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Large orders of $1/n$-expansion for multidimensional problems

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Abstract

The asymptotics of large orders of the $1/n$-expansion is investigated for multidimensional problems of quantum mechanics and atomic physics, including those with separable variables (the hydrogen molecular ion H_2^+), and those where separation of variables is impossible (a hydrogen atom in electric and magnetic fields). It is shown that the parameters of the asymptotics can be found by means of calculating sub-barrier trajectories with the help of the "imaginary time" method, as well as by solution of the eikonal equation.

1. The $1/n$-expansion is widely used in quantum mechanics and atomic physics, see e.g. Refs. [1–12]. The energy eigenvalues (which are complex for quasistationary states, $E=E_r-\frac{1}{2}i\Gamma$) are represented in the form of an expansion [2,4,5]

$$\epsilon=\epsilon^{(0)}+\frac{\epsilon^{(1)}}{n}+\ldots+\frac{\epsilon^{(k)}}{n^k}+\ldots, \tag{1}$$

where n is the principal quantum number, $\epsilon=n^2E_{nl}$ is the "reduced" energy of the nl state and k is the order of the $1/n$-expansion. This method was successfully applied to the problems of atoms in strong external fields [3,5–7], the hydrogen molecular ion H_2^+ [6,8,9], etc. [2].

At present the behaviour of large orders of the $1/n$-expansion, i.e. of the coefficients $\epsilon^{(k)}$ with $k\gg 1$, has been investigated numerically [9,11] and analytically [12,13]. Here we continue our previous investigations [11–13] and present some results for multidimensional problems of quantum mechanics.

In the problems considered earlier the asymptotics has the form [11,13]

$$\epsilon^{(k)}\approx k!a^k k^\beta(c_0+c_1/k+\ldots), \quad k\to\infty \tag{2}$$

or

$$\epsilon^{(k)}\approx k!k^\beta\,\mathrm{Re}(c_0a^k)[1+O(k^{-1})]\,. \tag{2'}$$

Here a, β, c_0, etc. are calculable constants, the numerical values of which depend on the problem considered. For the one-dimensional case (e.g. for a potential with spherical symmetry) the asymptotical parameter a can be calculated from the equation [12]

$$a^{-1}=2^{3/2}\int_{r_1}^{r_2}[U(r)-\epsilon^{(0)}]^{1/2}\,\mathrm{d}r\,, \tag{3}$$

where $U(r)=n^2V(n^2r)+(2r^2)^{-1}$ is the effective potential including the centrifugal energy, $V(r)$ is the initial potential in the Schrödinger equation and

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$r_0<r<r_2$ is the sub-barrier region [1]. Since the energy $\epsilon^{(0)}$ corresponds to the minimum of the potential U, two turning points coincide, $r_1=r_0$. The applications of Eq. (3) to the bound and quasistationary states in the Yukawa and Hulthen potentials can be found in Refs. [12,13].

2. Here we consider the problem of two Coulomb centres,

$$V(r)=-(Z_1/r_1+Z_2/r_2)\,,$$
$$r_{1,2}=[\rho^2+(z\pm\tfrac{1}{2}R)^2]^{1/2}\,. \qquad (4)$$

Proceeding to the elliptic coordinates $\xi=(r_1+r_2)/R$, $\eta=(r_1-r_2)/R$ and performing the scaling transformation [2]

$$E=\lambda\epsilon,\quad R'=\lambda R,\quad r=\lambda r,\quad \lambda=\frac{1}{m^2-1}\approx n^{-2}\,,$$

we arrive at the Schrödinger equations with the effective energy e and effective potentials $U(\xi)$ and $V(\eta)$,

$$e=\tfrac{1}{4}\epsilon R'^2=\frac{ER^2}{4n^2}\,,$$

$$V(\eta)=\frac{1}{2(1-\eta^2)^2}+\frac{\beta R'}{1-\eta^2} \qquad (5)$$

(here $Z_1=Z_2=1$, which corresponds to the hydrogen molecular ion H_2^+, $m=0,\pm1,\pm2\ldots$ is the magnetic quantum number and R is the internuclear distance). The potential $V(\eta)$ is shown in Fig. 1. If $R'>R_*=3^{3/2}\times2^{-2}$, then

$$a^{-1}=2\int_{-\eta_0}^{\eta_0}|p_\eta|\,\mathrm{d}\eta$$
$$=4\left(\frac{\eta_0}{1-\eta_0^2}-\mathrm{Arth}\,\eta_0\right)>0\,, \qquad (6)$$

which coincides with Eq. (28) in Ref. [12], see also Ref. [8]. The value $R=R_*$ corresponds to the collision of two classical electron orbits in the field of two Coulomb centres and is determined from the condition that the frequency of small oscillations near the equilibrium orbit turns to zero (compare with the analogous calculations in Ref. [6]). If $R'<R_*$, then $\eta_0=0$ and the turning points are complex, $\eta_1^2=1+(2e)^{-1}<0$. Therefore,

$$a^{-1}=2^{3/2}\int_0^{\eta_1}[V(\eta)-V(0)]^{1/2}\,\mathrm{d}\eta$$
$$=-2(\mathrm{Arth}\,\zeta-\zeta)<0 \qquad (7)$$

