables the values of the quantities

$$\delta^{(0,1,2)} = \frac{g_{nn_r,cr}^{(1/n)}}{g_{nn_r,cr}^{\text{exact}}} - 1 \quad (2.40)$$

are given. Here $g_{nn_r,cr}^{\text{exact}}$ are the exact values of the critical parameter ξ , which are derived by means of the numerical solution of the Schrödinger equation. Indexes 0, 1, and 2 are corresponding to the order of the terms taken into account in $1/n$ -expansion in Eq. (2.35).

Finally, let us consider the Hulthén potential. In the first order of $1/n$ -expansion we find

$$g_{nn_r,cr}^{(1/n)} = g_0 n^2 \left[1 - \frac{2n_r+1}{n} \left(1 - \sqrt{r_{0,cr}-1} \right) \right],$$

where $g_0 = 0.7721$ and $r_{0,cr} = 1.5936$ (see the previous Problem). Comparison of results of $1/n$ -expansion with exact calculations is presented in Table 2.9.

Table 2.9 Comparison of results of $1/n$ -expansion with exact calculations

l	0	0	0	1	1	1
n_r	0	1	2	0	1	2
$g_{nn_r}^{\text{exact}}$	0.5	2	4.5	2.7486	5.3623	9.0505
$\delta_{nn_r}^{(0)}$	0.54	0.54	0.54	0.12	0.30	0.36
$\delta_{nn_r}^{(1)}$	0.19	0.012	-0.047	-0.0054	-0.0016	-0.027

It follows from these Tables that though zero approximation has a great error at $l \sim 1$, calculations taking into account terms of the first and the second order in $1/n$ increase the accuracy of calculations essentially. Analogous situation occurs also for other smooth short-range potentials, as a rule.

Problem 2.5

Find the energy spectrum of bound s-states for a particle in the central potential $U(r)$ using $1/N$ -expansion. Choice of the parameter N is based on the dimension of the space. Illustrate the exactness of results on the examples of power potentials.

Solution

Analogous to the derivations in $1/n$ -expansion method, we present the potential energy in the form

$$U(r) = U_0 v\left(\frac{r}{R}\right) \equiv \frac{\hbar^2}{mR^2} N^2 g v\left(\frac{r}{R}\right).$$

Then $1/N$ -expansion gives:

$$U_{\text{eff}} = \frac{\hbar^2}{mR^2} N^2 \left\{ g v\left(\frac{r}{R}\right) + \frac{R^2}{8r^2} - \frac{R^2}{2Nr^2} + \frac{3R^2}{8N^2r^2} \right\},$$

$$E_{nn_r} = \frac{\hbar^2}{mR^2} N^2 \left\{ \varepsilon^{(0)} + \frac{1}{N} \varepsilon_{n_r}^{(1)} + \frac{1}{N^2} \varepsilon_{n_r}^{(2)} + \dots \right\}.$$

(see Eq. (2.17)). Further we put $R = 1$. In the point of classical equilibrium of a particle we have

$$gr_0^3 v'(r_0) = \frac{1}{4}, \quad \varepsilon^{(0)} = \frac{1}{8r_0^2} + g v(r_0).$$

The next, oscillator, approximation of 1/N-expansion gives:

$$\varepsilon_{n_r}^{(1)} = \omega \left(n_r + \frac{1}{2} \right) - \frac{1}{2r_0^2}; \quad \omega = \left\{ \frac{3}{4r_0^4} + gv''(r_0) \right\}^{1/2}.$$

Corrections of the second order on 1/N can be derived by the same method as in the case of 1/n-expansion (see Eq. (2.15)).

In the case of s -states for the power potential

$$U(r) = \frac{G}{\nu} r^\nu \equiv \frac{\hbar^2}{mR^2} N^2 \left(\frac{r}{R} \right)^\nu, \quad \text{where} \quad R = \left(\frac{\hbar^2 N^2}{mG} \right)^{\frac{1}{\nu+2}},$$

($g = 1$ here and thereafter, in the sakes of simplicity) we obtain according to above formulas:

$$r_0 = 2^{-\frac{2}{\nu+2}}, \quad \omega = 2^{\frac{2-\nu}{2+\nu}} (\nu + 2)^{1/2}.$$

Hence, the 1/N-expansion for the energy takes the form

$$E_{nn_r}(1/N) = \left[\frac{\hbar^2 N^2}{m} (4G)^{2/\nu} \right]^{\frac{\nu}{\nu+2}} \times \left\{ \frac{\nu+2}{8\nu} + \frac{1}{2N} \left[\left(n_r + \frac{1}{2} \right) (\nu+2)^{1/2} - 1 \right] + \dots \right\}. \quad (2.41)$$

In the case of $\nu = 2$ and $G = m\omega_0^2$ we obtain from (2.41) that

$$E_{nn_r} = \hbar\omega_0 \left(2n_r + \frac{N}{2} \right),$$

which coincides with exact expression for energies of s -states of N -dimensional harmonic oscillator (it is clear without further derivations that corrections of next orders, $\varepsilon^{(k)}$ with $k \geq 2$ vanish).

