High-order asymptotic behavior of the coefficients of 1/*D*-expansion for Hooke's law potential

Let us consider here *D*-dimensional spherically-symmetric potential

$$V(r) = r^2 / 2 + \lambda / r\,. \qquad (1)$$

D-dimensional radial Schrödinger equation has a form

$$\left(-\frac{1}{2}\frac{d^2}{dr^2} + \frac{(D-1)(D-3)}{8r^2} + V(r) - E\right)\psi(r) = 0\,. \qquad (2)$$

(for s-states). After the scaling transformation $r = r' D^{1/2}$, we arrive to the equation

$$\left(-\frac{1}{2D^2}\frac{d^2}{dr'^2} + \frac{1-4D^{-1}+3D^{-2}}{8r'^2} + \frac{r'^2}{2} + \frac{\lambda'}{r'} - E'\right)\psi'(r') = 0\,, \qquad (3)$$

where $\lambda' = \lambda D^{-3/2}$ and $E' = ED^{-1}$ are the rescaled parameter and the energy.

I. Model-0

We suppose that the parameter λ' **does not depend on *D*** i.e. $\lambda = \lambda' D^{3/2}$ depends on *D*. Further, we shall refer only to the scaled version of the Schrödinger equation (3). All primes will be omitted for simplicity, e. g. we shall use the scaled energy and the parameter λ' without primes.

The energy is expanded in negative powers of *D*:

$$E(\lambda, D) = \sum_{k=0}^{\infty} E_k D^{-k}\,. \qquad (4)$$

Here, we present the results for the parameters a and C_0 in the asymptotic formula for the large-order coefficients

$$E_k \sim k^{-3/2} k!(C_0 a^k + C_0 * a*^k), \quad k \to \infty. \qquad (5)$$

Let us consider the equation of general form

$$\left(-\frac{\delta^2}{2}\frac{d^2}{dr^2}+V_{\mathrm{eff}}(r)-\frac{\delta+O(\delta^2)}{2r^2}-E\right)\psi(r)=0\,, \qquad (6)$$

where $V_{\mathrm{eff}}(r)$ is any potential having a methastable minimum. The following formulas (8) - (16) hold for arbitrary potentials, although finally we restrict ourselves to potentials like

$$V_{\mathrm{eff}}(r)=\frac{1}{8r^2}+\frac{\mu r^2}{2}+\frac{\lambda}{r}\,. \qquad (7)$$

The typical form of such effective potential for negative parameters μ and λ is shown on the following figure:

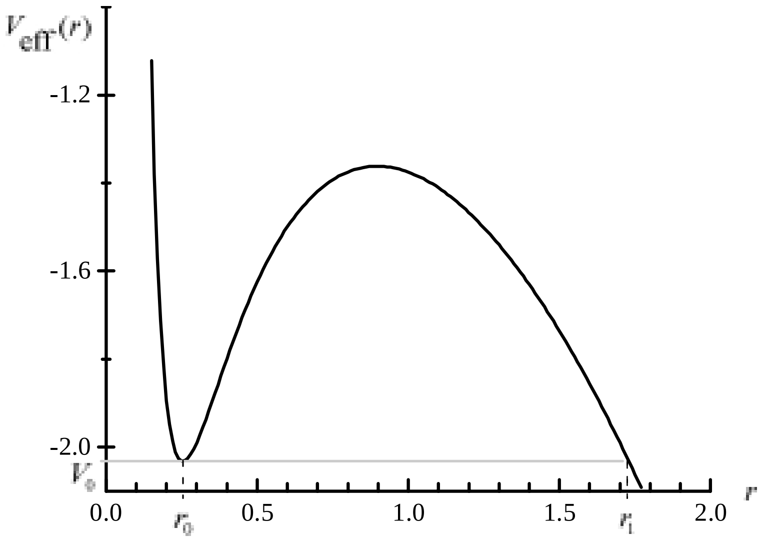

Fig. 1. A plot of the potential $V_{\mathrm{eff}}(r)=\frac{1}{8r^2}+\frac{\mu r^2}{2}+\frac{\lambda}{r}$ for $\mu=\lambda=-1$

In equation (6), δ plays a role of Planck's constant $\hbar$. At small δ, the particle performs small oscillations around the minimum r_0. The quasiclassical decay rate is roughly proportional to the tunneling probability

$$W \sim \exp(-2S/\delta)\,, \qquad (8)$$

where

$$S = \int_{r_0}^{r_1} p(r)dr, \quad p(r) = \left[2(V_{\text{eff}}(r) - V_0)\right]^{1/2}, \tag{9}$$

is a classical action along a subbarrier trajectory (meaning of r_0, r_1, and V_0 is evident from Fig. 1). Because of possibility of ionization, the state has an exponentially small width $\Gamma = \hbar W$ and the energy has an imaginary part $\operatorname{Im} E = \Gamma / 2$. According to Dyson's argument, the instability of a state leads to the divergence of the perturbation series. We evaluate large-order behavior of the coefficients in the expansion (4) using dispersion relations for the energy:

$$E_k = \frac{1}{2\pi i} \oint \frac{E(\delta)}{\delta^{k+1}} d\delta, \tag{10}$$

where the integration is done along a small circle embracing the point $\delta = 0$. The integral (10) may be reduced to

$$E_k = \frac{1}{2\pi} \int_0^\infty \frac{\Gamma(\delta)}{\delta^{k+1}} d\delta. \tag{11}$$

(see, e. g. C. M. Bender, T. T. Wu, Phys. Rev. D, 7, 1620, 1973; we conjecture that the function $E(\delta)$ have suitable analytic properties).

