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Large orders of the $1/n$ expansion in quantum mechanics

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The asymptotics of large orders of the $1/n$ expansion in quantum mechanics has been found. It is shown that the coefficients $\epsilon^{(k)}$ grow as $k!a^k$ with $k\to\infty$, and the dependence of the parameter a on the coupling constant is investigated.

1. Introduction

At present the $1/n$ expansion is widely used in various quantum-mechanical problems, see e.g. refs. [1–10] and references therein. We consider below the version of the method proposed in ref. [7], which is applicable not only for a discrete spectrum, but also in the case of quasistationary states (resonances). The energy eigenvalues which are complex in the last case ($E_{nl}=E_r-\frac{1}{2}i\Gamma$), can be represented in the form of an expansion in powers of the "small parameter" $1/n$,

$$\epsilon=\epsilon'-i\epsilon''=\epsilon^{(0)}+\frac{\epsilon^{(1)}}{n}+...+\frac{\epsilon^{(k)}}{n^k}+... , \tag{1}$$

where $n=n_r+l+1$ is the principal quantum number, l is angular momentum, $\epsilon=2n^2E_{nl}$ is the "reduced" energy of the nl state, $\epsilon''=n^2\Gamma_{nl}$ and k is the order of the $1/n$ expansion.

The behavior of the coefficients $\epsilon^{(k)}$ for $k\gg 1$ not only presents some theoretical interest, but is of considerable importance in calculating the energy E_{nl} with high accuracy using expansion (1). It is known that the divergence of the perturbation theory series (PT) in quantum mechanics and field theory is connected with the instability of the vacuum state when the coupling constant g changes its sign (the so-called "Dyson phenomenon", established for the first time in QED [11] and later considered for the anharmonic oscillator [12,13], Stark [14–16] and Zeeman [17] effects, and other quantum-mechanical problems).

As a rule, the asymptotics of large orders of PT has the form

$$E_k\simeq(k\alpha)!a^kk^\beta\left(c_0+\frac{c_1}{k}+\frac{c_2}{k^2}+...\right)$$
$$\equiv(k\alpha+\beta)!a^k\left(c_0'+\frac{c_1'}{k}+...\right), \tag{2}$$

where $E(g)=\sum_k E_kg^k$, $z!\equiv\Gamma(z+1)$ and $\alpha>0$, β, a, c_0, c_1 etc. are calculable constants.

In eq. (1) the expansion parameter is $1/n$ (instead of the coupling g), which does not enter into the Hamiltonian explicitly, and the coefficients $\epsilon^{(k)}$ are rather complicated functions of g, contrary to the case of higher PT orders. So some modification of Dyson's arguments is needed, which is given below.

2. Asymptotics of large orders of the 1/n expansion

Using recurrence relations [#1], we have computed 30–50 coefficients $\epsilon^{(k)}$; eq. (2) for them was checked for $k\gg 1$ and the parameters of the asymptotics α, a, ... were determined numerically. These calculations have been done for the following problems: the funnel potential

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[#1] See ref. [18]. The numerical methods we have used will be described elsewhere.

$$V(r)=-r^{-1}+gr, \quad g>0\,, \tag{3}$$

the Stark effect in hydrogen and its spherical model (which corresponds to $g\to -g$ in eq. (3)), and the screened Coulomb potential

$$V(r)=-r^{-1}f(x), \quad x=\mu r\,, \tag{4}$$

where μ^{-1} is the screening radius and atomic units are used, $\hbar=m=e=1$. These examples embrace a wide class of potentials used in physics, including the short-range Yukawa and Hulthen potentials [#2], the confining potential (3), frequently used in QCD, and potentials with a barrier.

In all the cases considered it turned out that $\alpha=1$, e.g. $\epsilon^{(k)}\sim k!$. The dependence of the parameter a in eq. (2) on the parameters in the problems is also of some interest, and $\nu=n^2\mu$ is the right parameter for the screened potentials (4), with $\mu=g^{1/2}$ and $f(x)=1-x^2$ in the case of potential (3). Finally, $\nu=n^2\varepsilon^{1/2}\equiv F^{1/2}$ for the Stark problem, where F is the "reduced" electric field ($F=\varepsilon/\varepsilon_a$, ε is an external field and $\varepsilon_a\sim\bar{r}^{-2}\sim n^{-4}$ is the atomic field in the electron orbit with principal quantum number n).