$(0<\zeta<1)$. The dependence of the variable ζ on the reduced internuclear distance $R'=n^{-2}R$ is determined parametrically,

$$\zeta=(2e+1)^{1/2}=(1-3\tau)^{1/2}(1-\tau)^{-1}\,,$$
$$R'=\tau^{1/2}(1-\tau)^{-2},\quad 0<\tau<\tfrac{1}{3} \qquad (8)$$

($\tau=\frac{1}{3}$ corresponds to $\zeta=0$ and $R'=R_*$). So, the asymptotical parameter $a(R)$ in Eq. (2) is obtained in analytical form for any R.

From Eqs. (6)–(8) it follows that at $R'\to R_*$,

$$a(R)=A_-|h|^{-3/2}[1+\mathrm{O}(h)],\quad h=\frac{R'-R_*}{R_*}\,, \qquad (9)$$

where $A_+=3^{-1/2}$ and $A_-=-(2/3)^{1/2}$. Calculation of the parameter a by Eqs. (6)–(8) gives curve 1 in Fig. 2.

If $Z_1\neq Z_2$, the potential $V(\eta)$ is not symmetrical any more, see Fig. 1c. The calculations are performed in a similar way as in the case $Z_1=Z_2$, but the analytical formulae become more complicated (the calculation details will be published elsewhere). Just as for the discrete states in the Yukawa potential [4], the turning point r_2 moves into the complex plane, the parameter a becomes complex and Eq. (2′) holds. Here $|a(R)|<\infty$ for any R (see Fig. 2), since the collision of classical orbits does not occur at $Z_1\neq Z_2$, as opposed to the case of two equal charges. Note that the parameter $a(R)\to0$ at $R\to0$ and $R\to\infty$. In these limiting cases the problem of two Coulomb centres is reduced to the hydrogen-like atom.

Let us compare these results with that of Ref. [9], where large-order dimensional perturbation theory for the H_2^+ ion was considered and the singularity of the

[1] An analogous, though more complicated, formula can be obtained for the pre-exponential factor c_0. It can be also shown that $\beta=-\frac{3}{2}$ for nodeless states in a spherically symmetrical potential [12].

[2] Further we consider the states with a maximal possible value of $m=n-1$ and choose $\lambda=1/(n^2-2n)$. If the value $\lambda=n^{-2}$ is chosen, the parameters a and β in Eq. (2) remain the same, unlike the pre-exponential coefficients c_0, c_1, etc. Evidently, for the highly excited states, $n\gg1$, both values of the scaling factor λ are equivalent.