Further, we shall use more precise quasiclassical formula for the width including pre-exponential factor:

$$\Gamma(\delta) = \sqrt{\frac{\omega^3 \delta}{\pi}} (r_1 - r_0) \exp(-2S/\delta + I_1 + I_2 + O(\delta)). \tag{12}$$

where I_1, I_2 are the following integrals:

$$I_1 = \int_{r_0}^{r_1} \left[\frac{\omega}{p(r)} - \frac{1}{r - r_0}\right] dr, \quad I_2 = \int_{r_0}^{r_1} \frac{r^{-2} - r_0^{-2}}{p(r)} dr. \tag{13}$$

Here,

$$\omega = \left[\frac{d^2}{dr^2} V_{\text{eff}}(r_0) \right]^{1/2} \tag{14}$$

is the frequency of small vibrations. Derivation of this result is lengthy and it is omitted here. It may be reproduced by a method described in [A. Schmid. Ann. Phys. (N. Y.) 1986, v. 170, no. 2, p. 333 - 369]. Inserting (12) into (11), we arrive to

$$E_k \sim C_0 a^k k^{-3/2} k! \left(1 + O(1/k)\right), \tag{15}$$

where the parameters a and C_0 are:

$$\begin{aligned} &a = (2S)^{-1}, \\ &C_0 = \frac{1}{2a^{1/2}} \left(\frac{\omega}{\pi} \right)^{3/2} (r_1 - r_0) \exp(I_1 + I_2), \end{aligned} \tag{16}$$

The parameter a is the most important in asymptotic formula (15). As a result of the divergence behavior (15), the Borel function for the series (4) has a singularity at $\delta = \delta_0$, where $\delta_0 = a^{-1} = 2S$.

Now, let us return to our specific potential (7). We rewrite the integrand in (9) as

$$2(V_{\text{eff}}(r) - V_0) = \frac{\mu}{r^2} \left(r^4 - \frac{2V_0}{\mu} r^2 + \frac{2\lambda}{\mu} r + \frac{1}{4\mu} \right). \tag{17}$$

Introducing the equilibrium radius r_0 which is a double root of the polynomial in rhs of eq. (17), we factorize this polynomial:

$$\begin{aligned} &r^4 - \frac{2V_0}{\mu} r^2 + \frac{2\lambda}{\mu} r + \frac{1}{4\mu} = (r - r_0)^2 (r - r_1)(r - r_2) = \\ &r^4 - (2r_0 + r_1 + r_2) r^3 + (r_1 r_2 + 2r_0 r_1 + 2r_0 r_2 + r_0^2) r^2 - (2r_0 r_1 r_2 + r_0^2 r_1 + r_0^2 r_2) r + r_0^2 r_1 r_2 \end{aligned} . \tag{18}$$

Equating coefficients before r^2 and r^0 in eq. (18), we arrive to the system of equations for determining the turning points r_1 and r_2:

$$\left. \begin{aligned} r_1 + r_2 &= -2r_0 \\ r_1 r_2 &= \frac{1}{4\mu r_0^2} \end{aligned} \right\}. \tag{19}$$

Its solution is

$$r_{1,2} = -r_0 \pm \left(r_0^2 - \frac{1}{4\mu r_0^2} \right)^{1/2}. \tag{20}$$

The positive turning point r_1 shown on the Figure 1 corresponds to a plus sign in eq. (20). The action integral (9) now reads

$$S = \int_{r_0}^{r_1} \left[\mu (r - r_1)(r - r_2) \right]^{1/2} (r - r_0) r^{-1} dr \,, \tag{21}$$

Substituting the expressions for r_1 and r_2 into eq. (21), we obtained (using *Mathematica*) some analytic expressions for this integral, and also for integrals I_1 and I_2. Then, we analytically extend these results to positive $\mu = 1$ that corresponds to the potential in our Schrödinger equation (3),

$$V_{\text{eff}}(r) = \frac{1}{8r^2} + \frac{r^2}{2} + \frac{\lambda}{r}. \tag{22}$$