In the case of $\nu = 1$ we obtain from Eq. (2.41) for ground state, $n_r = 0$:

$$\begin{aligned} E_0(1/N) &= \frac{3}{2} \left(\frac{NG}{2} \right)^{2/3} \left\{ 1 + \frac{1}{N} \left(\frac{2}{\sqrt{3}} - \frac{4}{3} \right) + \frac{1}{N^2} \left(\frac{4}{3\sqrt{3}} - \frac{20}{27} \right) + \dots \right\} \\ &= \frac{3}{2} \left(\frac{NG}{2} \right)^{2/3} \left\{ 1 - 0.17863N^{-1} + 0.02906N^{-2} + \dots \right\}. \end{aligned} \quad (2.42)$$

Here $\hbar = m = 1$ and the correction $\varepsilon_{n_r}^{(2)}$ is taken into account. In the case of $N = 3$ we obtain from Eq. (2.42) that

$$E_0 = 1.8549G^{2/3}.$$

This value differs by 0.05 % only from the exact value of the energy of ground state. It should be noted that in the case of one-dimensional potential, $U(x) = G|x|$, Eq. (2.42) gives ($N = 1$) the energy $E_0 = 0.8036G^{2/3}$, that is also near to the exact value of $0.8086G^{2/3}$.

Finally, let us discuss shortly the case of Coulomb potential, $\nu = -1$. In the case of ground state we obtain the next expansion:

$$E_0(1/N) = -\frac{2mG^2}{\hbar^2 N^2} \left\{ 1 + \frac{2}{N} + \frac{3}{N^2} + \cdots \right\}. \quad (2.43)$$

Convergence of $1/N$ -expansion in this case is, obviously, poor compared to the previous case. It is explained by the fact that in one-dimensional Coulomb potential ($N = 1$) the falling of a particle to the origin occurs. Therefore, the case of $N = 1$ is the singularity for the function $E_0(1/N)$, so that $E_0(1) = -\infty$. Therefore, it is useful to substitute the parameter of expansion $N \rightarrow N - 1$. It is interesting that after this substitution according to Eq. (2.43) we obtain:

$$E_0 = -\frac{2mG^2}{\hbar^2 (N - 1)^2}.$$

This expression coincides with the exact value of the energy of the ground state for N -dimensional Coulomb potential.

2.2 Wave Functions of 1/n-Expansion

Problems and Solutions

Problem 2.6

Find the next correction to the unperturbed wave function (2.12) with respect to $1/n$ -expansion for a particle in a central potential. Investigate the accuracy of the obtained result on the examples of solvable potentials at $n \sim 1$.

Solution

The perturbed wave function is calculated according to general formulas of the perturbation theory (see [1], Sect. 38). The perturbation is given by Eq. (2.13). Taking into account the well-known values of dipole matrix elements for linear oscillator, we obtain that the most important is the odd part $V^{(-)}$ of the potential (2.13). It results in terms of the order of $1/\sqrt{n}$, while the even part $V^{(+)}$ results in terms of the order of $1/n$.

We restrict ourselves by states with $n_r = 0$. Non-zero matrix elements for the harmonic oscillator with the frequency ω_0 are (here $\hbar = m = 1$):

$$\langle 1 | x | 0 \rangle = \frac{1}{\sqrt{2\omega_0}}, \quad \langle 1 | x^3 | 0 \rangle = \frac{3}{(2\omega_0)^{3/2}}, \quad \langle 3 | x^3 | 0 \rangle = \frac{\sqrt{6}}{(2\omega_0)^{3/2}}.$$

In our case $\omega_0 = n\omega$, where the frequency ω is given by Eq. (2.11). In the first order perturbation theory the wave function is [1]:

$$\chi_{n0} = \chi_{n0}^{(0)} + \sum_k' \frac{\langle k | V^{(-)} | 0 \rangle}{-k\omega} \chi_{nk}^{(0)}. \quad (2.44)$$

