Asymptotic form of higher orders of the $1/n$ expansion for multidimensional problems

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The asymptotic form of higher orders of the $1/n$ expansion is analyzed for multidimensional problems of quantum mechanics and atomic physics. Problems in which variables can and cannot be separated are discussed. Examples of the former are the molecular hydrogen atom and the Stark effect; an example of the latter is the hydrogen atom in electric and magnetic fields. The asymptotic form is always factorial. Its parameters can be calculated through a calculation of electron tunneling trajectories by the "imaginary time" method. Possible types of singularities of the asymptotic parameter a at the collision point of the classical solutions are determined.

1. INTRODUCTION

Although the $1/n$ expansion, also known as dimensional scaling, is still a new method in quantum mechanics and field theory, it has already found numerous applications (see, for example, Refs. 1–4). In particular, it has been applied successfully to the hydrogen atom in strong electric and magnetic fields,[5–8] the Yukawa and Hulthén potentials,[9,10] and the problem of two Coulomb centers (the molecular hydrogen ion H_2^+; Refs. 11–14). The present state of this method, various versions of it, and applications in the theory of atoms and molecules, quantum chemistry, etc., are discussed in a collection of papers.[4]

Interest has recently been attracted to the asymptotic form of higher orders of the $1/n$ expansion. In addition to being of theoretical importance, this topic is important for calculations on atomic states at a spectroscopic accuracy. This question has been studied by numerical methods[13,15] and also analytically.[14,16] In the present paper, which is a continuation of Ref. 14, we look at the asymptotic form of higher orders of the $1/n$ expansion for potentials which are not spherically symmetric.

Let us outline the paper. Section 2 contains the formulation of the problem and a brief discussion of results. Section 3 deals with the problem of two Coulomb centers (the molecular ion H_2^+) and compares our analytic expressions with numerical calculations.[13] Section 4 deals with the hydrogen atom in electric and magnetic fields. Using this example, we show that a calculation of an electron tunneling trajectory by the "imaginary time" method[17,18] also yields parameters of the asymptotic behavior in multidimensional problems, in which variables cannot be separated in the Schrödinger equation. The Stark effect and the Zeeman effect in the hydrogen atom are analyzed in Sec. 5. Section 6 contains a qualitative analysis of the singularities of the asymptotic parameter a near the collision point of the classical solutions ($\nu=\nu_*$ in the notation of Refs. 8 and 10). The results are briefly discussed in Sec. 7, which is the final section of this paper.

Technical details of the calculations and some of the lengthier equations are set aside in appendices. This paper uses atomic units.

2. ASYMPTOTIC FORM OF HIGHER ORDERS OF THE $1/n$ EXPANSION

The literature reveals various versions of dimensional scaling, which differ in certain details (e.g., the "displaced" $1/n$ expansion[4,9]). Below we discuss a version of this method which was proposed in Ref. 10 and which can be used for both a discrete spectrum and quasistationary states (resonances). Some corresponding examples can be found in Refs. 6 and 10. A similar approach was recently developed by Kais and Herschbach.[19]

The energy eigenvalues (which are complex in the case of quasistationary states: $E_{nl}=E_r-i\Gamma/2$) can be expanded in powers of the "small parameter" $1/n$:

$$\epsilon=2n^2E_{nl}=\epsilon^{(0)}+\frac{\epsilon^{(1)}}{n}+\ldots+\frac{\epsilon^{(k)}}{n^k}+\ldots, \tag{2.1}$$

where $n=n_r+l+1$ is the principal quantum number of the level ($n_r=0,1,2,\ldots$ is fixed; $l\to\infty$), ϵ is the "reduced" energy, and k is the order of the $1/n$ expansion. The coefficients $\epsilon^{(k)}$ can be calculated from recurrence relations which are convenient for numerical calculations. The results of numerical calculations of higher orders of the $1/n$ expansion, up to $k\sim 40$, are reported in Refs. 13 and 16.

For all problems discussed below, the asymptotic expression for $\epsilon^{(k)}$ is of the Dyson form:[20]

$$\epsilon^{(k)}\approx k!a^kk^b\left(c_0+\frac{c_1}{k}+\ldots\right), \quad k\to\infty, \tag{2.2}$$

or

$$\epsilon^{(k)}\approx k!k^b(a_c^kc_c+a_c^{*k}c_c^*)$$
$$\approx \text{const}\cdot\Gamma(k+b+1)\,|a_c|^k\cos(k\delta+\delta_0), \tag{2.3}$$

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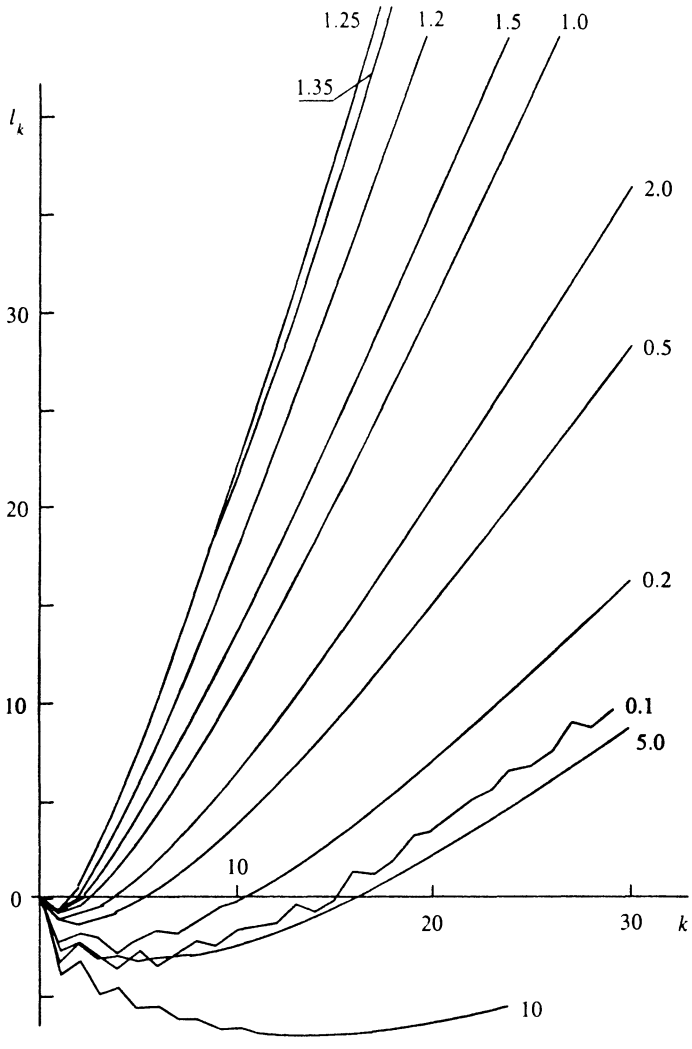

FIG. 1. Higher orders of the $1/n$ expansion for the problem of two centers with $Z_1=Z_2=1$ and $m=n-1$ (nodeless states). The curves are labeled with the values of the "reduced" distance $R[l_k=\log|\epsilon^{(k)}(R)|]$.

where a,b, etc., are some constants which can be calculated (a_c and c_c are complex; $\delta=\arg a_c$). The nature of the a symptotic behavior [i.e., Eq. (2.2) or (2.3)] may vary with a variation in the coupling constant or in other parameters of the problem; see Ref. 11 and especially Fig. 1.

For spherically symmetric potentials $V(r)$, the calculation of the asymptotic parameters a and c reduces to quadratures.[14,21] We begin our analysis of multidimensional problems with the case in which variables can be separated in the Schrödinger equation. We then move on (Sec. 4) to the general case, which requires a new approach.