The final results are:

$$\begin{aligned} S &= \frac{1}{2} \log\left(\frac{2r_0^2 B}{1 + 4r_0^4 + A} \right) + \frac{1 - 12r_0^4}{2R} \log\left(\frac{B}{R + A} \right) \pm \frac{\pi}{2} i, \\ I_1 &= -\frac{A}{R} \log\left(\frac{R + A}{R - A} \right) + \log\left(\frac{2A^2}{B(R - B)} \right), \\ I_2 &= 2 \log\left(\frac{2r_0^2 B}{1 + 4r_0^4 + A} \right) + \frac{1}{r_0^2} \log\left(\frac{R + A}{B} \right) \pm 2\pi i. \end{aligned} \tag{23}$$

Here,

$$R = 4r_0^2, \quad A = \left(1 + 12r_0^4\right)^{1/2}, \quad B = \left(4r_0^4 - 1\right)^{1/2}, \tag{24}$$

r_0 is a positive root of the fourth-order algebraic equation

$$r^4 - \lambda r - 1/4 = 0. \tag{25}$$

Another quantities that enter eq. (16) are: $r_1 = B/(2r_0) - r_0$, and $\omega = 2A/R$. Our results were checked using an attached *Mathematica* program.

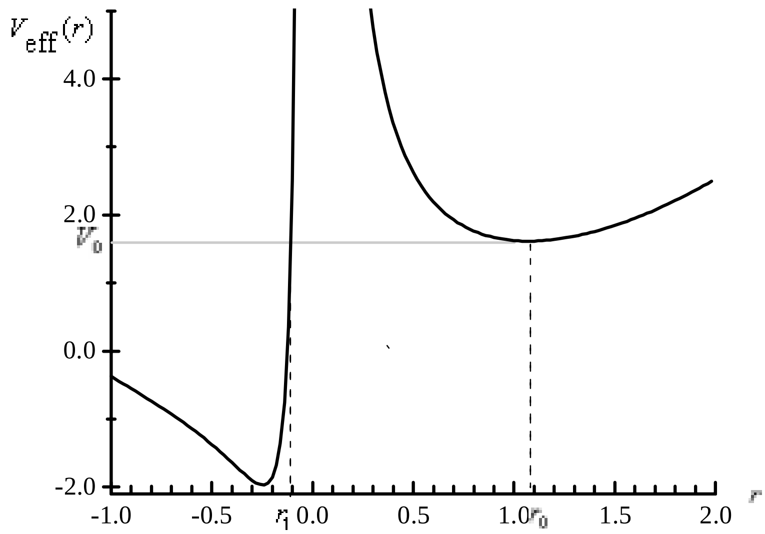

Fig. 2. A plot of a potential $V_{\text{eff}}(r) = \dfrac{1}{8r^2} + \dfrac{\mu r^2}{2} + \dfrac{\lambda}{r}$ for $\mu = \lambda = 1$

Note that the integral I_1 is real, and the integrals S and I_2 are imaginary. Moreover, their imaginary parts are constants equal to $\pm\pi/2$ and $\pm 2\pi$, correspondingly. The explanation of this fact is simple. The integrand $\dfrac{\omega}{p(r)} - \dfrac{1}{r - r_0}$ is a purely real function in the interval $[r_1, r_0]$ without singularities, so I_1 is real (here, $r_1 < 0$ and $r_0 > 0$ are real numbers, see Fig. 2). The integrand $p(r) \sim \dfrac{1}{2r}$ at $r \to 0$, and it has a pole at the origin, so the integral S has an imaginary part $\pm\pi/2$ (the sign depends on the route of the integration). The integrand $\dfrac{r^{-2} - r_0^{-2}}{p(r)} \sim \dfrac{2}{r}$ at $r \to 0$, so the integral I_2 has an imaginary part $\pm 2\pi$ for the same reason. Note also that the imaginary part of I_2 equal to $\pm 2\pi$ is inessential for us because I_2 stands in the formula (16) under an exponent.

Note that the reciprocal of the parameter *a* (equal to 2*S*) represents the nearest to the origin singularity of the Borel function, δ_0. Its imaginary part always equals to $\pm\pi$, and the real part grows monotonicly from zero to infinity when λ varies in the interval $[0,\infty)$. The dependence of $|\delta_0|$ on λ is shown on Fig. 3.