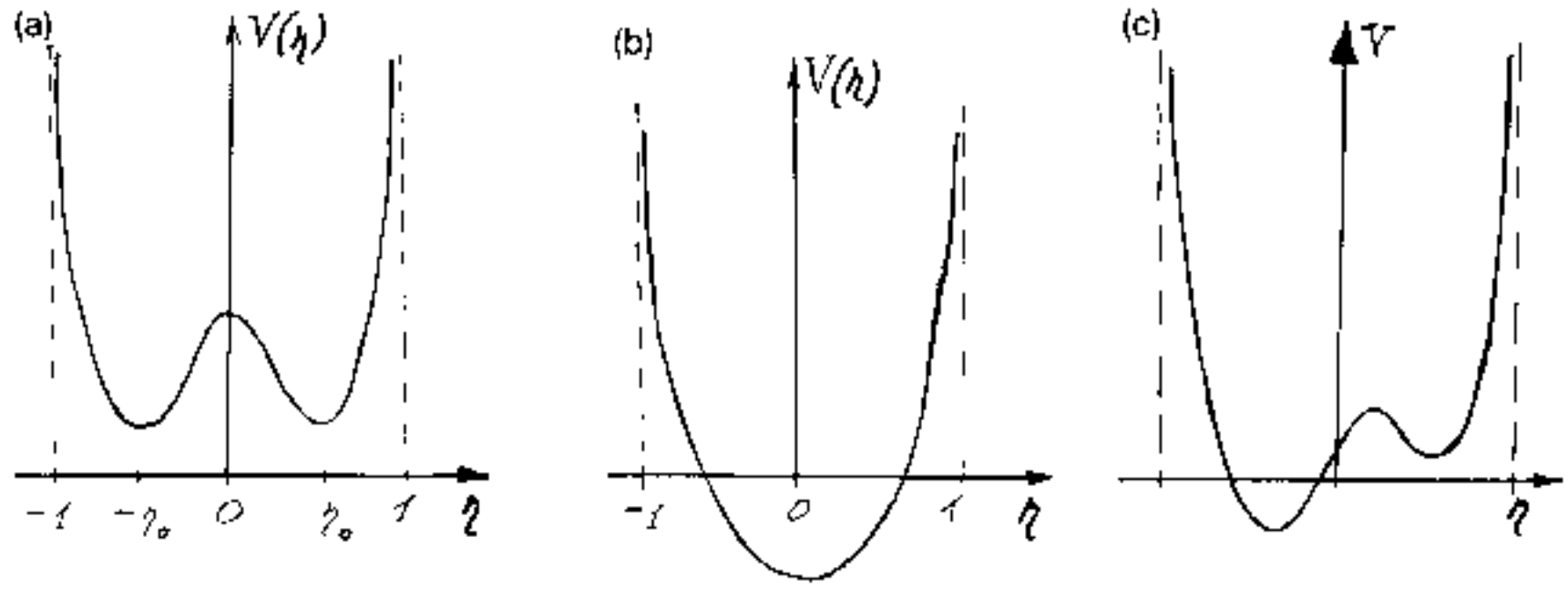

Fig. 1. The effective potential $V(\eta)$: (a) at $R'>R_*=1.299$, (b) at $0<R'<R_*$, (c) for $Z_1\neq Z_2$. Here $R'=n^{-2}R$, R is the internuclear distance.