3. THE PROBLEM OF TWO CENTERS

The nonrelativistic problem of two Coulomb centers,[22,23]

$$V(\mathbf{r})=-\frac{Z_1}{r_1}-\frac{Z_2}{r_2},$$
$$r_{1,2}=\sqrt{\rho^2+(z\pm R/2)},\quad \rho=\sqrt{x^2+y^2}, \tag{3.1}$$

is of interest in the theory of molecules, μ catalysis, etc. In this case the coefficients of the $1/n$ expansion in (2.1) depend on the internuclear distance R. The first term, $\epsilon^{(0)}$, corresponds to the energy of an electron in a classical orbit. We first consider the case $Z_1=Z_2=1$ (the molecular hydrogen ion) and the states with $m=n-1$ and $n\to\infty$ (or, equivalently, $n=1$ and $D\to\infty$, where D is the dimensionality of the space[12,13]). An equation for $\epsilon^{(0)}(R)$ follows in a straightforward way from the condition for an equilibrium of the forces acting on an electron in its proper frame of reference.[11] The first two terms of the $1/n$ expansion can be written in parametric form:

$$\epsilon^{(0)}=-2(1-\tau)^2(1+\tau),$$
$$\epsilon^{(1)}=2(1-\tau)^3[(1+3\tau)^{1/2}+(1-3\tau)^{1/2}-2], \tag{3.2}$$
$$\tilde{R}=\tau^{1/2}(1-\tau)^{-2}.$$

The succeeding coefficients $\epsilon^{(k)}$ can be calculated from recurrence relations. Here we have $0<\tau<1/3$ (these values correspond to $\tilde{R}<R_*=3^{3/2}\cdot 2^{-2}$), and the quantities $\epsilon=n^2E$ and $\tilde{R}=n^{-2}R$ are "reduced" values of the electron energy and of the distance between the Coulomb centers.

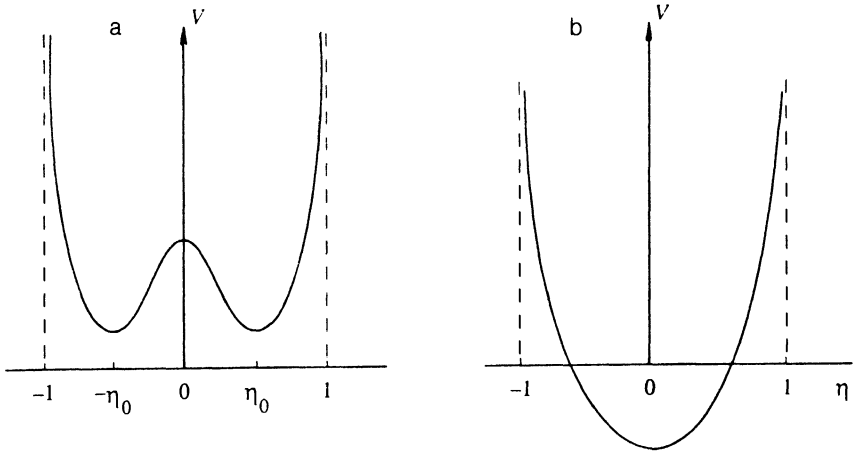

FIG. 2. Profile of the effective potential along the variable η in the problem of two centers with $Z_1=Z_2$. a) $R>R_*$; b) $R<R_*$.

For brevity we will be omitting the tilde from $\tilde{R}$ (for the ground term we have $n=1$, and the difference between $\tilde{R}$ and R disappears).

A numerical analysis[11,13] shows that we have $\epsilon^{(k)} \propto k!$ as $k\to\infty$. The asymptotic parameter a satisfies $a<0$ at $R<R_*$ and $a>0$ at $R>R_*$; $a(R)$ increases sharply as R approaches R_* (as is clear from Fig. 1). We will show that the R dependence of a can be derived in analytic form.

Transforming to the elliptical coordinates[22]

$$\xi=(r_1+r_2)/R, \quad \eta=(r_1-r_2)/R,$$

and carrying out the gauge transformation

$$E=\lambda\epsilon, \quad \tilde{R}=\lambda R, \quad \mathbf{r}=\lambda\mathbf{r},$$

$$\lambda=(m^2-1)^{-1}\approx n^{-2}, \tag{3.3}$$

$$\psi=[(\xi^2-1)(1-\eta)^2]^{-1/2}\chi_1(\xi)\chi_2(\eta)\exp(im\varphi),$$

we find one-dimensional Schrödinger equations of the type

$$\lambda^2 d^2\chi_1/d\xi^2+2[e-U(\xi)]\chi_1=0,$$

in which $\lambda\to 0$ plays the role of Planck's constant, and the effective energy e and the effective potentials U and V are given by

$$e=\tfrac{1}{4}\epsilon\tilde{R}^2=\tfrac{1}{4}\lambda ER^2,$$

$$U(\xi)=\frac{1}{2(\xi^2-1)^2}-R\frac{Z_+\xi-\beta}{\xi^2-1}, \tag{3.4}$$

$$V(\eta)=\frac{1}{2(1-\eta^2)^2}+R\frac{Z_-\eta-\beta}{1-\eta^2},$$

where $Z_\pm=(Z_1\pm Z_2)/2$, and β is a separation constant. At this point we set $Z_+=1$ and $Z_-=0$; these values correspond to the H_2^+ ion. We consider two cases.

1) $R>R_*=1.299\,038\ldots$. The potential $V(\eta)$ is a two-well potential (Fig. 2a) in which there are symmetric and antisymmetric states with slightly different energies (but with identical $1/n$ expansions). The $1/n$ expansion is constructed around one of the minima ($\eta=\pm\eta_0$ in Fig. 2a). Its divergence stems from the possibility that an electron will tunnel from one minimum to the other along an instanton trajectory. In this case, a summation of series (2.1) by the Borel method leads to $\Gamma/2$, the imaginary part of the energy, which is equal to the tunneling probability.[1)]

In the limit $n\to\infty$, with the quantum numbers $n_\xi=n_\eta=0$, the $1/n$ expansion for the energy leads to the equations

$$U(\xi_0)=V(\eta_0)=e, \quad U'(\xi_0)=V'(\eta_0)=0, \tag{3.5}$$

whose solution is

$$R=\frac{8\xi_0^3}{(\xi_0^2-1)(\xi_0^2+1)^2}, \quad \epsilon_0=-\frac{[(3\xi_0^2-1)(\xi_0^2+1)]^2}{32\xi_0^6},$$

$$\eta_0=\sqrt{\frac{3\xi_0^2-\xi_0^4}{3\xi_0^2-1}}=\sqrt{1-(-2e)^{-1/2}}, \tag{3.6}$$

$$e=-\frac{1}{2}\left(\frac{3\xi_0^2-1}{\xi_0^4-1}\right)^2, \quad \beta R=\sqrt{-2e},$$

as can be verified quite simply by direct substitution of these expressions into (3.5). Here ξ_0, $\pm\eta_0$ are the elliptical coordinates of the equilibrium classical orbit,[2)] and we have $1<\xi_0\leqslant\sqrt{3}$ and $-\infty<e<-1/2$. Since we have $V(\eta)-V(\eta_0)=-e[(\eta^2-\eta_0^2)/(1-\eta^2)]^2$, we can write (cf. Ref. 14)

$$\frac{1}{a}=2\int_{-\eta_0}^{\eta_0}|p_\eta|d\eta=4\left(\frac{\eta_0}{1-\eta_0^2}-\operatorname{Arth}\eta_0\right), \tag{3.7}$$

with the R dependence of η_0 being found from Eqs. (3.6). Assuming $\tau=\xi_0^{-2}$, we can write these equations in the simpler form

$$\eta_0=\sqrt{\frac{3\tau-1}{3\tau-\tau^2}}, \quad R=\frac{8\tau^{3/2}}{(1-\tau)(1+\tau)^2}, \quad \frac{1}{3}<\tau<1. \tag{3.8}$$

In particular, with $\tau=1/3$ we have $\xi_0=\sqrt{3}$, $\eta_0=0$, $R=R_*$, and $e=-1/2$. Expression (3.7) for the barrier transmission was derived in Ref. 12, but it was not pointed out there that this expression also determines the asymptotic parameter a.

In the limit $\eta\to 0$ we have

TABLE I. Borel parameter δ_0 for the molecular hydrogen ion.