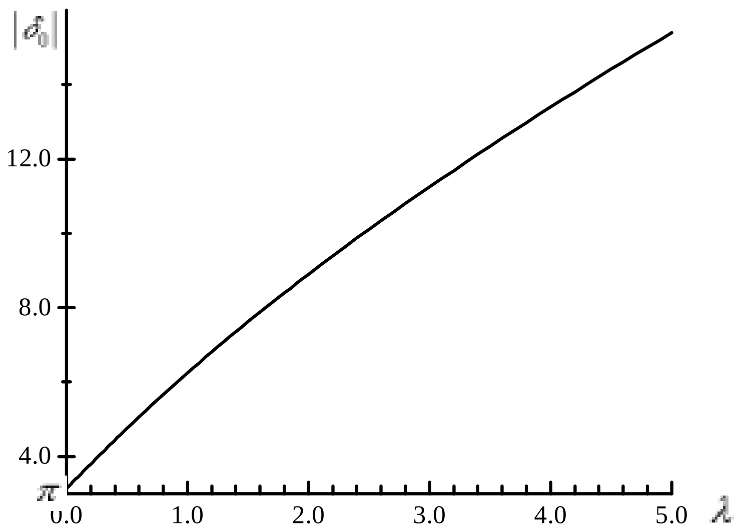

Fig. 3. Dependence of $|\delta_0|$ on λ

As for pre-factor C_0, its modulus also grows from zero to infinity (see Fig. 4) while $\mathrm{Arg}\, C_0 = \frac{1}{2}\mathrm{Arg}\, S$ (see eq. 16).

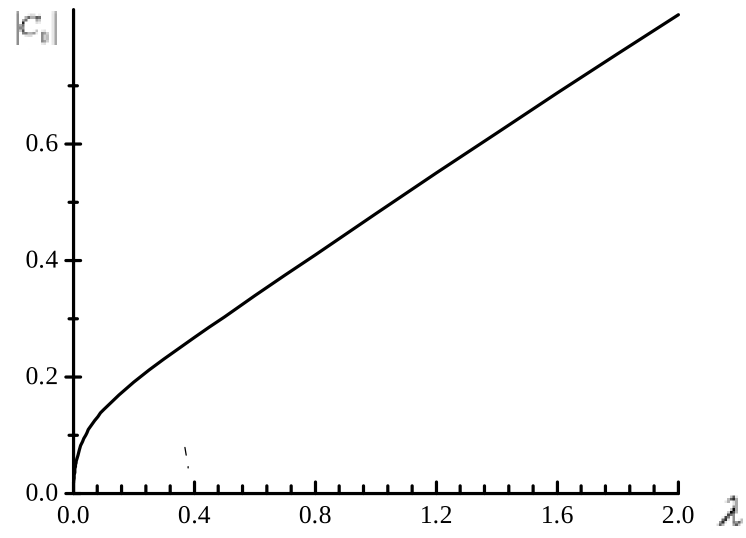

Fig. 4. Dependence of $|C_0|$ on λ

Also, note that there are no unstable states in a potential (22), because there are no real positive turning points. We suggest, that the parameters of the large-order behavior may be calculated via analytic continuation of their values as functions of μ from negative μ to positive μ. The resulting large-order asymptotic formula (5) has two complex-conjugate terms, originating from two complex-conjugate integration paths, embracing the singularity at the origin.

The growth of asymptotic-approximation coefficients E_k^{as} given by formula (5) is shown on Figure 5.

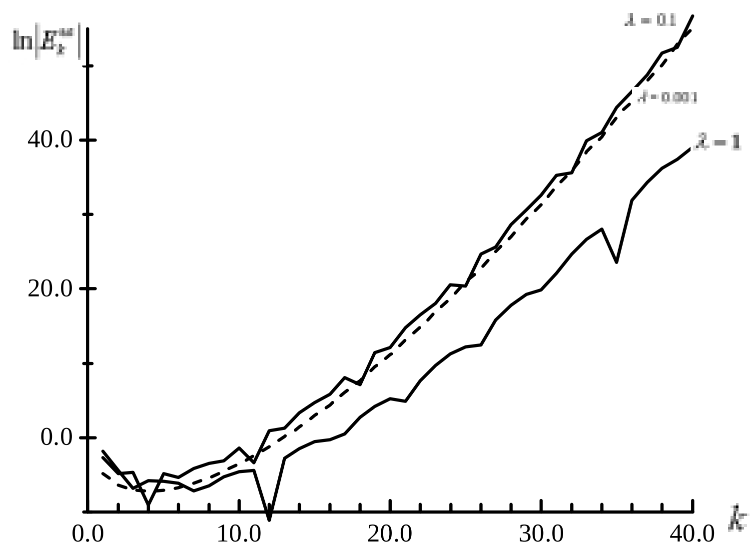

Fig. 5. Growth of E_k^{as} given by (5) with increase of the order k

For smaller λ, the Borel singularity is closer to the origin, so the series diverges stronger. But for very small λ, the Borel singularities become stable at points $\pm\pi i$, and pre-factor diminishes with decreasing of λ, so coefficients diminish also. So, our result for $\lambda \to 0$ is consistent with the fact that for a pure harmonic oscillator all coefficients but the first one are zero. Our result is also consistent with Coulomb limit, since Borel singularity goes away to infinity when $\lambda \to -\infty$.

Of cause, formula (5) is not exact one since there are also terms of order $\sim k^{-3/2} k! a^k \cdot 1/k$ etc. To check its accuracy, we calculated coefficients E_k using enclosed FORTRAN program. They are listed in Table 1 for different λ. The ratio E_k / E_k^{as} is shown in Table 2. This ratio vs. k is also plot on Fig. 6.