Using the explicit form (2.12) of unperturbed wave functions, we obtain:

$$\begin{aligned} \chi_{n0}(r) &= \left(\frac{n\omega}{\pi}\right)^{1/4} \\ &\times \left\{ 1 - \left[\left(\frac{\alpha}{\omega^{3/2}} + \frac{1}{(\omega r_0^2)^{3/2}} \right) \sqrt{\omega} (r - r_0) + \frac{n\alpha}{3\omega} (r - r_0)^3 \right] \right\} \\ &\times \exp \left[-\frac{n\omega}{2} (r - r_0)^2 \right]. \end{aligned} \quad (2.45)$$

The parameter α is determined by Eq. (2.14). At $n \gg 1$ the wave function (2.45) describes a particle in a region $|r - r_0| \sim (n\omega)^{-1/2}$ where this function is localized. The correction in square brackets of Eq. (2.45) is of the order of magnitude $1/\sqrt{n}$.

Equation (2.45) is asymptotically exact one at $n \rightarrow \infty$. Its accuracy is $\sim 1/n$. We illustrate its accuracy on the example of Coulomb potential $U(r) = -n^2/r$ in the most unfavorable cases for 1/n-expansion: $n = 1$ ($l = 0$) and $n = 2$ ($l = 1$). We obtain $r_0 = 1$, $\omega = 1$, $\alpha = 1$. Equation (2.45) takes the form:

$$\chi_{n0}(r) = \left(\frac{n}{\pi}\right)^{1/4} \exp \left[-\frac{n}{2} (r - 1)^2 \right] \left\{ 1 + \frac{n}{3} (r - 1)^3 \right\}. \quad (2.46)$$

Exact wave functions of $1s$ - and $2p$ -states are of the form

$$\chi_{1s}(r) = 2r \exp(-r); \quad \chi_{2p}(r) = 8\sqrt{\frac{2}{3}} r^2 \exp(-2r) \quad (2.47)$$

(it should be noted that the Bohr radius is $a_B = n^{-2}$). In order to compare wave functions (2.46) with (2.47), we give two Tables (2.10) and (2.11)

In these Tables the values of the quantities are presented:

$$\delta^{(0,1)}(r) = \frac{\chi_{n0}^{(0,1)}(r)}{\chi_{n0}(r)} - 1.$$

Table 2.10 Comparison of wave functions (2.46) with (2.47) for $n = 1$ ($l = 0$), $n_r = 0$

r	0.5	1.0	1.5
$\delta^{(0)}$	0.099	0.021	-0.010
$\delta^{(1)}$	0.047	0.021	0.032

Table 2.11 Comparison of wave functions (2.46) with (2.47) for $n = 2$ ($l = 1$), $n_r = 0$

r	0.5	1.0	1.5
$\delta^{(0)}$	0.16	0.010	-0.049
$\delta^{(1)}$	0.061	0.010	0.030

Here $\chi_{n0}(r)$ is the exact wave function (2.47), while $\chi_{n0}^{(0,1)}(r)$ is the wave function in the approximation of 1/n-expansion (zero and first approximation, respectively).

It is seen that in nodeless states ($n_r = 0$) 1/n-expansion describes quite well the wave functions even at $n \sim 1$, in the vicinity of their maxima ($r \approx 1$). It should be noted that the position of maximum, i.e., $r_0 = 1$ is the same for exact wave functions and for the wave functions of 1/n-expansion.

Problem 2.7

Using 1/n-expansion, find the wave function of nl -level in classically forbidden region. Calculate the asymptotic coefficient C_{nl} in the origin $r \rightarrow 0$ and investigate its accuracy.

Solution

In classically forbidden region the parabolic expansion of effective potential is incorrect when r is far from the equilibrium point r_0 . Then, the Eq. (2.12) for the wave function is invalid (see also the previous Problem). Instead of this, the wave function can be found using WKB-approximation. Radial Schrödinger equation taking into account the expansions (2.7) and (2.8) is of the form

$$\frac{1}{2}\chi''(r) - n^2 \left[gv(r) + \frac{1}{2r^2} - \varepsilon^{(0)} - \frac{2n_r + 1}{2nr^2} - \frac{1}{n}\varepsilon_{n_r}^{(1)} \right] \chi(r) = 0. \quad (2.48)$$

We neglected here the terms $\sim 1/n^2$.