The $1/n$ expansion is constructed around the classical equilibrium point $x_0(\nu)$ in the effective potential including centrifugal energy. Here we confine ourselves to the $l=n-1\gg 1$ states with no radial nodes. The quasiclassical momentum is

$$p(r)=\frac{1}{n}\,[-\varphi(y,\nu)]^{1/2}\,,$$

$$\varphi=y^{-2}-2y^{-1}f(\nu y)-\epsilon^{(0)}\,, \tag{5}$$

where $y=n^{-2}r$ and $\epsilon^{(0)}$ is the energy of a classical particle at rest at the equilibrium point, $x_0=\nu y_0$. The quantities $x_0(\nu)$ and $\epsilon^{(0)}(\nu)$ are determined by the equations [7]

$$\nu=xf-x^2f', \quad \epsilon^{(0)}=(xf')^2-f^2|_{x=x_0}\,. \tag{6}$$

We assume the potential to be of the form shown in fig. 1. The width of the highly excited, $n\gg 1$, levels is (within exponential accuracy)

[#2] When $f(x)=\exp(-x)$ and $x[\exp(x)-1]^{-1}$ in eq. (4), we obtain the Yukawa and Hulthen potentials, frequently used in nuclear physics; $f(x)=x\exp(-x^2)$ corresponds to the Gaussian potential, $f(x)=1-x^2$ to the funnel potential (3), etc. In fact, an arbitrary central potential $V(r)$ can be written in the form of eq. (4), if the condition $0<f(0)<\infty$ is ignored.