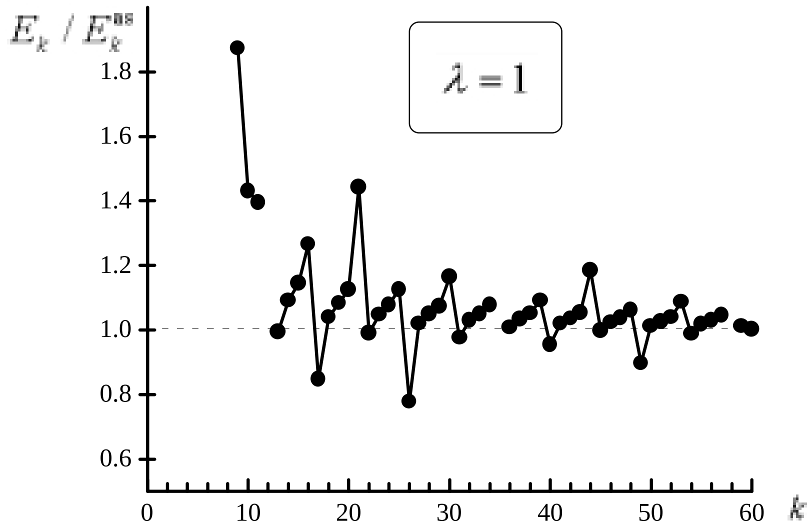

Fig. 6. Accuracy of the asymptotic formula (5) for coefficients E_k

The accuracy of the asymptotic formula is reasonably good beginning from $k \sim 10$. There are few missed points on Fig. 6 because they have very strong deviation from 1.0, namely E_k / E_k^{as} equal to -24.7 and -8.06 for k equal 35 and 58, correspondingly. In these cases, $\text{Arg}(C_0 a^k)$ is close to $(n+1/2)\pi$, $\text{Re}(C_0 a^k)$ is near zero, and the asymptotic expression (5) is small. So, the next correction to (5) of order $\sim k^{-3/2} k! a^k \cdot 1/k$ can not be omitted.

The deviation from one at large $k \sim 60$ for λ smaller than ~ 0.1 (see Table 2) is probably a result of round-off errors in our numerical calculations.

I. A. Summary

Here, the results will be presented in a more formal and concise form convenient to computations.

We deal with a Schrödinger equation

$$\left(-\frac{\delta^2}{2}\frac{d^2}{dr^2}+\frac{1-4\delta+3\delta^2}{8r^2}+\frac{r^2}{2}+\frac{\lambda}{r}-E\right)\psi(r)=0\,.$$

The eigenvalue is expanded in a power series

$$E=\sum_{k=0}^{\infty}E_k\delta^k\,.$$

We found that for large k

$$E_k\sim\frac{8A^2Br_0^4}{(R-B)(1+4r_0^4+A)^2}\left(\frac{R-A}{R+A}\right)^{\omega/2}\left(\frac{R+A}{B}\right)^{1/r_0^2}(r_1-r_0)\left(\frac{\omega}{\pi k}\right)^{3/2}\mathrm{Re}\left(\delta_0^{1/2-k}\right)k!\,.$$

In this formula, r_0 is a positive root of an equation

$$r^4-\lambda r-1/4=0\,,$$

$R=4r_0^2$, $A=\left(1+12r_0^4\right)^{1/2}$, $B=\left(4r_0^4-1\right)^{1/2}$ are variables introduced to make formulas more short, $r_1=B/(2r_0)-r_0$, $\omega=2A/R$, and

$$\delta_0=\log\left(\frac{2r_0^2B}{1+4r_0^4+A}\right)+\frac{1-12r_0^4}{R}\log\left(\frac{B}{R+A}\right)+\pi i,$$

is one of the complex-conjugate Borel singularities.

I. B. Small λ limit

We used an enclosed *Mathematica* program to derive the following expansions valid at $\lambda\to 0$:

$$\omega = 2 + O(\lambda)\,,$$

$$r_0 = \sqrt{2}\,/\,2 + O(\lambda)\,,$$

$$r_1 = -\sqrt{2}\,/\,2 + O(\lambda^{1/2})\,,$$

$$S = \pm\frac{i\pi}{2} + \left(1 + \frac{5}{2}\ln 2 - \ln\lambda\right)\frac{\lambda}{\sqrt{2}} + O(\lambda^2 \ln\lambda)\,,$$

$$I_1 = -\frac{5}{4}\ln 2 + \frac{1}{2}\ln\lambda + O(\lambda^{1/2})\,,$$

$$I_2 = \pm 2\pi i + O(\lambda\ln\lambda)\,.$$

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II. Model-3/2

We suppose that the unscaled parameter λ does not depend on D i.e. the scaled parameter in eq. (3) **depends on** $\boldsymbol{D}$**:** $\lambda' = \lambda\delta^{3/2}$**.** Here, we shall refer only to the scaled version of the Schrödinger equation (3). For simplicity, we shall use the scaled energy E' without prime.