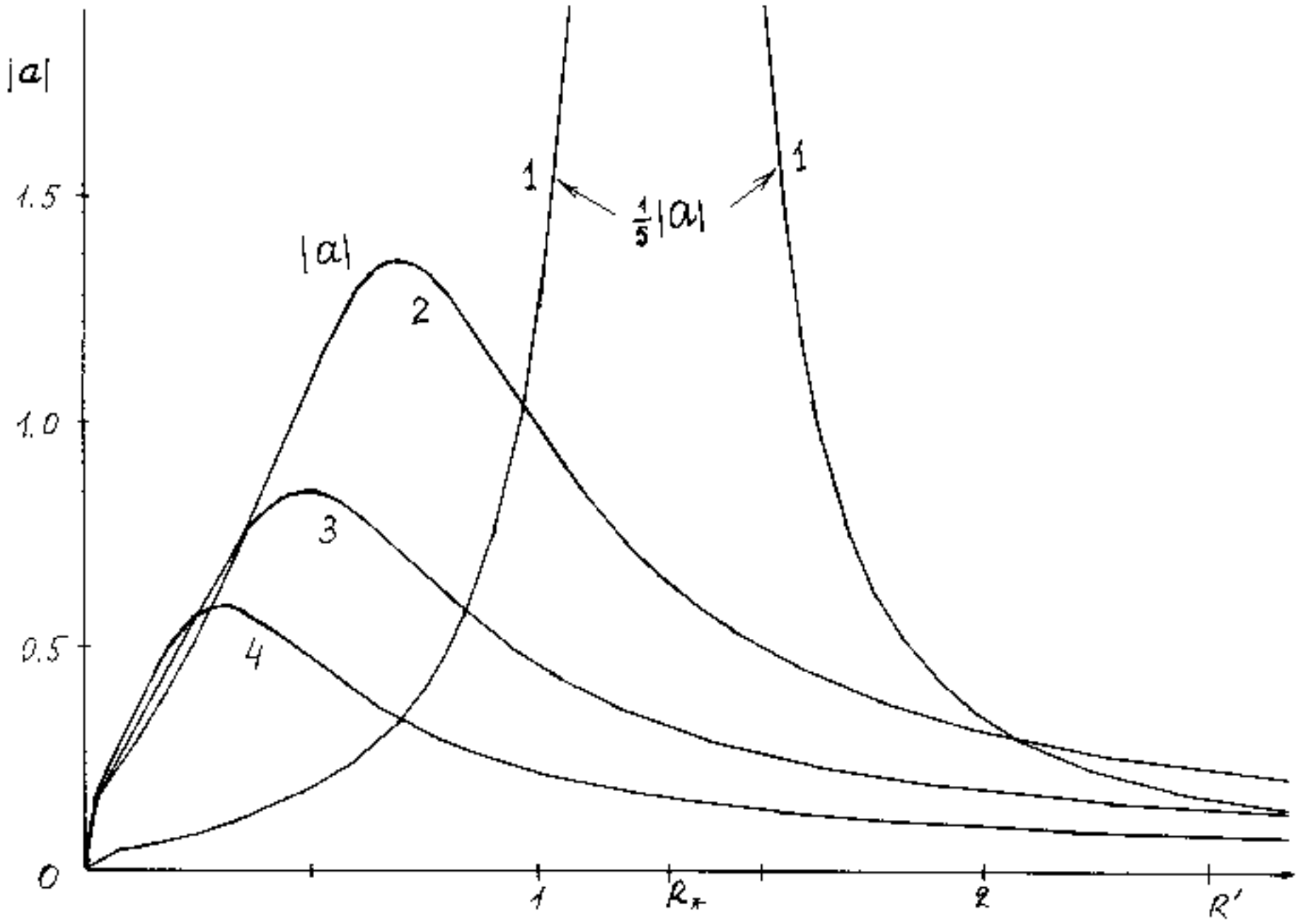

Fig. 2. The parameter of the asymptotics (2) for the problem of two Coulomb centres. Curves 1–4 correspond to $Z_1/Z_2=1$, $\frac{3}{2}$, 2 and 3.

Borel transform closest to the origin, $\delta_0=(2a)^{-1}$, was calculated numerically with the help of the quadratic Padé approximants. The agreement between Ref. [9] and our formula (7) is excellent, see Table 1. Note that only the case of $R'<R_*$ was considered in Ref. [9], where $a(R')<0$, so the series (2) is alternating in sign and the singularity of the Borel transform does not lie on the path of integration.

3. We consider a hydrogen atom in external fields, the case of uniform and parallel fields $\mathscr{E}$ and $\mathscr{H}$ and $(0, 0, n-1)$ states with magnetic quantum number $m=n-1$, which correspond to circular electron orbits (at $n\gg 1$). The $1/n$-expansion is constructed around the classical orbit with radius $r_0=r_0(F, B)$, determined from the equation [7]

$$r(1-F^2r^4)^2(1+\tfrac{1}{4}B^2r^3)=1 \qquad (10)$$

(we use atomic units, $\hbar=e=m_e=1$, and reduced variables $F=n^4\mathscr{E}$ and $B=n^3\mathscr{H}$, convenient in the case of Rydberg, $n\gg 1$, states).

To determine the asymptotical parameter a the "imaginary time" method was used, previously developed [14] for calculation of the tunneling probability through barriers, varying in time (e.g. in the theory of multiphoton ionization of atoms and ions by a strong light wave [15], as well as for calculation of e^+e^- pair production from vacuum by a varying

Table 1
Values of the Borel parameter δ_0 for the hydrogen molecular ion

$1.5R$	δ_0	Method of calculation
0.2	−1.720950	a
0.4	−1.062376	a
0.6	−0.705527	a
0.8	−0.474800620	a
	−0.474795	c
1.0	−0.313841191	a
	−0.31384121	c
1.2	−0.19751662152	a
	−0.19751661876	c
1.4	−0.112797	a
1.6	−0.052563	a
1.8	−0.013569	a
2.0	0.003681	b
2.2	0.038463	b
2.5	0.119351	b
3.0	0.294164	b
5.0	1.202939	b
10.0	3.943259	b

Notations: (a) the calculation of $\delta_0=(2a)^{-1}$ by Eq. (7), (b) by Eq. (6), (c) δ_0 from Ref. [9]. Note that the definition of the scaled internuclear distance in Ref. [9] differs from ours by the factor $\frac{3}{2}$.

electric field [16]). The classical trajectory $r(t)$, which joins the point r_0 of maximum effective potential $\tilde{U}$,

$$\tilde{U}(r)=-U=\frac{1}{r}-\frac{1}{2\rho^2}+Fz-\tfrac{1}{8}B^2\rho^2\,,$$

$$\rho=(x^2+y^2)^{1/2}\,, \tag{11}$$

with the turning point $r_2\in\sigma$, was found by numerical integration (here σ is an isoenergetical surface, e.g. $U(r_2)=U(r_0)$). The condition $\dot{r}_0=\dot{r}_2=0$ selects the sub-barrier trajectory, which minimizes Im S [14]. Then the parameter $a=a(F, B)$ in Eq. (2) is equal to

$$a=(2\,\mathrm{Im}\,S)^{-1},\quad S=\int_{r_0}^{r_2}\boldsymbol{p}\,\mathrm{d}\boldsymbol{r}=\int_0^{\infty}\dot{r}^2\,\mathrm{d}t\,, \tag{12}$$