$\frac{3}{2}\tilde{R}$	δ_0	Calculation method	$\frac{3}{2}\tilde{R}$	δ_0	Calculation method
0.2	−1.720 950	A	1.6	−0.052 563	A
0.4	−1.062 376	A	1.8	−0.013 569	A
0.6	−0.705 527	A	2.0	0.003 681	B
	≈−0.7	C	2.2	0.038 463	B
0.8	−0.474 800 620	A	2.4	0.089 708	B
	−0.474 795	C	3.0	0.294 164	B
1.0	−0.313 841 191	A	4.0	0.720 999	B
	−0.313 841 21	C	5.0	1.202 939	B
1.2	−0.197 516 621	A	7.0	2.253 090	B
	−0.197 516 618	C	10.0	3.943 259	B
1.4	−0.112 797	A			

Note. Here $\delta_0=(2a)^{-1}$, where a is the asymptotic parameter in (2.2). Calculation method A is based on Eq. (3.9), method B is based on Eq. (3.7), and method C is that of Ref. 13. For convenience in comparison with Ref. 13, we show values of $1.5\tilde{R}$, where $\tilde{R}$ is the reduced distance between the Coulomb centers.

$$V(\eta)-V(0)=\begin{cases}-[\sqrt{-2e}-1]\eta^2+\ldots, & e<-1/2,\\ \eta 4/2+\ldots, & e=-1/2,\\ (e+1/2)\eta^2+\ldots, & -1/2<e<0,\end{cases}$$

from which we see that the effective potential $V(\eta)$ changes in form at $R=R_*$.

2) $R<R_*$ (Fig. 2b). In this case we have $-1/2<e<0$ and

$$V(\eta)-V(0)=\frac{\eta^2}{(1-\eta^2)^2}\left[\frac{1}{2}+e(1-\eta^2)\right].$$

The point $\eta_0=0$ is thus an equilibrium point, and the turning points move out into the complex plane: $\eta_{1,2}^2=1+1/2e<0$. Hence

$$\frac{1}{a}=2^{3/2}\int_0^{\eta_1}\frac{\eta\sqrt{\eta_1^2-\eta^2}}{1-\eta^2}d\eta=-2(\mathrm{Arth}\,\zeta-\zeta), \quad (3.9)$$

where

$$\zeta=\sqrt{2e+1}=\frac{\sqrt{1-3\tau}}{1-\tau}, \quad 0<\tau<\frac{1}{3}, \quad (3.10)$$

and the parameter $\tau=\tau(\tilde{R})$ is defined as in (3.2). In contrast with the preceding case we have $a(R)<0$ here, and the stable classical orbit is symmetric: $\eta_0=0$, $r_1=r_2$. The variable τ has a simple geometric meaning: $\tau=\cos^2\alpha$, where α is the angle at a Z vertex of the triangle (Z,Z,e). From the equations above we find

$$\tau=\begin{cases}R^2-4R^4+22R^6-140R^8+\ldots, & R\to 0,\\ 1-2R^{-1}+4R^{-2}-7R^{-3}+\ldots, & R\to\infty,\end{cases} \quad (3.11)$$

$$a(R)=\begin{cases}-\dfrac{1}{2\Lambda}[1+(1-\ln 2)\Lambda^{-1}+O(\Lambda^{-2})], & R\to 0,\\ \dfrac{1}{2R}+\dfrac{\ln 2R}{2R^2}+O\left(\dfrac{(\ln R)^2}{R^3}\right), & R\to\infty,\end{cases} \quad (3.12)$$

where $\Lambda=-\ln R$. We also note that $a(R)$ has a power-law singularity as $R\to R_*$:

$$a(R)=A_\pm|h|^{-3/2}\{1+O(h)\}, \quad (3.13)$$

where $A_+=1/\sqrt{3}$, $A_-=-\sqrt{2/3}$, and $h=(R-R_*)/R_*\to\pm 0$.

Equations (3.7) and (3.9) completely determine[3)] the dependence of the parameter a on the internuclear distance R. Let us compare these equations with the results derived by Lopez-Cabrera *et al.*,[13] who calculated higher orders of the $1/D$ expansion for the molecular hydrogen ion. Using numerical methods, they studied the singularities of the Borel transform $F_B(\delta)$:

$$\sum_k \epsilon^{(k)}\delta^k=\int_0^\infty e^{-t}F_B(\delta t)dt, \quad \delta=\frac{1}{D}. \quad (3.14)$$

If the singularity closest to zero is at the point $\delta=\delta_0$ and is of the form $F_B(\delta)\propto(\delta_0-\delta)^{-\rho}$, then we have $\epsilon^{(k)}\propto k!(2\delta_0)^{-k}k^{\rho-1}$ as $k\to\infty$. We thus have the following relationships between parameters:

$$a=\frac{1}{2\delta_0}, \quad b=\rho-1, \quad n=\frac{D-1}{2}. \quad (3.15)$$

In addition, the gauge transformation used in Ref. 13 differs from (3.3), so the numerical value of the reduced distance R in Ref. 13 differs from that in the present paper by a factor of 1.5. The region $R<R_*$ was studied in Ref. 13, and it was shown by numerical methods that we have $\delta_0(R)<0$ and $\rho=-1/2$ in this region. These results correspond to a square-root branch point in the Borel transform. As can be seen from Table I, the values of the Borel parameter δ_0 given in Ref. 13 (they were calculated by the method of quadratic Padé–Hermite approximants) are in complete agreement with the analytic expression (3.9). Table I also shows several values of δ_0 for the region $R>R_*$,

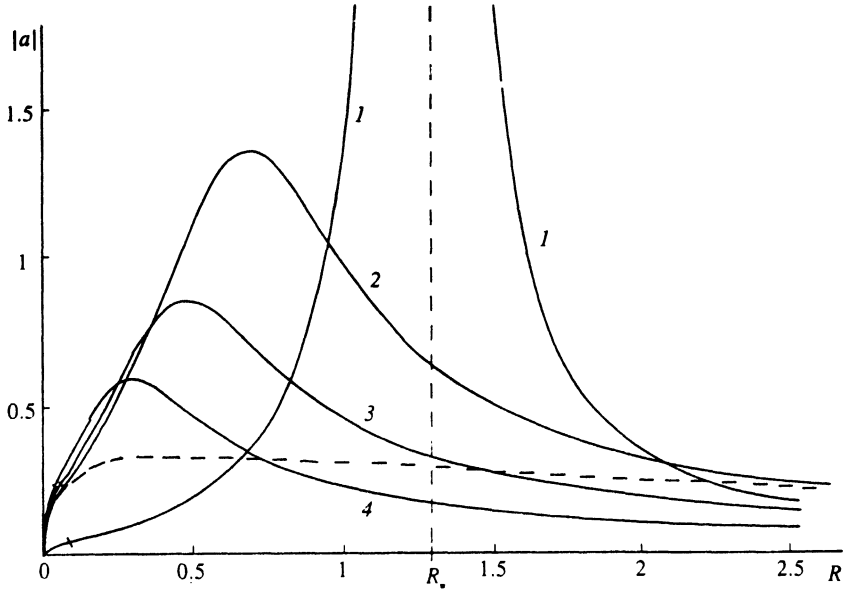

FIG. 3. The parameters $|a|$ (solid curves *1–4*) and $|a_c|$ (dashed curve) versus the internuclear distance R. Here we have $Z_1=1$ in all cases. *1,2,3,4*—$Z_2=1,1.5,2,3$, respectively; dashed curve: $Z_1=Z_2=1$. For curve *1*, the ordinate scale has been changed by a factor of 5; i.e., values of $0.2\,|a(R)|$ are plotted.

for the case in which the singularity of the Borel transform $F(\delta)$ lies on the positive semiaxis, so that series (2.1) is no longer sign-varying. The effect is to complicate the summation of this series by ordinary methods.

To conclude this section of the paper, we note that in addition to the turning points in the coordinate η which we discussed above, there are also some turning points in ξ. Since the potential $U(\xi)$ has a unique minimum $\xi=\xi_0$ in the interval $1<\xi<\infty$, these points can either be complex or lie in the nonphysical region $\xi<1$. As a result, the possibility of tunneling in the potential $U(\xi)$ leads to a complex parameter a_c and to the appearance of terms like (2.3) in the asymptotic behavior. The details are in Appendix A.