The expansion for the energy is:

$$E(\lambda, D) = \sum_{N=0}^{\infty} E_{N/2}\delta^{N/2}\,. \tag{26}$$

To evaluate the width, we use the approximation given by (12):

$$\Gamma(\delta) = \sqrt{\frac{\omega^3\delta}{\pi}}(r_1 - r_0)\exp(-2S/\delta + I_1 + I_2)\,. \tag{27}$$

although it is no more an asymptotic formula. To obtain an asymptotic expression for the width, we expand all quantities entering (27) for small δ using small-λ expansions from I. B subsection (there we make a substitution $\lambda \to \lambda\delta^{3/2}$ according to our new scaling):

$$\omega = 2 + O(\delta^{3/2}),$$

$$r_0 = \sqrt{2}/2 + O(\delta^{3/2}),$$

$$r_1 = -\sqrt{2}/2 + O(\delta^{3/4}),$$

$$S = \pm\frac{i\pi}{2} + \left(1 + \frac{5}{2}\ln 2 - \ln\lambda - \frac{3}{2}\ln\delta\right)\frac{\lambda}{\sqrt{2}}\delta^{3/2} + O(\delta^3 \ln\delta),$$

$$I_1 = -\frac{5}{4}\ln 2 + \frac{1}{2}\ln\lambda + \frac{3}{4}\ln\delta + O(\delta^{3/4}),$$

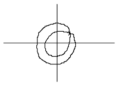
$$I_2 = \pm 2i\pi + O(\delta^{3/2}\ln\delta). \tag{28}$$

After substitution of eqs. (28) into (27) we arrive to the asymptotic formula:

$$\Gamma(\delta) = -2^{3/4}\pi^{-1/2}\lambda^{1/2}\delta^{5/4}\exp(\pm i\pi/\delta)\left[1 + \frac{3}{\sqrt{2}}\lambda\delta^{1/2}\ln\delta + (2\ln\lambda - 2 - 5\ln 2)\frac{\lambda}{\sqrt{2}}\delta^{1/2} + O(\delta^{1/4})\right]. \tag{29}$$

Then we shall use dispersion relations for the series (26) to obtain high-order behavior of their coefficients. The formula analogous to (10) is:

$$E_{N/2} = \frac{1}{4\pi i}\oint\frac{E(\delta)}{\delta^{N/2+1}}d\delta, \tag{30}$$

where the integration is done along a contour embracing the origin twice:  . After inflating of this contour, the integral (30) may be reduced to

$$E_{N/2} = \frac{1}{4\pi}\int_0^\infty\frac{\Gamma(\delta)}{\delta^{N/2+1}}d\delta. \tag{31}$$

in a way similar to the integral (10). Inserting (29) into (31), we find

$$E_k \sim -2^{-1/4}\lambda^{1/2}\pi^{-k-1/4}k^{-9/4}k!$$
$$\cdot\mathrm{Re}\left\{\exp\left(\frac{5}{4}i\pi(1/2 - N)\right)\left\{1 - \frac{3}{2}(1+i)\pi^{1/2}\lambda k^{-1/2}\ln k + \left[\frac{3}{4}i\lambda\pi\ln\pi + (\ln\lambda - 1 - \frac{5}{2}\ln 2)\lambda\right](1+i)\pi^{1/2}k^{-1/2}\right\}\right\}$$
(32)

where $k = N/2$. Here, we summed two complex-conjugate terms corresponding to two possible signs in (29).

A leading term in the expansion (32) is

$$\tilde{E}_k \sim -2^{-1/4}\lambda^{1/2}\pi^{-k-1/4}k^{-9/4}k!\cos\left(\frac{5}{4}\pi(1/2-N)\right) \tag{33}$$

Note that there is an ambiguity in deriving formulas (32) and (33) because we can consider i entering $\exp(\pm i\pi/\delta)$ equally as $\exp(i\pi/2)$ and $\exp(5i\pi/2)$. We choose the last expression, because in this case the asymptotical formula appears to work better (it was tested by comparison with exact coefficients).

A ratio $E_{N/2}/\tilde{E}_{N/2}$ vs $N/2$ is shown on Fig. 7.