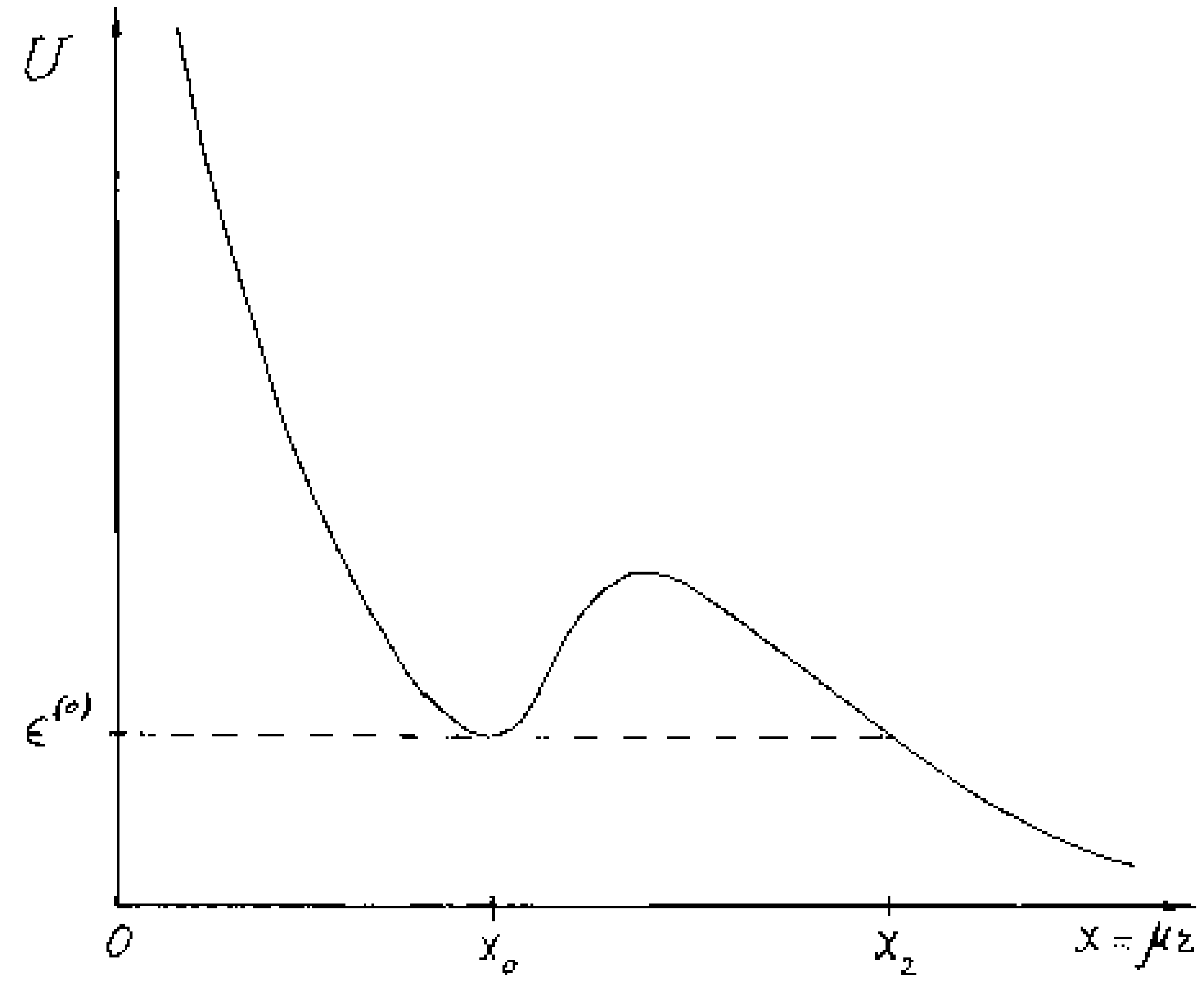

Fig. 1. An effective potential U (qualitatively).

$$\Gamma_n\approx \text{const}\times\exp(-2nQ)n^{\sigma}\,,$$

$$Q(\nu)=\int_{y_0}^{y_2} dy\,[\varphi(y,\nu)]^{1/2}\,, \tag{7}$$

where y_0, y_2 are the turning points, see fig. 1, and σ depends on the problem considered. Supposing analyticity in the variable $\lambda=1/n$ and using the dispersion relations in λ, we obtain

$$\epsilon^{(k)}\approx k!a^kk^{\sigma+1}c_0[1+O(1/k)], \quad k\to\infty\,,$$

$$a=[2Q(\nu)]^{-1}\,. \tag{8}$$

When $y\to y_0$, then $\varphi(y,\nu)=\omega^2y_0^{-4}(y-y_0)^2+...$, where ω is the dimensionless frequency of vibrations around the equilibrium point $x_0(\nu)$. For sufficiently small values of ν this point is real, as well as all the coefficients $\epsilon^{(k)}$ in (1). With ν increasing the value $\nu=\nu_*$ is achieved, when the collision of two classical orbits occurs, corresponding to the stable (x_0) and unstable equilibrium points in the effective potential. The value ν_* is determined by the first of eqs. (6) with $x=x_*$, while x_* is a root of the equation $f-xf'-x^2f''=0$. It can be shown that for $\nu\to\nu_*$

$$\omega=C(1-\nu/\nu_*)^{1/4}\,,$$

$$a(\nu)\simeq A(1-\nu/\nu_*)^{-5/4}\,, \tag{9a}$$

where

$$A=a_1(1+xf'''/3f''|_{x=x_*})^{3/4}=\tfrac{5}{96}C^3\,,$$

$$a_1=2^{-17/4}\times3^{-1/4}\times5=0.19967\,. \tag{9b}$$

Note that asymptotics (8) follows from the dispersion relation

$$\epsilon^{(k)}=\frac{1}{\pi}\int_0^\infty \mathrm{d}\lambda\,\frac{\Gamma_n}{\lambda^{k+3}}\,,\quad \lambda=1/n\,,$$

and from eq. (7) for the widths of highly excited states with $n\gg1$. To obtain eq. (9a) one should consider the integral (7) for $Q(\nu)$ in the case when the turning points y_0, y_2 are nearby, and the function $\varphi(y,\nu)$ is considerably simplified. The details will be published elsewhere.

For $\nu>\nu_*$, the coefficients $\epsilon^{(k)}$ and parameter $a(\nu)$ become complex. Evidently, this solution has no direct physical sense in classical mechanics, but proceeding to quantum mechanics it allows one to calculate easily, within the $1/n$ expansion, not only the position E_r, but also the width Γ_n of the quasistationary state (see refs. [7–9]).