The results calculated for the asymptotic parameters a and a_c are shown in Fig. 3, from which we see that we have $|a|>|a_c|$ for $R>0.0858$. The contribution of the complex singularity at $\delta_c=1/2a_c$ to the asymptotic behavior of $\epsilon^{(k)}$ becomes significant at $R\lesssim 0.2$, where it is manifested in oscillations of the coefficients of the $1/n$ expansion with increasing k [see (2.3)]. Oscillations of this sort have indeed been observed in numerical calculations of $\epsilon^{(k)}$ both at $R\leqslant 0.2$ and at $R\gtrsim 5$ (see Fig. 1 and Ref. 11).

4. THE HYDROGEN ATOM IN EXTERNAL FIELDS; THE IMAGINARY-TIME METHOD

The problem of the hydrogen atom in an electric field $\mathscr{E}$ and a magnetic field $\mathscr{H}$ is more complicated. In this problem, variables cannot be separated in the Schrödinger equation. We assume that the fields are uniform and parallel, and we consider states with magnetic quantum number $m=n$—1. These are the states which are closest to classical mechanics in the limit $n\to\infty$ (Ref. 27). Higher-order perturbation theories for this problem are discussed in Ref. 28.

The $1/n$ expansion is constructed around the classical orbit, whose radius $r_0=r_0(F,B)$ is found from the equation[4)]

$$r(1-F^2r^4)^2(1+\tfrac{1}{4}B^2r^3)=1. \tag{4.1}$$

Here $F=n^4\mathscr{E}$; $B=n^3\mathscr{H}$; and F, B, and r are "reduced" variables. We should take that root of Eq. (4.1) which becomes equal to unity when the external fields are turned off:

$$r_0(F,B)=1+2F^2-\tfrac{1}{4}B^2+\ldots .$$

It can be shown (Appendix B) that the effective potential $U(\rho,z)$ for this problem has a minimum (which corresponds to a point of stable equilibrium, r_0) only in weak magnetic fields, $F<F_*(B)$. At $F=F_*$, the barrier disappears from the potential $U(\rho,z)$. Following Ref. 6, we call this field the "classical ionization threshold." For the calculation of $F_*(B)$ we note that at $F=F_*(B)$ the two roots of Eq. (4.1) coalesce. Hence we find the dependence of F_* on B, which can be conveniently written in parametric form $(0<u<1)$:

$$\begin{aligned} F_*&=2^{12}\cdot 3^{-9}\sqrt{1+2u}\,(1-\tfrac{1}{4}u)^6(1-u)^{-2},\\ B&=2^9\cdot 3^{-11/2}\sqrt{u}\,(1-\tfrac{1}{4}u)^{9/2}(1-u)^{-2}. \end{aligned} \tag{4.2}$$

In particular, with $u=0$ we have

$$\begin{aligned} &F_*(0)=2^{12}\cdot 3^{-9}=0.2081, \quad B=0,\\ &r_*=3^4\cdot 2^{-6}=1.2656 \end{aligned} \tag{4.3}$$

[these values correspond to the Stark effect in the hydrogen atom for Rydberg states (0,0,n—1) with $n\gg 1$]. The other limiting case $u\to 1$ corresponds to an ultrastrong magnetic field; the asymptotic expression for $F_*(B)$ is given in Appendix B [Eq. (B6)]. A calculation from (4.2) yields the curve in Fig. 4 for $F_*(B)$. The magnetic field stabilizes the classical orbit, so $F_*(B)$ increases along with B.

At $F>F_*(B)$, the radius of the orbit and the coefficients $\epsilon^{(k)}$ of the $1/n$ expansion become complex. Such a solution has no physical meaning in classical mechanics, but when we go over to quantum mechanics it is specifi-

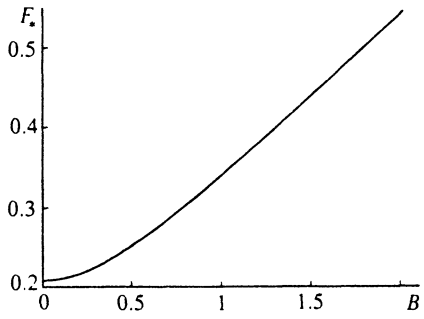

FIG. 4. The critical field F_* (atomic units).

cally this solution which makes it possible to describe (within the framework of a $1/n$ expansion) not only the shift but also the width of the quasistationary levels in a strong field.[10]

Let us examine the asymptotic form of higher orders of the $1/n$ expansion. To determine the parameter a in (2.2) we use the imaginary-time method, which was developed previously for calculating the probability of particles tunneling through an oscillating barrier. This method has been used in the theory of multiphoton ionization of atoms and ions by the field of an intense light wave[17,18] and also in the problem of e^+e^- pair creation from vacuum in a variable electric field.[30] It was also applied to steady-state problems in Ref. 31.[5)] For $0<F<F_*$ we have

$$a=\frac{1}{2\,\mathrm{Im}\,S},\quad S=\int_{\mathbf{r}_0}^{\mathbf{r}_2}\mathbf{p}d\mathbf{r}=\int_0^\infty \mathbf{r}^2dt, \tag{4.4}$$

where the action S is calculated along a tunneling trajectory which connects the minimum of potential (B2), $\mathbf{r}_0=(\rho_0,z_0)$, with the turning point $\mathbf{r}_2$, which lies on the constant-energy surface σ: $U(\mathbf{r})=U(\mathbf{r}_0)$. Here we have $\dot{\mathbf{r}}_0=\dot{\mathbf{r}}_2=0$ (this condition singles out from the bundle of classical trajectories that for which $\mathrm{Im}\,S$ reaches a minimum;[18] this circumstance determines the exponential factor in the tunneling probability and thus the asymptotic parameter a). The σ surface is the boundary of the classically allowed region, and the electron trajectory which we are seeking is analogous to an instanton tunneling trajectory. Since the potential U is quadratic in $\mathbf{r}$—$\mathbf{r}_0$ near $\mathbf{r}_0$, the time of motion of the particle along this trajectory is infinite. This circumstance is reflected in (4.4).

A tunneling trajectory satisfies the classical equations of motion but with an imaginary time $t=i\tau$. In the numerical integration it is convenient to treat the variable τ as a "physical" time,

$$\frac{d^2\mathbf{r}}{d\tau^2}=-\nabla\tilde{U},\quad \tilde{U}=-U \tag{4.5}$$

(the potential changes sign in the process), and to integrate this equation starting from some point $\mathbf{r}_2'\in\sigma$. In varying $\mathbf{r}_2'$, we need to ensure that the trajectory ends at the point of the minimum, $\mathbf{r}_0$.

Figure 5 shows a contour map of the effective potential $\tilde{U}(\rho,z)$. We see that the tunneling trajectory runs along the crest of the potential $\tilde{U}$ on which the saddle point $s=(\rho_s,z_s)$ lies. The potential $\tilde{U}$ is approximated near $\mathbf{r}_0$ by an "inverted-oscillator potential," so all trajectories are unstable.