where $\dot{r}=\mathrm{d}r/\mathrm{d}t$ and $t=\mathrm{i}\tau$ is "imaginary time". Note that $\tilde{U}$ differs in sign from the potential U entering the Schrödinger equation, which exactly corresponds to the description of the sub-barrier motion of a particle in terms of the imaginary time method. Since $\ddot{r}=\nabla U=0$ at $r=r_0$, the time of motion τ along the above trajectory is infinite. The lines of constant potential $\tilde{U}$ (dashed curves) and a few classical trajectories (solid curves) are given in Fig. 3. The integral S in Eq. (12) was calculated from the initial point $r_2\in\sigma$ to the point r_m of closest approach of the trajectory to the point of unstable equilibrium r_0. Since the potential $\tilde{U}(r)$ is approximated at $r\approx r_0$ by the potential of the "upturned oscillator", any trajectory is unstable. The trajectories in Fig. 3 correspond to initial deviations $\Delta\rho$, shown in Table 2. Although it is impossible to get from $r_2\in\sigma$ precisely to r_0 in numerical calculations, the value of Im S is readily determined. It can be shown that at small $\Delta\rho$

$$|1-\mathrm{Im}\,S/S_0|\sim(\Delta\rho/L)^2,$$

$$\tau\sim\frac{1}{\omega_1+\omega_2}\ln(L/|\Delta\rho|)\,, \tag{13}$$

where $L=|r_2-r_0|$, ω_i are the frequencies of normal vibrations at $r\approx r_0$, and the action S_0 corresponds to the above trajectory, which connects the point r_0 with the isoenergetic surface σ.

The results of the calculations (at $F<F_*$) are shown in Fig. 4. Here F_* is the classical ionization threshold, $F_*(B)=0.2081$, 0.2207, 0.2532 and 0.3449 at $B=0$, 0.25, 0.5 and 1.0. At $F\to F_*$ the points r_2 and r_0 converge, and the potential (11) takes the form $V=V_0+\alpha q-\frac{1}{3}\beta q^3$, where $\alpha\propto F_*-F\to 0$ and $\beta\sim 1$. Taking Eq. (3) into account, we find that

$$a^{-1}=2\int_{q_0}^{q_2}(-p^2)^{1/2}\,\mathrm{d}q\propto\alpha^{5/4},$$

$$a\propto(F_*-F)^{-5/4}\,. \tag{14}$$

So the parameter a has a power singularity at $F=F_*$ of the same type as in the one-dimensional case [12].

4. Let us also give a brief description of the alternative calculation method for the action S along the sub-barrier trajectory, based on solution of the Hamilton–Jacobi (HJ), or eikonal equation,

$$(\nabla S)^2=2(U-U_0),\quad U_0=U(r_0)\,. \tag{15}$$

Choosing the origin at the point r_0 and axes x, y (normal coordinates), we get at $r\approx r_0$