3. Some examples

(a) We begin with the potential (4), where

$$f(x)=\exp(-x)x^{\lambda-1}\,,\quad \lambda>0 \tag{10}$$

($\lambda=1$ corresponds to the Yukawa potential, $\lambda=2$ to the exponential potential). The equations for x_0 and ω take the following form,

$$[x_0^{\lambda+1}+(2-\lambda)x_0^{\lambda}]\exp(-x_0)=\nu\,,$$

$$\omega^2=\lambda-\frac{x_0(1-\lambda+x_0)}{2-\lambda+x_0}\,,$$

hence

$$x_*=\lambda+\tfrac12[(1+4\lambda)^{1/2}-1]\,,$$

$$\nu_*=\frac{1}{2\lambda}[1+(1+4\lambda)^{1/2}]x_*^{\lambda+1}\exp(-x_*)\,,$$

$$A=\tfrac{5}{96}[1+4\lambda-(1+4\lambda)^{1/2}]^{3/4}\,. \tag{11}$$

(b) For the generalized funnel potential

$$V(r)=-\frac{1}{r}+\frac{g}{N}r^N\,,\quad N>-1\,, \tag{12}$$

we get ($g<0$)

$$\nu_*=(N+1)(N+2)^{-(N+2)/(N+1)}\,,$$

$$A=\tfrac53\times2^{-17/4}(N+2)^{3/4}=a_1[\tfrac13(N+2)]^{3/4}\,, \tag{13}$$

where a_1 is the coefficient in eq. (9b).

(c) Consider the Stark effect in a hydrogen atom for the (n_1, n_2, m) state, where n_1, n_2, m are the parabolic quantum numbers and $n=n_1+n_2+|m|+1$. Using the results of refs. [9,18], we obtain for $n\gg1$:

$$a=\tfrac32F[-\epsilon^{(0)}(F)]^{-3/2}/J(F)\,, \tag{14a}$$

where $\epsilon^{(0)}$ is the first term in expansion (1), $F=n^4\varepsilon$,

$$J(F)=\frac32\int_{u_1}^{u_2}\frac{\mathrm{d}u}{u}(A'-B'u+u^2-u^3)^{1/2}\,, \tag{14b}$$

$$A'=m^2F^2(-\epsilon^{(0)})^{-3},\quad B'=4\beta_2F(\epsilon^{(0)})^{-2}$$

and $\beta_2=\beta_2(F)$ is the separation constant corresponding to the parabolic coordinate $\eta=r-z$.

Hence, in the region of weak fields

$$a=\tfrac32F-\frac{9}{4n}(2n_2+|m|+1)F^2\ln F$$
$$+O(F^2)\,. \tag{15}$$

The $(0, 0, n-1)$ states correspond to circular electron orbits perpendicular to the direction of the electric field ε. In this case the integral $J(F)$ can be expressed through elementary functions and

$$a=\frac12\left(z+\frac{z^3}{3(1-z^2)}-\mathrm{Arth}\,z\right)^{-1}\,, \tag{16}$$

where

$$z=(1-3\tau)^{1/2}(1-\tau)^{-1},\quad \tau(1-\tau^2)^4=F\,,$$
$$0<\tau<\tfrac13\,. \tag{17}$$

The collision of two classical solutions occurs at $\tau=\frac13$, or $F=F_*=2^{12}\times3^{-9}=0.2081$, where the parameter of the asymptotics behaves similarly to eq. (9a):

$$a(F)=Af^{-5/4}(1+bf^{1/2}+b_1f+\ldots)\,, \tag{18}$$

$A=2^{-3/4}\times3^{-3/2}\times5=0.5722$ and $f=1-F/F_*\to0$ (for details of the calculation see appendix).

(d) The formulae for the funnel potential (3) can be obtained from the preceding ones when substituting $g\to-g$,