The trajectories in Fig. 5 correspond to the initial excursions $\Delta\rho=\rho_2'-\rho_2$ shown in Table II. Because of the exponential instability of the trajectory, an excursion $\Delta\rho\sim10^{-6}$ grows to a size visible to the eye as the point $\mathbf{r}_0$ is approached. It is not possible (in the numerical calculation) to go from $\mathbf{r}_2'$ to $\mathbf{r}_0$ in the literal sense. Accordingly, the integral in (4.4) is evaluated from $\mathbf{r}_2'$ to the point $(\mathbf{r}_m)$

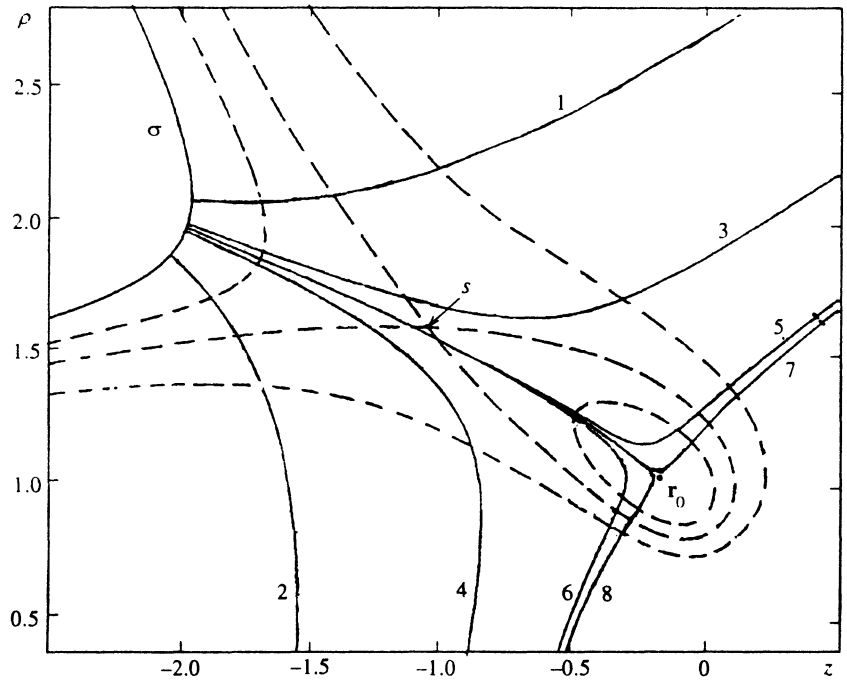

FIG. 5. Tunneling trajectories in the "imaginary time" method. Solid curves *1–8*—Classical trajectories, with the parameter values in Table II; dashed curves—constant-energy surfaces for potential (B2); *s*—saddle point. Here $F=0.15$ and $B=0.2$.

TABLE II. Parameters of tunneling trajectories.

No.	$\Delta\rho$	$F=0.15,\ B=0.2$			$F=0.5,\ B=2$		
		Δr	Im S	τ	Δr	Im S	τ
1	0.1	1.40	0.34	6.16	0.871	0.019	0.65
2	−0.1	1.40	0.42	4.92	1.03	0.061	0.55
3	0.01	0.692	0.393	8.35	0.651	0.045	1.62
4	−0.01	0.675	0.412	7.80	0.634	0.066	1.55
5	10^{-4}	0.135	0.40106	11.35	0.356	0.0813	3.45
6	-10^{-4}	0.134	0.40126	11.24	0.348	0.0869	3.39
7	10^{-6}	0.0247	0.4011264	13.93	0.146	0.08793	4.97
8	-10^{-6}	0.0246	0.4011278	13.91	0.145	0.08836	4.93
—	10^{-8}	0.0045	0.40112688	16.45	0.0526	0.088423	6.36
—	-10^{-8}	0.0045	0.40112689	16.45	0.0526	0.088438	6.35
—	≈ 0	≈ 0	0.40112688	≈ 20	≈ 0	0.088444	≈ 8.5

Note. Here $\Delta r = |\mathbf{r}_m - \mathbf{r}_0|$, τ is the time it takes the particle to move from the point $\mathbf{r}_2'$ to $\mathbf{r}_0$, and $\mathbf{r}_m$ is the point of the trajectory which is closest to $\mathbf{r}_0$. Here Nos. 1–8 correspond to the case $F=0.15$, $B=0.2$, and the corresponding trajectory numbers in Fig. 5.

at which the trajectory comes closest to the point $\mathbf{r}_0$. With increasing field B, and as F approaches $F_*(B)$, the trajectories become more unstable, since the crest of the potential $U(\rho,z)$ becomes progressively sharper.

Figure 6 shows the results calculated for the asymptotic parameter $a=a(F,B)$ as a function of the ratio F/F_* [numerically, we have $F_*(B)=0.2081$, 0.2532, and 0.3449 for $B=0$, 0.5, and 1.0, respectively]. As in the other cases, we find $a\to\infty$ as $F\to F_*$. A numerical analysis shows that the "critical exponent" of the singularity in $a(F,B)$ does not depend on B and that it has a value of $-5/4$ [cf. (5.12)] as in the Stark effect.

The calculation method described above is valid if the tunneling trajectory is real (after transformation to the imaginary time τ), with the consequence that the asymptotic parameter a has real values. In the case at hand, the situation corresponds to the region $0<F<F_*(B)$. At $F>F_*$, the turning points $\mathbf{r}_0$ and $\mathbf{r}_2$ and the tunneling trajectory become complex, complicating the numerical calculations. Although it appears that no difficulties of a fundamental nature arise here,[6)] a calculation of a in the region $F>F_*(B)$ by the imaginary-time method requires further research. The corresponding curves in Fig. 6 were constructed by other methods: in the case $B=0$, they were constructed from analytic expression (5.9), while in the case with a magnetic field (the dashed curves) they were calculated through a numerical analysis of higher orders of the $1/n$ expansion (cf. Ref. 16).

As $F\to 0$, the stopping point $\mathbf{r}_2$ goes off to infinity. However, there is a pair of complex-conjugate turning

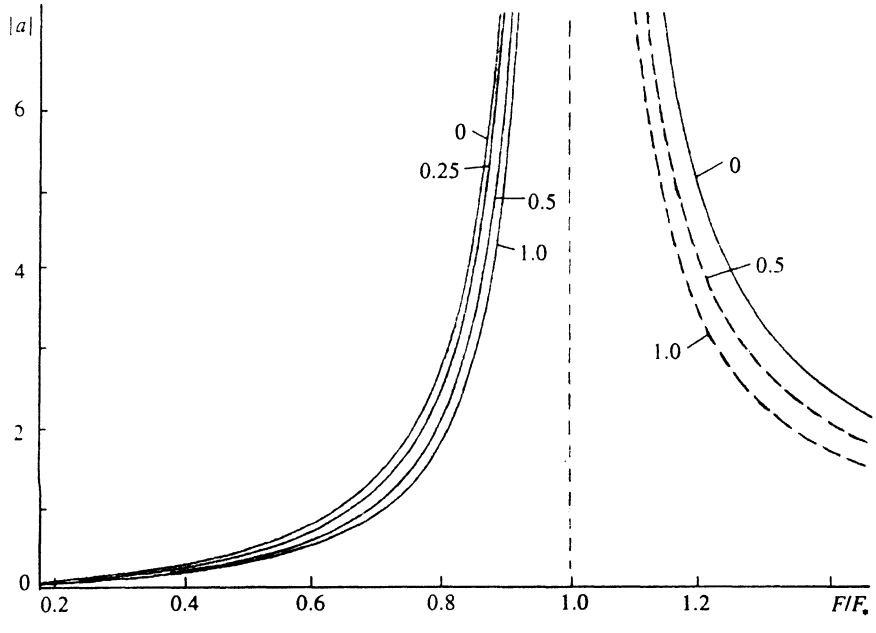

FIG. 6. Asymptotic parameter $a(F,B)$ as a function of F/F_*, where $F^*(B)$ is given in Fig. 4. The curves are labeled with the value of the magnetic field $B=n^3\mathscr{H}$. Curves with $F<F^*$ have been calculated by the imaginary-time method; those with $F>F^*$ were calculated using other methods, as indicated in the text.

points, so we have the characteristic asymptotic behavior in (2.3) and complex values of the parameter $a(B)$ (see the following section of this paper).

5. ZEEMAN AND STARK EFFECTS

If one of the fields ($\mathscr{E}$ or $\mathscr{H}$) is zero, the asymptotic form of the coefficients $\epsilon^{(k)}$ can be found analytically.