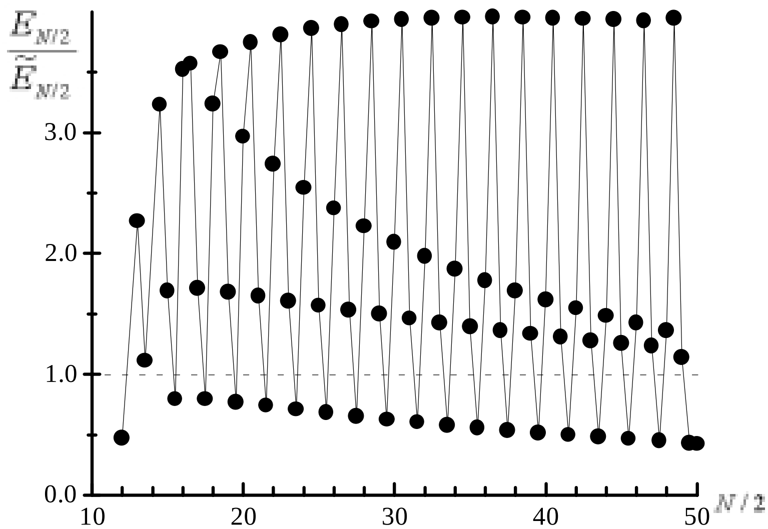


Fig. 7. Ratio of coefficients for Model-3/2 $E_{N/2}$ to their high-order approximation (33) at $\lambda = 2^{-3/2}$

The deviation of this ratio from one even for large $N \sim 100$ is probably a result of the next correction in (32) of order $\sim k^{-1/2}\ln k$ equal 0.6 at $N \sim 100$. However, an incorporation of the next-order correction does not improve an accuracy. It may be because of poor convergence of the asymptotic expansion (32). Note that errors in our expressions for these corrections are possible, because of cumbersome calculations.

III. Comparison of convergence for the two models

Usually, convergence of series is characterized by a radius of convergence. Since we deal with factorially divergent series with zero radius of convergence, the growth of coefficients of the series may be characterized by a radius of convergence of its Borel transform that is a distance of a nearest Borel singularity from the origin. It was found that the Borel singularities for Model-0 are $2\,\mathrm{Re}\,S(\lambda)\pm i\pi$, see Fig. 8, and they are always $\pm i\pi$ for Model-3/2.

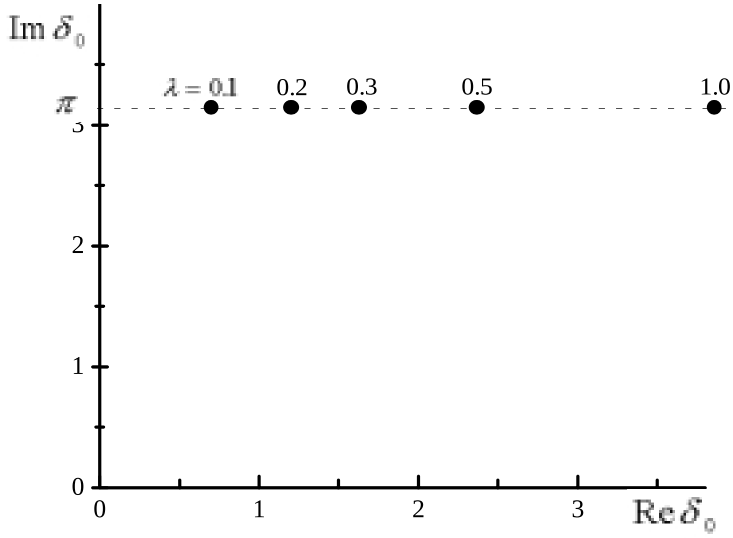


Fig. 8. Position of Borel singularity in an upper-half plane for Model-0 at different λ

So, the divergence of coefficients at large orders is always stronger for Model-3/2. However, for small λ the Borel singularities are almost the same, but pre-factorial factor $k^{-9/4}$ for Model-3/2 is less than $k^{-3/2}$ for Model-0, and so coefficients are also less. Dependence of E_k on λ for both models is illustrated on Fig. 9. One can see that coefficients for Model-3/2 become smaller only for very small λ, and this range of small λ is more narrow for larger k.

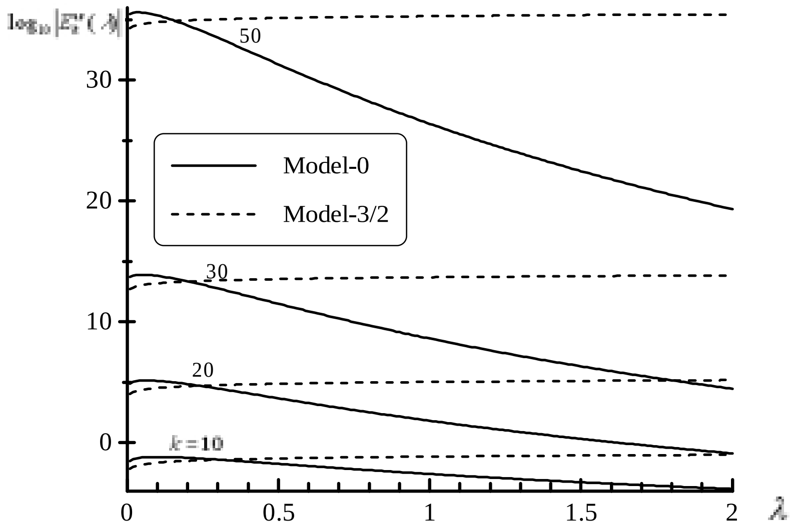


Fig. 9. Dependence of coefficients E_k given by asymptotic formulas (5) and (33) on λ. To avoid rapid oscillations of $\cos k\varphi$ where $\varphi = \mathrm{Arg}\,\delta_0$, we replaced $\log_{10}|\cos k\varphi|$ by its averaged value -0.30103. All curves tend to $-\infty$ for extremely small λ.