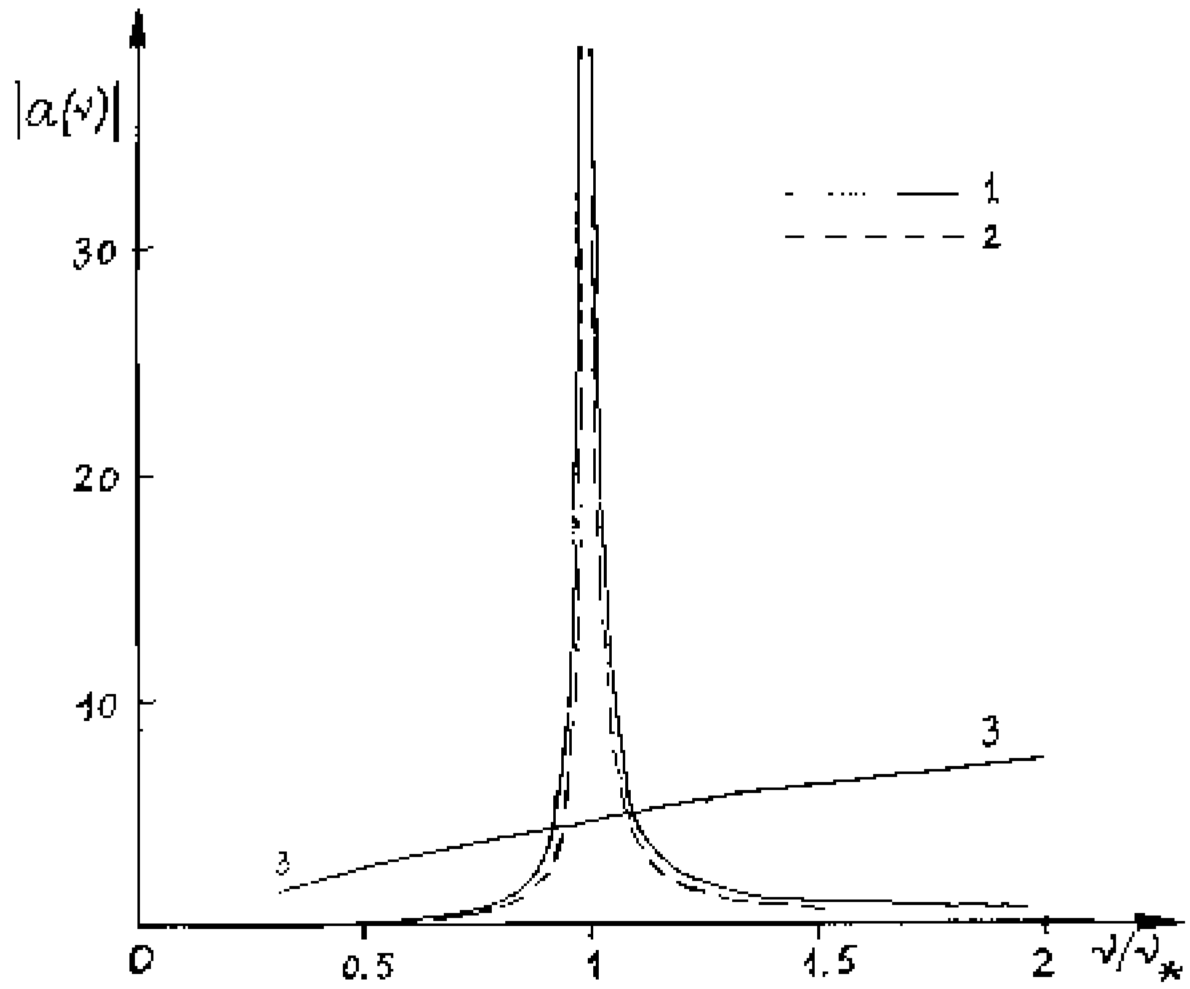

Fig. 2. $|a(\nu)|$ versus ν/ν_*. Curves (1)–(3) correspond to the Stark effect, its spherical model and the funnel potential. In the latter case the values of $|a|$ are multiplied by 10^2.

$$\nu = x_0 + x_0^3 ,$$

$$z = \omega = [(1+3x_0^2)/(1+x_0^2)]^{1/2} . \qquad (19)$$

So, $z > 1$ and Arth z = Arth $z^{-1} \pm \frac{1}{2}\pi i$. Therefore, the asymptotical parameter a becomes complex, which corresponds to oscillations of the coefficients $\epsilon^{(k)}$ with $k \to \infty$. In particular, for $g \to \infty$ we have: $z \to 3^{1/2}$,

$$a(\infty) = \tfrac{1}{2}[3^{1/2} - \ln(2+3^{1/2}) + i\pi]^{-1} \qquad (20)$$

and $|a(\infty)| = 0.1578$ (compare with fig. 2).

The parameters a for the Stark effect, the spherical model (12) with $N=1$ and the funnel potential (3) are shown in fig. 2 by curves (1)–(3), respectively. Note that $a(\nu) \to \infty$, when $\nu \to \nu_*$. Thus, the coefficients $\epsilon^{(k)}(\nu)$ grow sharply, and the $1/n$ expansion itself is no longer applicable in this region. This was observed already in the first attempts to sum series (1) for $\nu \approx \nu_*$ [7], and the underlying reason becomes clear from fig. 2. However, for $\nu > \nu_*$, the parameter $a(\nu)$ decreases with ν increasing, and the applicability of the $1/n$ expansion is restored. In this region the coefficients $\epsilon^{(k)}$ in eq. (1) are complex, thus the first few terms of expansion (1) determine the width of a quasistationary state with a reasonably high accuracy.