We begin with the case $\mathscr{H}=0$. To calculate the parameter a, we change the sign of B^2 in effective potential (B2); i.e., we go over to an imaginary magnetic field. By virtue of the symmetry of the problem, we can restrict the discussion to tunneling trajectories which lie in the plane $z=0(\rho\equiv r)$. The problem thus reduces to a one-dimensional problem:

$$V(r)=-\frac{1}{r}-\frac{1}{2}gr^2, \quad g=\frac{1}{4}\mathscr{H}^2. \tag{5.1}$$

In this case the turning points r_0 and r_2 are real, and a calculation of the barrier transmission yields

$$a=\frac{1}{2}\left[\frac{\sqrt{3}(1-z^2/2)}{\sqrt{1-z^2}}\operatorname{arctg}\frac{\sqrt{3}z}{2\sqrt{1-z^2}}-\operatorname{Arth}\frac{3z}{z^2+2}\right]^{-1}, \tag{5.2}$$

where $z=\sqrt{4-3r_0}$, and $r_0=r_0(\lambda)$ is found from the equation

$$r=1+\lambda r^4, \quad \lambda=n^6g=\tfrac{1}{4}B^2. \tag{5.3}$$

Here B is the reduced magnetic field [see (4.1)], and we have $1<r_0<\infty$. The value $\lambda=\lambda_*=27/256$ or $B=B_*=3^{3/2}\cdot 2^{-3}=0.6495$ corresponds to the collision of the two classical solutions (in this case we have $r_0=4/3$, $z\to 0$, and $a=\frac{10}{3}z^{-5}+\ldots\to\infty$).

To go from (5.2) to the corresponding expression for the Zeeman effect, we need to change the sign of the coupling constant (g and λ). In this case, $r_0(\lambda)$ remains real, and the variable z changes from 1 to 2:

$$r_0=1-\lambda+4\lambda^2+\ldots, \quad z=1+\tfrac{3}{2}\lambda-\tfrac{57}{8}\lambda^2+\ldots, \quad \lambda\to 0,$$

$$r_0=\lambda^{-1/4}-\tfrac{1}{4}\lambda^{-1/2}+\ldots, \quad z=2-\tfrac{3}{4}\lambda^{-1/4}+\ldots, \quad \lambda\to\infty.$$

In this case there is no collision of solutions. Noting that we have $\operatorname{Arth}[3z/(z^2+2)]=\operatorname{Arth} z+\operatorname{Arth}(z/2)$, we find

$$\operatorname{Arth}\frac{3z}{z^2+2}=\operatorname{Arth}\frac{z^2+2}{3z}\pm i\frac{\pi}{2}, \quad 1<z<2, \tag{5.4}$$

where the plus and minus signs correspond to the upper and lower edges of the cut. Similarly, we find

$$u=\frac{\sqrt{3}z}{2\sqrt{1-z^2}}=\pm iv^{-1},$$

$$u\operatorname{arctg}u=-v^{-1}\left(\operatorname{Arth}v\pm i\frac{\pi}{2}\right), \tag{5.5}$$

where

$$v=\frac{2}{\sqrt{3}}\frac{\sqrt{z^2-1}}{z}, \quad 0<v<1.$$

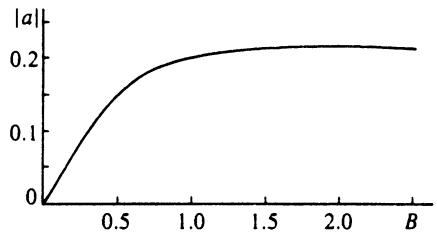

FIG. 7. Plot of $|a(B)|$ for the Zeeman effect in the hydrogen atom.

Substituting these expressions into (5.2), we find an explicit expression for the parameter $a(B)$, which is complex [see (B8)]. The two possible signs of the imaginary part correspond to two complex-conjugate branch points, δ_0 and δ_0^*, of the Borel transform; as a result, we find the asymptotic behavior in (2.3).

The dependence of $|a|$ on the field B is shown by the curve in Fig. 7, which has a maximum at $B=B_m\approx 1.95$; here we have $|a(B_m)|=0.2133$. In the strong-field limit we have $|a(\infty)|=1/2\pi=0.1592$, but this limit is reached very slowly:

$$|a(B)|=\frac{1}{2\pi}\left[1+\frac{1}{\sqrt{2}}B^{-1/2}-\frac{1}{16\pi^2}B^{-1}\ln^2 B+O\left(\frac{\ln B}{B}\right)\right]. \tag{5.6}$$

(See Appendix B.) This result explains the shape of the curve in Fig. 7.

We turn now to the Stark effect ($B=0$). The probability for the ionization of a hydrogen atom in a weak electric field is[22,33]

$$\Gamma(\epsilon)=C_{n_1n_2m}F^{-p}\exp(-2n/3F),$$
$$C_{n_1n_2m}=(4n)^p e^{3(n_1-n_2)}/n_2!(n_2+|m|)!n^3, \tag{5.7}$$

where $n=n_1+n_2+|m|+1$, $p=n-n_1+n_2=2n_2+|m|+1$, and n_1, n_2, and m are parabolic quantum numbers. Using Stirling's formula, we find

$$a(F)=\frac{3}{2}F-\frac{9p}{4n}F^2\ln F+O(F^2), \tag{5.8}$$

$$\beta=\begin{cases}-2, & n_2\gg 1 \text{ (arbitrary } m),\\ n_2-3/2, & n_2\sim 1,\ m\gg 1,\\ 2n_2+|m|-1, & n_2,m\sim 1\end{cases} \tag{5.9}$$

[the exponent β in (2.2) thus depends on the quantum numbers].

In the semiclassical approximation it is a simple matter to write the barrier transmission [and thus the parameter $a(F)$] for all fields $F<F_*$ and for an arbitrary state (n_1,n_2,m). However, a rather complicated elliptic integral arises in the process. Let us consider states $(0,0,n-1)$ with

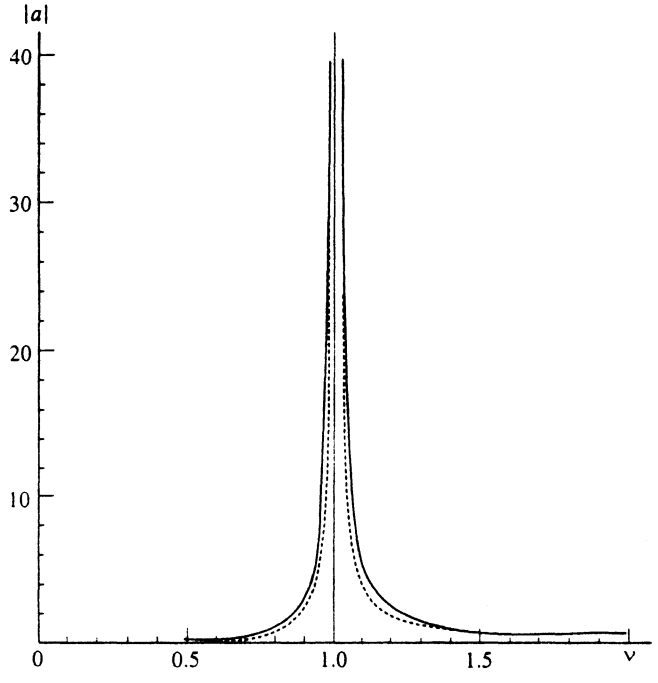

FIG. 8. Plot of $|a|$ versus $\nu=\sqrt{F/F_*}$ for the case of the Stark effect in the hydrogen atom ($F_*=0.2081$, solid curve) and corresponding spherical model ($F_*=0.1481$, dashed curve).

$n\gg 1$, for which the two turning points coalesce ($r_0=r_1$), so this integral can be expressed in terms of elementary functions:

$$a=\frac{1}{2}\left[z+\frac{z^3}{3(1-z^2)}-\operatorname{Arth} z\right]^{-1}, \tag{5.10}$$

where

$$z=\sqrt{1-3\tau}(1-\tau)^{-1}, \quad \tau(1-\tau^2)^4=F. \tag{5.11}$$

Corresponding to the interval $0<\tau<1/3$ are values $a(F)>0$. At $\tau=1/3$ or $F=F_*=2^{12}\cdot 3^{-9}$, the two classical solutions collide, and we find

$$a(F)=Af^{-5/4}(1+bf^{1/2}+b_1f+\ldots), \quad f=\frac{F-F_*}{F_*}\to 0, \tag{5.12}$$

where

$$A=5\cdot 2^{-3/4}\cdot 3^{-3/2}=0.5772, \quad b=-0.4770,\ldots .$$

At $F>F_*$, the quantities τ and a become complex. On the whole, the behavior of the parameter a with increasing F is the same as for a short-range potential (cf. Refs. 14 and 15 and Fig. 8 of the present paper).