$$U(x, y)=U_0+\tfrac{1}{2}\omega_1^2x^2+\tfrac{1}{2}\omega_2^2y^2+\ldots\,,$$

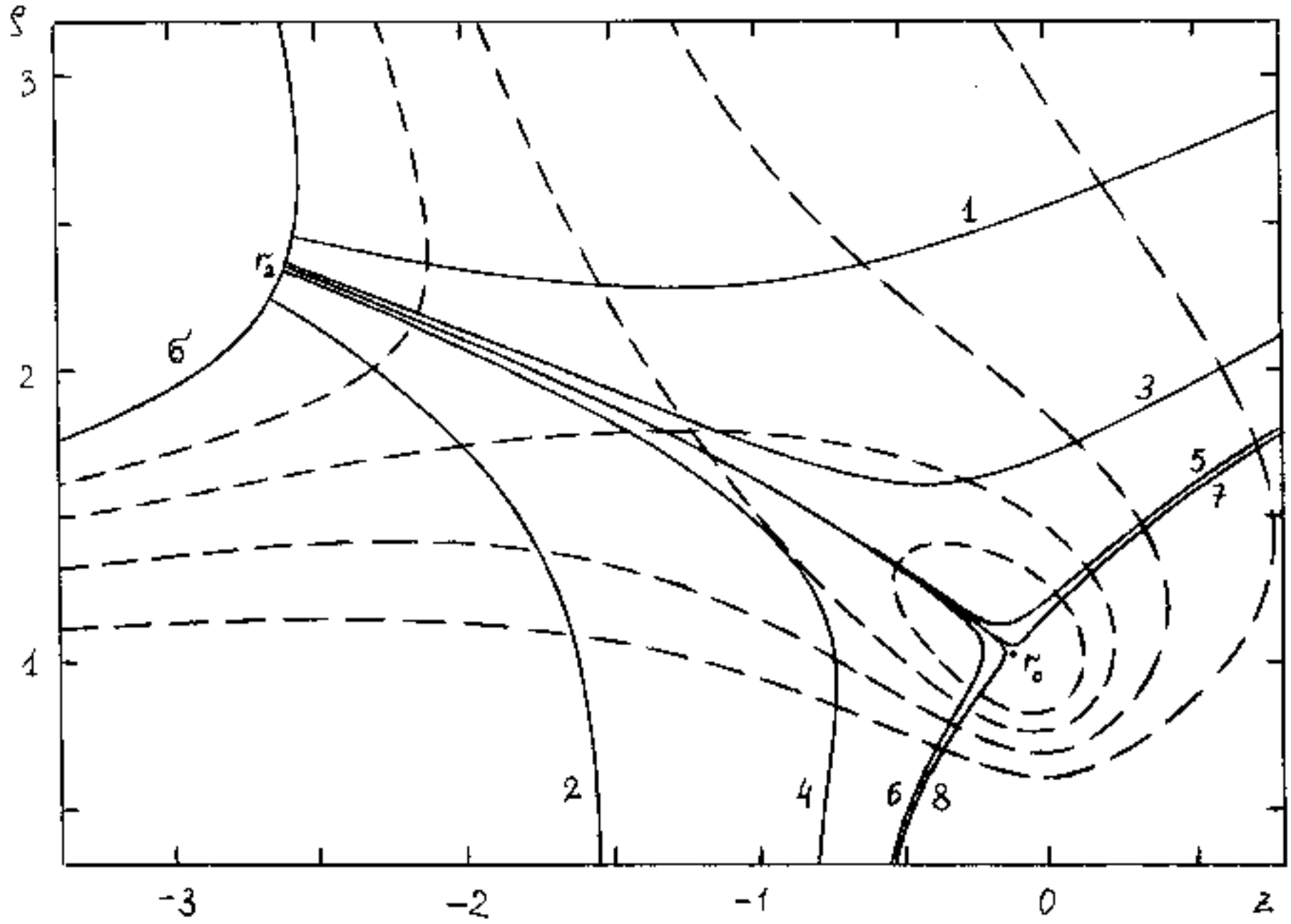

Fig. 3. The sub-barrier trajectories for the potential (11). The values of parameters for trajectories Nos. 1–8 are given in Table 2. Here ρ and Z are the cylindric coordinates of the electron, the nucleus (proton) is located at $\rho=z=0$.

Table 2
Convergence of the Im S values ($F=0.15$, $B=0.2$ and $F_*=0.2163$)

Imaginary time method					Solution of the HJ equation	
No.	$\Delta\rho$	Δr	τ	Im S	N	Im S
1	0.1	1.396	6.16	0.345	15	0.39924
2	−0.1	1.401	4.92	0.424	18	0.40072
3	0.01	0.692	8.35	0.393	28	0.4011278
4	−0.01	0.675	7.80	0.412	35	0.4011270
5	10^{-4}	0.1347	11.35	0.40106	38	0.401126879
6	-10^{-4}	0.1335	11.24	0.40126		
7	10^{-6}	0.0247	13.93	0.4011264		
8	-10^{-6}	0.0246	13.91	0.4011278		
–	10^{-8}	0.0045	16.45	0.40112688		
–	-10^{-8}	0.0045	16.45	0.40112689		
–	~ 0	$\sim 10^{-3}$	~ 20	0.401126879		

Nos. 1–8 in the table correspond to the numbers of the curves in Fig. 3. Here $\Delta r=|\boldsymbol{r}_m-\boldsymbol{r}_0|$ is the distance of closest approach of the classical trajectory to the point of (unstable) equilibrium $\boldsymbol{r}_0$, τ is the time of motion from the initial point $\boldsymbol{r}_2$ to $\boldsymbol{r}_m$.

$$S(x,y)=\int_0^x \dot{x}\,\mathrm{d}x+\int_0^y \dot{y}\,\mathrm{d}y$$

$$=\tfrac{1}{2}(\omega_1 x^2+\omega_2 y^2)+\ldots. \qquad (16)$$

Substituting the expansions

$$U=\sum_{j,k=0}^{\infty} u_{jk}x^j y^k,\quad S=\sum_{j,k} s_{jk}x^j y^k \qquad (17)$$