Similar results were obtained also for the Yukawa and Hulthen potentials, see fig. 3.

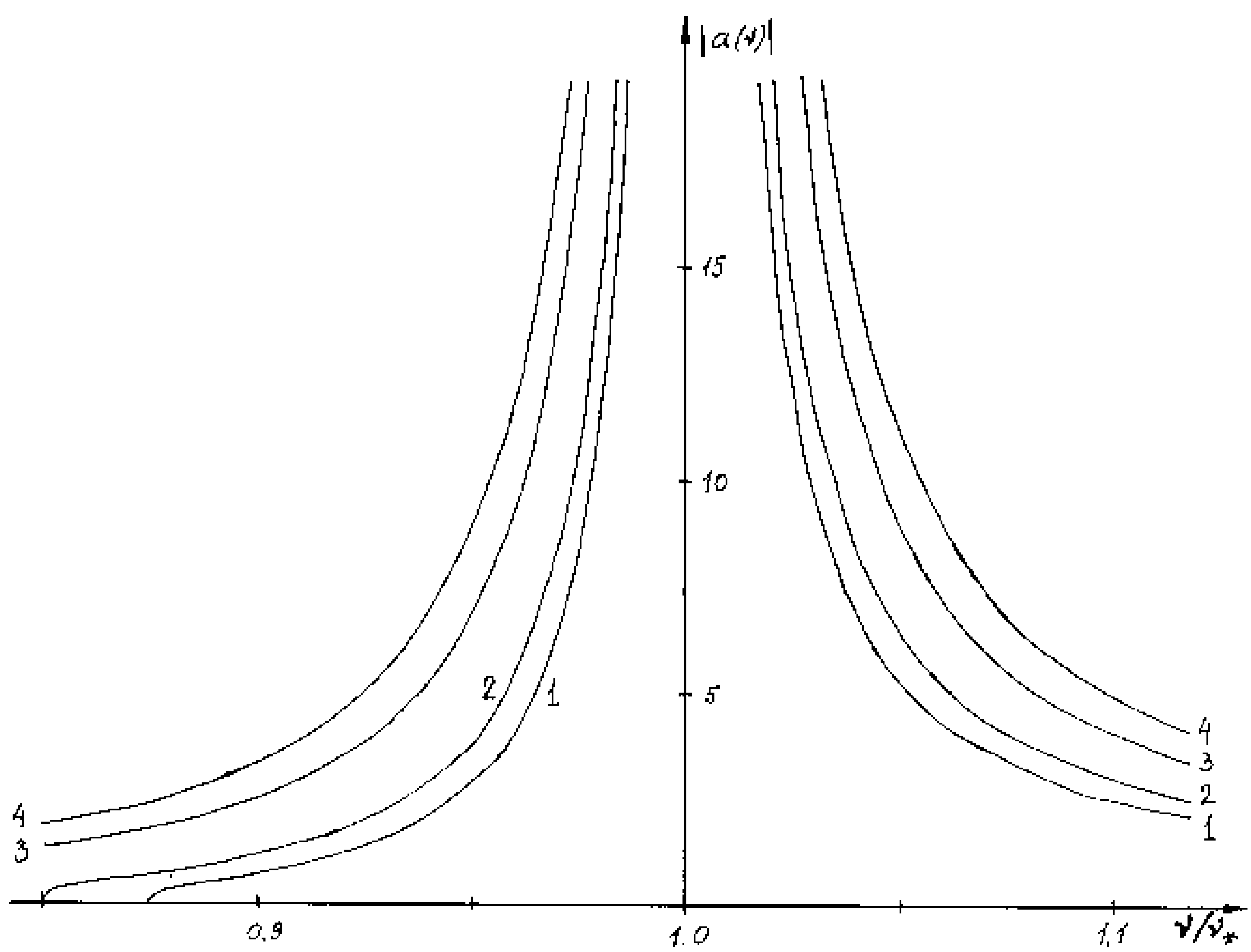

Fig. 3. The same as fig. 2 for the Yukawa potential ($\nu_* = 0.8400$, curve (1)), the Hulthen potential ($\nu_* = 1.5234$, curve (2)) and the funnel potentials (12) with $N=1$ and 2 ($\nu_* = 0.3849$, curve (3), and $\nu_* = 0.4725$, curve (4)).