6. NATURE OF THE SINGULARITY IN THE ASYMPTOTIC PARAMETER *a*

As we mentioned above, at $\nu>\nu_*$ the equilibrium point $x_0(\nu)$ about which the $1/n$ expansion is constructed migrates into the complex plane, and the effective potential U does not have a minimum at real values $0<x<\infty$. This situation is modeled by the following example:

$$U(x)=U_0+\alpha q-\tfrac{1}{3}\beta q^3, \tag{6.1}$$

where $q=x-(2x_0+x_2)/3$, and x_0 and x_2 are turning points. The quantity $a\propto\nu_*-\nu$ vanishes at $\nu=\nu_*$; $\beta>0$ is a coefficient of order unity. Setting $q=(\alpha/\beta)^{1/2}\xi$, we have

$$U=U_0+\alpha^{3/2}\beta^{-1/2}\left(\xi-\frac{1}{3}\xi^3\right), \quad \frac{1}{a}=2\int_{q_0}^{q_2}|p|\,dq=c_1\alpha^{5/4}, \tag{6.2}$$

where the numerical value of the constant $c_1>0$ is not important for our purposes (the tunneling region corresponds to $-1<\xi<2$, and the maximum of the potential to $\xi=\xi_m=1$). In (6.2) we used $E=U(q_0)=U(q_2)$.

The oscillation frequency of the particle about the point q_0 is $\omega=(4\alpha\beta)^{1/4}$. In the limit $\nu\to\nu_*$ we thus have

$$\omega\propto(\nu_*-\nu)^{1/4}, \quad a\sim(\nu_*-\nu)^{-5/4}. \tag{6.3}$$

These results were derived in Ref. 14 by a less transparent method. The frequency ω vanishes as $\nu\to\nu_*$, indicating that the equilibrium point becomes unstable.

Equations (5.3) describe the most typical situation, but we can also look at the more general case

$$U=U_0+\alpha q-\frac{q^N}{N}, \quad \alpha\propto\nu_*-\nu, \tag{6.4}$$

where $N=3,5,\ldots$ is an odd number [in this case the potential has an inflection point at $\nu=\nu_*$, as for (6.1)]. Here we always have $\xi_0=-1$ and $\xi_m=1$, but ξ_2 depends on N. Repeating the calculations, we find

$$\omega\propto(\nu_*-\nu)^{N-2/2(N-1)}, \qquad a\propto(\nu_*-\nu)^{-N+2/2(N-1)}, \quad \nu\to\nu_*. \tag{6.5}$$

With increasing N, the singularity of $a(\nu)$ becomes weaker; we have $a(\nu)\propto\omega^{-1}\propto(\nu_*-\nu)^{-1/2}$ at $N\gg 1$. The classical energy has a branch point here,

$$\epsilon^{(0)}(\nu)=\epsilon_*+c_1(\nu_*-\nu)-c_2(\nu_*-\nu)^{N/N-1}+\ldots, \tag{6.6}$$

and it becomes complex at $\nu>\nu_*$ (Appendix C). In the usual case we would have $N=3$, and the exponents of the singularities in (6.5) and (6.6) would be $-5/4$ and $3/2$, respectively.[10,14]

For the problem of two Coulomb centers with $R=R_*$, there is a collision of three (rather than two) classical orbits; two of the three are stable, and the third is unstable.[11] This situation is described by the potential

$$U=U_0-\frac{1}{2}\alpha q^2+\frac{\beta}{N}q^N, \tag{6.7}$$

where $\alpha\propto\nu_*-\nu\to 0$, $\beta\sim 1$, and $N=4,6,8,\ldots$. As above, we set $q=(\alpha/\beta)^{1/N-2}\xi$; then $\xi_0=-1$ and $\xi_2=1$ are turning points, and we find

$$\omega=\sqrt{(N-2)\alpha},$$

$$p^2=-\frac{2}{N}\alpha^{N/N-2}\beta^{-2/N-2}(1-\xi^2)^2Q_N(\xi),$$

where $Q_4=1$, $Q_6=\xi^2+2$, $Q_8=\xi^4+2\xi^2+3$ etc. Hence

$$\omega \propto \sqrt{\nu_*-\nu}, \quad a \propto (\nu_*-\nu)^{-N+2/2(N-2)}, \quad \nu \to \nu_*. \tag{6.8}$$

For the problem of two centers we have $N=4$ and $a \propto (\nu_*-\nu)^{-3/2}$. We see that these results correspond to Eq. (3.13) when we note that the role of the parameter ν is being played by the internuclear distance R.

Finally, we consider the following question. The coefficients in conventional perturbation theory in powers of the coupling constant g can grow as $E_k \propto (k\alpha)!a^k$ with arbitrary $\alpha>0$. For the anharmonic one-dimensional oscillator

$$V(x)=\tfrac{1}{2}x^2+gx^N, \quad -\infty<x<\infty, \tag{6.9}$$

for example, we have[34,35] $\alpha=(N-2)/2$. The divergence of the $1/n$ expansion is always factorial; i.e., we have $\alpha=1$. What is responsible for this difference between the higher orders of perturbation theory and of the $1/n$ expansion?

As we know,[22] the formal parameter of the semiclassical expansion is Planck's constant $\hbar$, which goes over to $1/n$ in the final equations. Assuming analyticity in $1/n$, noting that the barrier transmission (to exponential accuracy) is

$$\Gamma \propto \exp\left(-\frac{2}{\hbar}\int |p|\,dq\right) \to \exp\left(-\frac{n}{a}\right), \tag{6.10}$$

and using the dispersion relations, we find[14] $\epsilon^{(k)} \propto k!a^k$ as $k\to\infty$. We thus always have $\alpha=1$ in the case of the $1/n$ expansion.

7. CONCLUSION

The $1/n$ expansion method has several features which distinguish it favorably from other methods—in particular, perturbation theory. Among these features are its close relationship with classical mechanics, its applicability to complicated problems with nonseparable variables, and the fact that just the first few terms of the $1/n$ expansion are often sufficient for highly accurate calculations of energies[10–13] and wave functions[36] (in particular, for nodeless states; this result can be explained by the theory of coherent states[27]).

On the other hand, one can also point out cases in which it is necessary to evaluate dozens of coefficients $\epsilon^{(k)}$ and to sum series (2.1) in order to calculate level energies accurately enough for comparison with experiment. In particular, this is the situation when F is close to F_* (for the Stark effect in a strong field[6]). In such cases, the asymptotic form of the coefficients $\epsilon^{(k)}$ as $k\to\infty$ becomes important: knowledge of this asymptotic form can be utilized to choose a suitable summation method and thus to improve the accuracy of energy calculations.

It has been shown in this paper that the asymptotic form of the higher orders of the $1/n$ expansion is factorial (by analogy with "Dyson's phenomenon"[20] for ordinary perturbation theory), and in many cases its parameters can be found analytically. For problems in which variables cannot be separated, as in the many-body problem, analytic calculations are hardly possible, but in such cases one can find the parameter a in (2.2) by calculating the tunneling trajectory of the particle by the imaginary-time method.

We wish to thank V. D. Mur for a useful discussion of these results and M. N. Markina for assistance in putting the manuscript together.

APPENDIX A

To evaluate the parameter a_c in (2.3), we work from an equation analogous to (3.7):

$$\frac{1}{a_c}=2^{3/2}\int_{\xi_0}^{\xi_1}[U(\xi)-U(\xi_0)]^{1/2}d\xi, \tag{A1}$$

where $\xi=(r_1+r_2)/R$, ξ_0 is the location of the absolute minimum of the potential $U(\xi)$ $(1<\xi_0<\infty)$, and ξ_1 is a turning point, which can lie either in the nonphysical region $\xi<1$ or in the complex plane. In either case the parameter a_c is complex.