into the HJ equation, we arrive at the recurrence relations

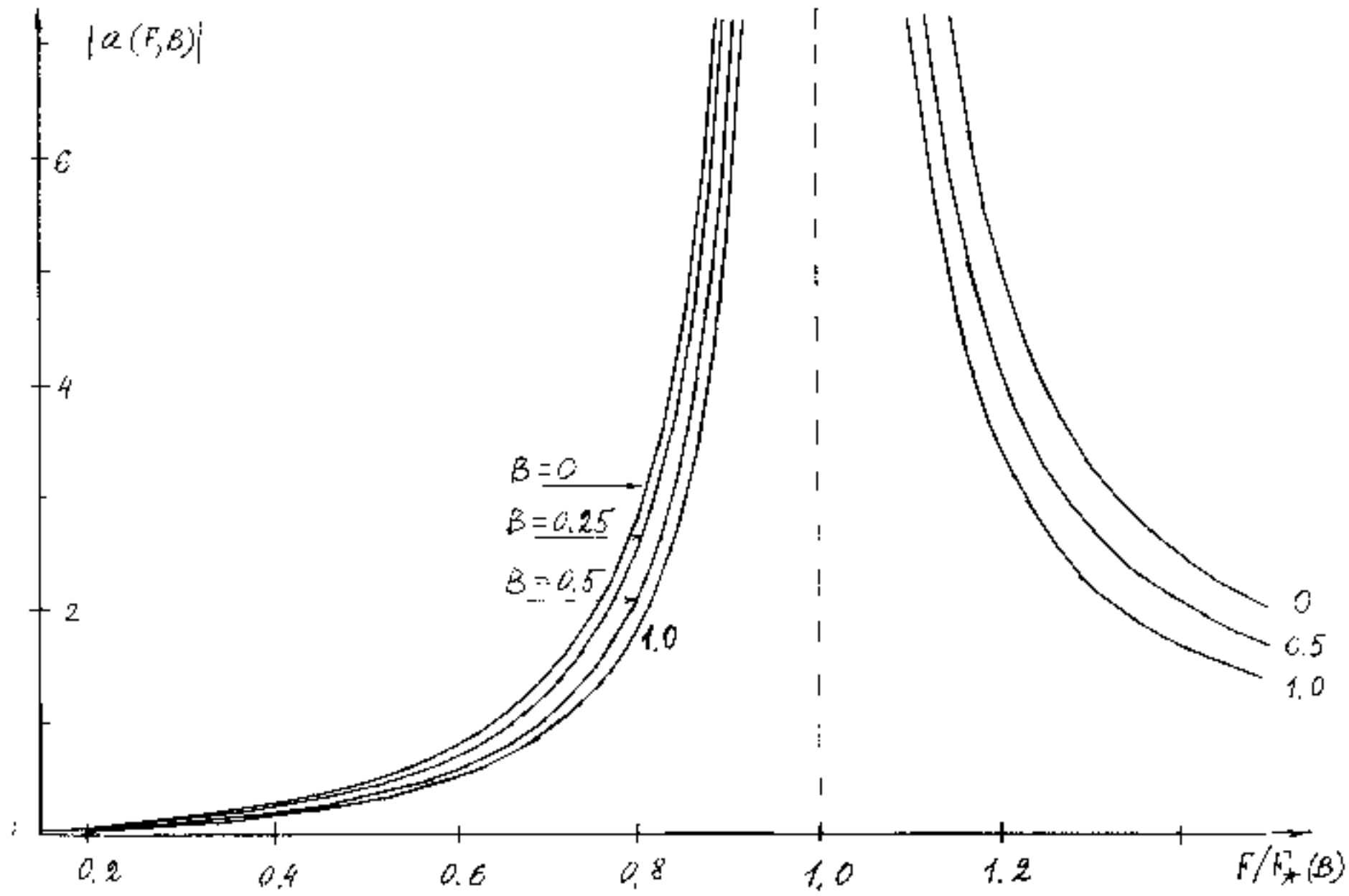

Fig. 4. The parameter $|a(F, B)|$ versus the ratio $F/F_*(B)$. The values of the reduced magnetic field B are shown besides the curves.

$$s_{jk}=(j\omega_1+k\omega_2)^{-1}\Bigg(u_{jk}-\tfrac{1}{2}\sum_{p=2}^{n-2}\sum_{q=0}^{p}[(q+1)\times(j-q+1)s_{q+1,l}s_{j-q+1,k-l}+(l+1)(k-l+1)s_{q,l+1}s_{j-q,k-l+1}]\Bigg) \qquad (18)$$

$(n=j+k\geqslant 3,\ l=p-q)$, from which the coefficients s_{jk} can be calculated subsequently. For example,

$$s_{03}=(3\omega_2)^{-1}u_{03},\quad s_{12}=(\omega_1+2\omega_2)^{-1}u_{12},$$
$$s_{21}=(2\omega_1+\omega_2)^{-1}u_{21},$$
$$s_{13}=(\omega_1+3\omega_2)^{-1}\times[u_{13}-2s_{12}(s_{21}+3s_{03})],\ \ldots. \qquad (17')$$

It is easy to obtain s_{jk} up to $n\sim 50$ with a computer, thus allowing one to use summation methods for divergent (or slowly convergent) series. So we proceed to a power series in one variable λ,

$$f(\lambda)\equiv S(\lambda x,\lambda y)=\sum_{n=0}^{\infty}f_n\lambda^n,$$

$$f_n=\sum_{j=0}^{n}s_{j,n-j}x^j y^{n-j} \qquad (19)$$

$(0<\lambda<1)$. Then the value $f(1)$ is calculated by Padé (PA) or Hermite–Padé (HPA) approximants.