4. $1/n$ expansion and the problem of two centres

The nonrelativistic problem of two Coulomb centres,

$$V(\boldsymbol{r})=-\frac{Z_1}{r_1}-\frac{Z_2}{r_2}, \quad r_{1,2}=[\rho^2+(z\pm\tfrac{1}{2}R)^2]^{1/2},$$
$$\rho=(x^2+y^2)^{1/2}, \tag{21}$$

is encountered frequently in different branches of physics, including the theory of molecules, μ catalysis, etc. In this case the coefficients $\epsilon^{(k)}$ depend on the internuclear distance R, where the first term $\epsilon^{(0)}$ corresponds to the electron energy on the classical orbit which is determined by the equilibrium condition of the forces acting on the electron in its rest frame. Here we confine ourselves to the case $Z_1=Z_2=1$ (the molecular ion H_2^+). For the states with $m=n-1$, $n\to\infty$ (or, equivalently, for $n=1$ and $D\to\infty$, where D is the space dimension) the equations can be written in a parametric form,

$$\epsilon^{(0)}=-2(1-\tau)^2(1+\tau),$$
$$\epsilon^{(1)}=2(1-\tau)^3\{(2n_1+1)[1+(1+3\tau)^{1/2}]$$
$$-(2n_2+1)[1-(1-3\tau)^{1/2}]\},$$
$$\tilde{R}\equiv n^{-2}R=\tau^{1/2}(1-\tau)^{-2}, \tag{22}$$

where $0<\tau<\frac{1}{3}$, $\tilde{R}<R_*=3^{3/2}\times2^{-2}=1.299$ and $E=n^{-2}\epsilon$ is the term energy, while $\tau=\cos^2\alpha$ and α is the angle at the Z vertex in a triangle (Z, Z, e). The numerical analysis shows [10,19,20] that the $\epsilon^{(k)}$ grow as factorials for $k\to\infty$, while the parameter $a=a(\tilde{R})$, see eq. (8), increases for $\tilde{R}\to R_*$. Here we present a few analytical results.

If $0<\tilde{R}<R_*$, then

$$a(\tilde{R})=-\tfrac{1}{2}(\mathrm{Arth}\,\zeta-\zeta)^{-1},$$
$$\zeta=(1-3\tau)^{1/2}(1-\tau)^{-1}, \tag{23}$$

and $\tau=\tau(\tilde{R})$ is determined as in the preceding equations. So the singularity of the Borel transform [20] closest to the origin is at $\delta_0=1/2a<0$. The series (1) is alternating in sign and can be summed with the help of Padé approximants. In a recent paper [20] the dependence of δ_0 on $\tilde{R}$ was established numerically with a high accuracy. The values of the parameter δ_0, given in ref. [20], are in very good agreement with the analytical formula (23).

When $\tilde{R}=R_*$, the three classical orbits (stable and unstable) coincide, so the rearrangement of the $1/n$ expansion occurs at this point. If $\tilde{R}>R_*$, we have

$$a(\tilde{R})=\tfrac{1}{4}[\zeta(1-\zeta^2)^{-1}-\mathrm{Arth}\,\zeta]^{-1} \tag{24}$$

and

$$\zeta=[(3\tau-1)/(3\tau-\tau^2)]^{1/2},$$
$$\tilde{R}=8\tau^{3/2}(1-\tau)^{-1}(1+\tau)^{-2}, \quad \tfrac{1}{3}<\tau<1.$$

In this case $a=1/2\delta_0>0$, so the terms of the $1/n$ expansions are of the same sign. The derivation of eqs. (23), (24) follows the same lines as eq. (16), and will be given in detail elsewhere. It is notable that the singularity of $a(\tilde{R})$ differs from eq. (9a) and is no longer symmetrical in this case:

$$a(\tilde{R})\simeq A_\pm|1-\tilde{R}/R_*|^{-3/2}, \quad \tilde{R}\to R_*, \tag{25}$$

where $A_+=3^{-1/2}$ for $\tilde{R}>R_*$ and $A_-=-(\frac{2}{3})^{1/2}$ for $\tilde{R}<R_*$.

5. Conclusion

Thus, large orders of the $1/n$ expansion increase as factorials. This explains why in many quantum-mechanical problems [#3] it is necessary to calculate ~30–50 coefficients $\epsilon^{(k)}$ and to use a summation method to obtain the energy ϵ_{nl} with the accuracy required for experiments. At present the summation of divergent series occurring in quantum mechanics is developed fairly well and, in principle, presents no insuperable difficulties.