Let us compare a rate of convergence of partial sums and Padé approximants for three-dimensional case with unscaled $\lambda = 2^{-3/2}$. The results are shown on Fig. 10.

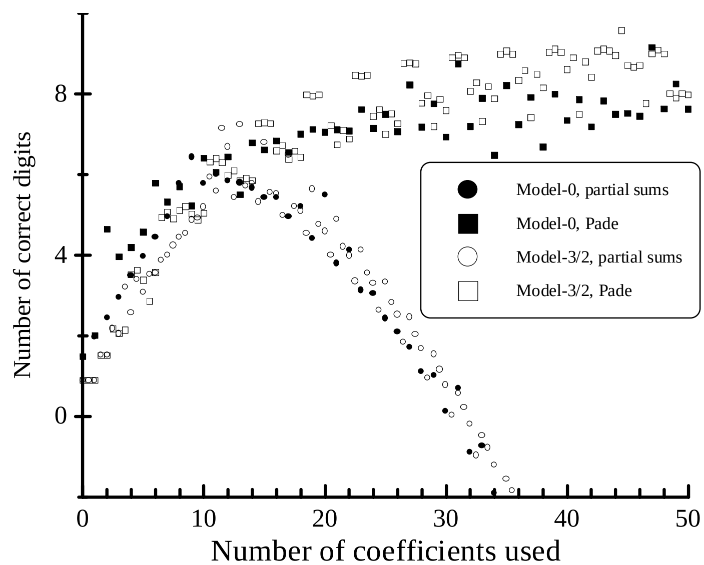


Fig. 10. Accuracy of summing of 1/*D*-expansion. Here, we plot $-\log_{10}|E_{\mathrm{sum}} - E|$ vs order k.

For Model-3/2, both partial sums and Padé approximants converge insignificantly better than for Model-0. It seems to contradict the fact that Model-3/2 coefficients are larger for $\lambda = 2^{-3/2}$, see Fig. 9. In fact, the value of λ for Model-0 is $3^{3/2}$ times less than for Model-3/2, because it is *scaled* $\lambda' = D^{-3/2}\lambda$. The dependence of the size of coefficients on *unscaled* λ for both models is shown on Fig. 11. One can see that actually Model-3/2 coefficients are slightly smaller for $\lambda = 2^{-3/2}$.

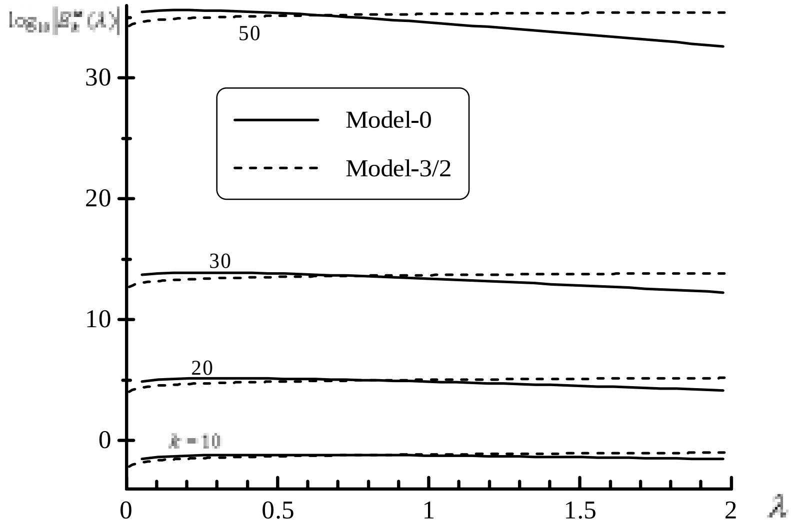


Fig. 11. Dependence of coefficients E_k given by asymptotic formulas (5) and (33) on *unscaled* λ for physical dimensionality $D = 3$. Compare with Fig. 9 and note a horizontal shift of all solid curves according to scaling $\lambda' = D^{-3/2}\lambda$.

The reverse situation (e. g. Model-0 has better convergence than Model-3/2) can be expected for $\lambda \sim 1$ and larger. A simple heuristic explanation of this fact is as follows. For Model-0, we incorporate a part of the term λr^{-1} into a zero-order harmonic approximation. In contrast, for Model-3/2 we treat this term entirely as a perturbation, even if it is not small. So, the magnitude of the perturbation is larger, and the series diverges stronger.