The sub-barrier trajectory ends at the turning point $\boldsymbol{r}_2$, where the line $S=S_0$ contacts the isoenergetic surface $U=U_0$, and $\partial_x S=\partial_y S=0$. The derivatives $\partial_i S$ have a square root singularity at $\boldsymbol{r}=\boldsymbol{r}_2$, therefore the calculation of $\boldsymbol{r}_2$ with high precision requires some effort [2]. Table 2 illustrates the rapid convergence of the S values with growing order of approximation (N is the number of the coefficients f_n included into calculation). It is evident from Table 2, that both methods used are in full agreement, thus providing the accuracy $\sim 10^{-8}$ in the S_0 values.

Note that the series (16) for $S(x, y)$ should be summed at the isoenergetic surface σ, where the anharmonicity of the potential $U(x, y)$ is not small any more. The precise values of S_0 can be obtained only due to the availability of high-order coefficients s_{jk} with $n=j+k\gg 1$ and the application of the effective methods for the summation of series [3].

[3] For this purpose, we have used a special modification of the HPA, where the solution of the equations for $\boldsymbol{r}_2$ was obtained by a minimization procedure (calculation details will be published elsewhere).

5. If $\mathscr{E}=0$ or $\mathscr{H}=0$, the parameter a can be calculated analytically. Let us consider the Zeeman effect for the $(0, 0, n-1)$ states in a hydrogen atom. It is convenient to begin with the case of imaginary magnetic field, or the funnel-like potential $V(r)=-r^{-1}-\frac{1}{2}gr^2$, where $g=-\frac{1}{4}\mathscr{H}^2>0$. Using Eq. (3) and calculating the penetrability of the barrier in this potential, after some algebra we get

$$(2a)^{-1}=\frac{3^{1/2}(1-\frac{1}{2}z^2)}{(1-z^2)^{1/2}}\operatorname{arctg}\frac{3^{1/2}z}{2(1-z^2)^{1/2}}$$

$$-\operatorname{Arth}\frac{3z}{z^2+2}, \qquad (20)$$

$$z=(1+\sigma)^{1/2}$$

$$=1+\tfrac{3}{8}B^2-\tfrac{57}{128}B^4+\ldots, \qquad B\to 0,$$

$$=2-3\times 2^{-3/2}B^{-1/2}+O(B^{-1}), \quad B\to\infty,$$

where $\sigma=3(1-r_0)$ and $r_0(B)$ is the radius of the classical orbit determined by Eq. (10). Since $z>1$, the value of a for the Zeeman effect is obtained from Eq. (20) with the help of analytic continuation, the parameter $a(B)$ becomes complex and finite for all B. In particular, in the region of weak magnetic fields

$$a(B)=\pm i\frac{B}{\pi}+\frac{2}{\pi^2}B^2\ln B+\ldots, \quad B\to 0 \qquad (21)$$

and $|a|=\pi^{-1}B+O(B^2)$. The parameter $|a(B)|$ has a maximum at $B=B_m\approx 1.95$, where $|a(B_m)|=0.2133$. Note that $|a(\infty)|=1/2\pi=0.1592$, but the limit is achieved only in very strong magnetic fields,

$$a(B)=\pm\frac{i}{2\pi}\left(1+(2B)^{-1/2}\right.$$

$$\left.+\frac{i}{2^{3/2}\pi}B^{-1/2}\ln B+\ldots\right), \qquad (22)$$

$$|a(B)|=\frac{1}{2\pi}\left(1+(2B)^{-1/2}\right.$$

$$\left.+\frac{1}{16\pi^2}\frac{\ln^2 B}{B}+O(B^{-1}\ln B)\right),$$

$$B\to\infty \qquad (22a)$$

Note that the two signs in Eqs. (21), (22) correspond to the complex conjugate singularities, δ_0 and δ_0^*, of the Borel function, so the asymptotics of $\epsilon^{(k)}$ is of the type (2′).

If $\mathscr{H}=0$ (the Stark effect in hydrogen), then $a(F)$ is determined by Eqs. (16), (17) in Ref. [13].

6. Thus, the coefficients of the $1/n$-expansion $\epsilon^{(k)}$ grow as $k!$ at $k\to\infty$, and the series (1) is divergent (analogous to the well-known "Dyson phenomenon" for the usual perturbation series in quantum mechanics and field theory [17]). In many cases the asymptotical parameters (a, β, etc.) can be found analytically, otherwise the calculation of the sub-barrier trajectory by the "imaginary time" method can be applied for the purpose. The use of the above parameters in the summation of series (1) considerably enhances the accuracy of the calculations of the energy eigenvalues by the $1/n$-expansion, as can be shown with a number of examples. However, this question would require too much space, so we shall leave it till a more detailed publication.

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