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Appendix

Calculating the integral in eq. (14b), we obtain

[#3] For example, when calculating complex energies of quasistationary states (n_1, n_2, m) for the Stark effect in hydrogen [8,9].

$$a = c/\phi(z)\,, \tag{A.1}$$

$$\phi(z) = z + \frac{z^3}{3(1-z^2)} - \text{Arth}\, z$$
$$= \tfrac{2}{15} z^5 (1 + \tfrac{10}{7} z^2 + \tfrac{5}{3} z^4 + \ldots)\,, \quad z \to 0\,, \tag{A.2}$$

where $c = \frac{1}{2}$ for the Stark effect in hydrogen, while the dependence of z and energy $\epsilon^{(0)}$ on the reduced electric field, $F \equiv \nu^2 = n^4 \varepsilon$, is determined parametrically, $\epsilon^{(0)} = -(1+3\tau^2)(1-\tau^2)^2$ and eqs. (17). For the spherical model (see eq. (12) with $N=1$ and $g<0$) we get: $c = \frac{1}{4}$,

$$z = [(1-3\tau)/(1-\tau)]^{1/2}, \quad \epsilon^{(0)} = -(1+3\tau)(1-\tau)\,,$$
$$\tau(1-\tau)^2 = F\,. \tag{A.3}$$

Note that in both cases the root $\tau = \tau(F) \to 0$ for $F \to 0$ should be chosen, and $\tau = \frac{1}{3}$ corresponds to the collision of two classical solutions (stable and unstable equilibrium points). It occurs at $F = F_*$, where $F_* = 2^{12} \times 3^{-9} = 0.2081$ for the Stark problem [8], $F_* = 2^2 \times 3^{-3} = 0.1481$ in the case of its spherical model. For $F \to F_*$ we put $\tau = \frac{1}{3}(1-t)$ and obtain from eq. (A.3) that

$$t^2 + \tfrac{1}{3} t^3 = \tfrac{4}{3} f, \quad z = [\tfrac{3}{2} t / (1 + \tfrac{1}{2} t)]^{1/2}\,, \tag{A.4}$$

$f = 1 - F/F_* \to 0$, while eqs. (17) yield

$$t^2 + \tfrac{1}{6} t^3 + \ldots + 2^{-12} t^9 = \tfrac{8}{9} f\,,$$
$$z = \tfrac{3}{2} t^{1/2} (1 + \tfrac{1}{2} t)^{-1}\,. \tag{A.5}$$

From eqs. (A.1)–(A.4) we obtain

$$z = (3f)^{1/4} [1 - 2 \times 3^{-3/2} f^{1/2} + O(f)]\,.$$

Hence, eq. (18) follows, where

$$A = 5/8 \times 3^{1/4} = 0.4749\,,$$
$$b = -20/7 \times 3^{3/2} = -0.5499\,,$$
$$b_1 = -0.6699 \tag{A.6}$$

(in the case of the spherical model). Analogous calculations for the Stark effect give

$$A = 5/2^{3/4} \times 3^{3/2} = 0.5722, \quad b = -0.4770\,. \tag{A.7}$$

These values are in agreement with the curves in fig. 2.

The parameter a of the asymptotics (8) in the weak field region can be calculated, when substituting expansions of $\epsilon^{(0)}$ and $J(F)$ for $F \to 0$ into eqs. (14). In this way, for an arbitrary (n_1, n_2, m) state in a hydrogen atom, we obtain

$$a(F) = \tfrac{3}{2} F (1 - \tfrac{3}{2} \rho F \ln F + kF + \ldots)\,, \tag{A.8}$$

where

$$k = \tfrac{3}{2} \{3 + (3 \ln 2 - 2)\rho$$
$$- \tfrac{1}{2} [(\rho + \mu) \ln(\rho + \mu) + (\rho - \mu) \ln(\rho - \mu)]\}\,,$$
$$\rho = (2n_2 + |m| + 1)/n = 1 - (n_1 - n_2)/n\,,$$
$$\mu = m/n\,.$$

In particular, $\rho = 1$ and $k = 3.579$ for the $(0, 0, n-1)$ states with $n \gg 1$, $k = 4.619$ for the ground state, $n = 1$.

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