The mathematical form of Eq. (2.48) is similar to Eq. (1.1), but the Planck constant is substituted by the parameter $1/n$. The limit $n \rightarrow \infty$ is corresponding to the WKB-

limit $\hbar \rightarrow 0$. This consideration allows to obtain the solution of Eq.(2.48) in the form of WKB-solutions, Eq. (1.5).

In particular, in the left classically forbidden region (from the equilibrium point r_0) the radial wave function is of the form (we take into account the boundary condition $\chi(0) = 0$):

$$\begin{aligned}\chi(r) &\approx \frac{C}{\sqrt{q(r)}} \exp \left\{ -n \int_r^a q(r') dr' \right\} \\ &\approx \frac{C}{\sqrt{q_0(r)}} \exp \left\{ -n \int_r^a \left[q_0(r') - \frac{2n_r + 1}{2nq_0(r')} \left(\frac{1}{r'^2} - \frac{1}{r_0^2} + \omega \right) \right] dr' \right\}.\end{aligned}\quad (2.49)$$

Here the notations are introduced

$$\begin{aligned}q(r) &= \left\{ q_0^2(r) - \frac{2}{n} \left(\frac{2n_r + 1}{2r^2} + \varepsilon_{n_r}^{(1)} \right) \right\}^{1/2}; \\ q_0(r) &= \left\{ 2 \left[gv(r) + \frac{1}{2r^2} - \varepsilon^{(0)} \right] \right\}^{1/2}.\end{aligned}\quad (2.50)$$

We used here expression (2.12) for $\varepsilon_{n_r}^{(1)}$ and expand over $1/n$. We omit in Eq. (2.49) terms of the order of $1/n$, since they are outside of accuracy of our approximation (in order to take them into account, we should use more exact WKB-solutions, see Ref.[1], Sect. 46).

We should determine now the normalized coefficient C in Eq.(2.49), which depends on the choice of a . The wave function (2.49) should be matched with the normalized oscillator wave function (2.12) in common region of their applicability:

$$1 \ll \sqrt{n\omega} |r - r_0| \ll \sqrt{n}. \quad (2.51)$$

Here, the left side of the inequality corresponds the condition of applicability of WKB-approximation (at $E = 0$) in the region where the harmonic oscillator potential occurs. Then we have

$$q_0(r) \approx \omega |r - r_0| \quad (2.52)$$

and (see Eq. (1.6))

$$\frac{1}{nq_0^2} \left| \frac{dq_0}{dr} \right| \ll 1.$$

Right side of the inequality (2.51) corresponds to the condition of applicability of parabolic expansion of the effective potential (i.e., condition of $1/n$ -expansion).

Let us discuss how to match the solutions. It is impossible to put $a = r_0$ in Eq. (2.49) directly, since the latter integral in Eq. (2.49) diverges when $a \rightarrow r_0$. This divergence does not depend on r ; therefore, it can be compensated by renormalization of the coefficient C . We pick out from the integrand the divergent part: according to (2.52) it is equal to $|r - r_0|^{-1}$. Then this integral takes the form

$$\int_r^a \frac{P_0(r)}{q_0(r)} dr = \int_r^a \left\{ \frac{P_0(r)}{q_0(r)} - \frac{1}{r_0 - r} \right\} dr + \ln \left(1 - \frac{r}{r_0} \right) - \ln \left(1 - \frac{a}{r_0} \right). \quad (2.53)$$

Here the notation is introduced

$$P_0(r) = \frac{1}{r^2} - \frac{1}{r_0^2} + \omega.$$

In the integral expression of right side of Eq. (2.53), we can put $a = r_0$. The contribution of the term $\ln(1 - a/r_0)$ can be included into still undetermined coefficient C , since it does not depend on the variable r . Then the wave function, Eq. (2.49) takes the form

$$\begin{aligned} \chi(r) = \frac{C'}{\sqrt{q_0(r)}} \exp \left\{ -n \int_r^{r_0} \left[q_0(r) - \frac{2n_r + 1}{2n} \left(\frac{P_0(r)}{q_0(r)} - \frac{1}{r_0 - r} \right) \right] dr \right. \\ \left. + \frac{2n_r + 1}{2} \ln \left(1 - \frac{r}{r_0} \right) \right\}. \end{aligned} \quad (2.54)$$

In the matching region determined by the conditions (2.51) we obtain

$$\chi(r) \approx C' \frac{1}{\sqrt{\omega r_0}} \left(\frac{r - r_0}{r_0} \right)^{n_r} \exp \left\{ -\frac{1}{2} n \omega (r - r_0)^2 \right\}, \quad (2.55)$$

while in this region the harmonic oscillator wave function (2.12) takes the form

$$\chi_{nn_r}^{(0)}(r) \approx \left[\frac{n\omega}{2^{2n_r} \pi (n_r!)^2} \right]^{1/4} (-1)^{n_r} [2\sqrt{n\omega} (r_0 - r)]^{n_r} \exp \left\{ -\frac{1}{2} n \omega (r - r_0)^2 \right\}. \quad (2.56)$$

Wave functions (2.55) and (2.56) should coincide each one other. Then we can calculate the coefficient C' :

$$C' = (-1)^{n_r} \left[\frac{n\omega^3 r_0^2}{\pi (n_r!)^2} \right]^{1/4} (2n\omega r_0^2)^{n_r/2}. \quad (2.57)$$

Table 2.12 The values of J_0 and J_1

ν	0	1	4	8
J_0	-0.67202	-0.55843	-0.43983	-0.38972
J_1	0.28381	0.34245	0.30358	0.16622

Expressions (2.54) and (2.57) determine the normalized radial wave function in the underbarrier region to the left from the point $r = r_0$. If $r \rightarrow 0$, we obtain $q_0(r) \approx 1/r$ and according to Eq. (2.54) we conclude that the radial wave function has correct limiting form near the origin:

$$\chi(r) \approx C_{nl} r^{l+1}.$$

Further, we can pick out divergent terms of Eq. (2.54) at $r \rightarrow 0$ by the method described just above. Then we can derive the asymptotic coefficient in the origin:

$$C_{nl}^{(1/n)} = C' r_0^{-l-1/2} \exp \{ - [n J_0 + (2n_r + 1) J_1] \}, \quad (2.58)$$

where the notations are introduced

$$J_0 = \int_0^{r_0} \left[q_0(r) - \frac{1}{r} \right] dr; \quad J_1 = \frac{1}{2} \int_0^{r_0} \left[\frac{r_0}{r(r_0 - r)} - \frac{P_0(r)}{q_0(r)} \right] dr. \quad (2.59)$$

Equation (2.58) is asymptotically exact at $n \rightarrow \infty$ and at fixed value of n_r . Its accuracy is of the order of $1/n$.

For nodeless states the Eq. (2.58) is valid with a good accuracy also at $n \sim 1$. As an example, we consider the case of power potentials $U(r) = r^\nu/\nu$. Simple numerical derivation according to Eq. (2.59) gives the values of parameters $J_0(\nu)$ and $J_1(\nu)$ presented in Table 2.12.

The case of $\nu = 0$ corresponds to the logarithmic potential $U(r) = \ln r$. The integrals in Eq. (2.59) are derived analytically in the cases of Coulomb potential ($\nu = -1$) and of the harmonic oscillator potential ($\nu = 2$):

$$J_0(\nu = -1) = -1; \quad J_1(\nu = -1) = 0; \quad J_0(\nu = 2) = -\frac{1}{2}; \quad J_1(\nu = 2) = \frac{1}{2} \ln 2. \quad (2.60)$$

(see also Problem 2.2 where parameters of $1/n$ -expansion are given for power potentials).

After derivation of parameters J_0, J_1 final value of the asymptotic coefficient can be found elementary using Eq. (2.58). Accuracy of such calculations for nodeless states in the case of power potentials is illustrated in Table 2.13. In this Table, the ratios

Table 2.13 Values of the ratio (η) according to Eq. (2.61)

	ν					
	-1	0	1	2	4	8
$l=0$	1.0209	1.0280	0.9952	0.9803	0.9900	1.0862
1	1.0104	1.0146	0.9976	0.9898	0.9984	1.0731
2	1.0070	1.0098	0.9984	0.9931	1.0002	1.0598
5	1.0035	1.0050	0.9992	0.9965	1.0009	1.0378

$$\eta = \frac{C_{nl}^{(1/n)}}{C_{nl}^{\text{exact}}}; \quad n = l + 1 \quad (2.61)$$

are calculated numerically in the case of power potentials $U(r) = r^\nu/\nu$. Here C_{nl}^{exact} is the exact value of the asymptotic coefficient, and $C_{nl}^{(1/n)}$ is derived using Eqs. (2.58–2.59).

It is shown from the Table 2.13 that maximum error occurs for C_{nl} at $\nu = 8$. It is explained by the fact that the power potential loses its smoothness at the increasing of ν . It is transformed into the infinitely deep spherical potential well in the limit of $\nu \rightarrow \infty$.

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