Assuming $R<R_*$ we have $\xi_0=\tau^{-1/2}$ and $\eta_0=0$ [since the potential $V(\eta)$ has a minimum at the origin] and thus

$$U(0)=V(0)=\frac{1}{2}-\beta R=-\frac{\tau(1+\tau)}{2(1-\tau)^2}.$$

The variable $\tau=\tau(R)$ is found from (3.2); it ranges from 0 to 1/3. According to (3.5) we have $U(\xi_0)=V(0)$ and thus $\xi_1=0$. Hence

$$\frac{1}{a_c}=\frac{2\sqrt{\tau^2+\tau}}{1-\tau}\int_0^{\xi_0}\frac{\xi_0-\xi}{\xi^2-1}\sqrt{\xi^2+\frac{2\xi_0}{\xi_0^2+1}}\,\xi\,d\xi$$

$$=\frac{2}{(1-\tau)\sqrt{1+\tau}}[\operatorname{Arth} u_1-\sqrt{(1+\tau)(1+3\tau)}]$$

$$-\operatorname{Arth} u_2 \pm i\pi, \tag{A2}$$

where $u_j=\sqrt{1-w_j^2}$,

$$w_1=\frac{\tau}{(1+2\tau)}, \quad w_2=\frac{\tau(1-\tau)}{(2+5\tau+\tau^2)}. \tag{A3}$$

The imaginary part of (A2) comes from the contour around the pole $\xi=1$ in the integral. Here u_i are very "listless" functions of R: $0.9798<u_1<1$ and $0.9983<u_2<1$ (for $R_*>R>0$).

Figure 3 shows a plot (the dashed curve) of $|a_c|$ constructed from Eq. (A2). We see that we have $|a_c|>|a|$ at $R<R_c=0.085\,806$. At sufficiently small distances R, the asymptotic behavior of the coefficients of the $1/n$ expansion is thus dominated by a term like that in (2.3). Numerical calculations show that the contribution of the oscillatory terms becomes appreciable as early as $R\sim 0.2$. This result is confirmed through a calculation of the closest singularities of Borel transform (3.14). With $R=0.1$ we thus find $\delta=-2.0031$ and $\delta_c=1.3262\pm i\pi/2$ $(|\delta|<|\delta_c|=2.056)$, while at $R=0.05$ we have $\delta=-2.6907$ and $\delta_c=2.0034\pm i\pi/2$, so in this case we have $|\delta|>|\delta_c|$.

At $R>R_*$, the calculations are similar, but they become more complicated because the turning point is $\xi_1\neq 0$. However, it turns out that we have $a(R)>|a_c(R)|$, so the

complex singularity at $\delta=1/2a_c$ does not contribute substantially to the asymptotic behavior of the coefficients of the $1/n$ expansion.

We note that we have $a_c/a\to -1$ both as $R\to 0$ and as $R\to\infty$.

Above we discussed the symmetric case, $Z_1=Z_2=1$. For $Z_1\neq Z_2$, the calculations are analogous, but the equations are quite a bit more complicated. Here it must be noted that tunneling can occur in either η or ξ. In the asymptotic behavior of the coefficients of the $1/n$ expansion, the dominant term is that for which $|a|$ is at its maximum:

$$|a(R)|=\max(|a_\xi|,|a_\eta|). \tag{A4}$$

Figure 3 shows results of a numerical calculation for several (Z_1,Z_2) pairs. Also shown here are values of R_c for a system of unequal charges: $R_c=0.0693$ for $Z_2=1.5$, $R_c=0.0588$ with $Z_2=2$, and $R_c=0.0458$ with $Z_2=3$ (with $Z_1=1$ everywhere).

APPENDIX B

States with parabolic quantum numbers $n_1=n_2=0$, $m=n-1$ correspond in the limit $n\to\infty$ to circular electron orbits, oriented perpendicular to the z axis, along which the fields $\mathscr{E}$ and $\mathscr{H}$ are directed. After the gauge transformation

$$\mathbf{r}\to n^2\mathbf{r},\quad U(\mathbf{r})\to n^{-2}U(n^2\mathbf{r}),$$
$$\mathscr{E}\to F=n^4\mathscr{E},\quad \mathscr{H}\to B=n^3\mathscr{H} \tag{B1}$$

the effective potential becomes

$$U(\mathbf{r})=-\frac{1}{\mathbf{r}}+\frac{1}{2\rho^2}+Fz+\frac{1}{8}B^2\rho^2 \tag{B2}$$

(ρ,z,φ are cylindrical coordinates). This potential has a minimum at the point $\mathbf{r}_0=(\rho_0,z_0)$, which satisfies the equations

$$r^{-3}+\tfrac{1}{4}B^2=\rho^{-4},\quad z=-Fr^3,\quad \rho^2+z^2=r^2$$

(for an equilibrium classical electron orbit). We then find Eq. (4.1) for the radius of the orbit, $r_0(F,B)$. After solving this equation, we find the other parameters of the orbit:

$$\rho_0=r_0(1-F^2r_0^4)^{1/2}=r_0^{3/4}(1+\tfrac{1}{4}B^2r_0^3)^{-1/4},$$
$$z_0=-Fr_0^3. \tag{B3}$$

At fixed B, the effective potential has a minimum only in weak electric fields $F<F_*(B)$. The solution of Eq. (4.1) accordingly remains real out to the point at which the roots collide. From this condition we can find the behavior of the "critical field" F_* as a function of B. Setting $F^2r_0^4=(1+2u)/9$, we find Eqs. (4.2), and the radius of the orbit is

$$r_*=r_0(F_*)=\tfrac{81}{64}(1-u)(1-\tfrac{1}{4}u)^{-3}. \tag{B4}$$

In particular, with $u=0$ (in the absence of a magnetic field; i.e., the Stark effect) we find (4.3). As $B\to\infty$, on the other hand, we find

$$u=1-(3B)^{-1/2}-\tfrac{1}{6}B^{-1}+..., \tag{B5}$$

and thus

$$\frac{F_*}{B}=c_0+c_1B^{-1/2}+c_2B^{-1}+c_3B^{-3/2}+..., \tag{B6}$$

where

$$c_0=3^{-3/2},\quad c_1=2/27=0.0741,$$
$$c_2=11/(2\cdot 3^{9/2})=0.0392,$$
$$c_3=7/324=0.0216,\quad c_4=0.0114,\ldots .$$

It can be seen from Fig. 4 that at $B\gtrsim 0.5$ the $F_*(B)$ dependence is approximately linear; the explanation lies in the numerically small values of the coefficients c_1 and c_3. As the magnetic field is strengthened, the radius of the equilibrium orbit, which corresponds to the field F_*, shrinks:

$$r_*=B^{-1/2}(3^{1/2}-\tfrac{1}{2}B^{-1/2}+...).\quad B\to\infty. \tag{B7}$$

APPENDIX C

For a potential (6.4) we have

$$p^2=2[U(q_0)-U(q)]=\text{const}\cdot\{\xi^N-N\xi-(N-1)\}, \tag{C1}$$

$$\omega=\sqrt{U''(q_0)}=\sqrt{N-1}\alpha^{N-2/2(N-1)}, \tag{C2}$$

where $q=\alpha^{1/N-1}\xi$, $\xi_0=-1$, and $\xi_m=1$. The right-hand turning point is $\xi_2=2$, 1.651, and 1.492 for $N=3$, 5, and 7. With increasing N, we find $\xi_2=1+(\ln 2N)/N+...\to 1$. We also find

$$a=C\omega^{-N+2/N-2}, \tag{C3}$$

where

$$C=2^{-3/2}N^{1/2}(N-1)^{N+2/2(N-2)}/J_N,$$
$$J_N=\int_{-1}^{\xi_2}\sqrt{N-1+N\xi-\xi^N}d\xi$$

(in the $N=3$ case, the integral can be evaluated analytically, and we have $C=5/6$). Using $\alpha\propto\nu_*-\nu\to 0$, we find (6.5).

In the course of an analytic continuation into the region $\nu>\nu_*$, the parameter $a(\nu)$ becomes complex, and its phase δ becomes ($\nu\approx\nu_*$)

$$\delta=\frac{\pi}{2}\frac{N+2}{N-1}. \tag{C4}$$

The splitting of the energies corresponding to the stable (q_0) and unstable (q_1) equilibrium points in potential (6.4) is

$$\Delta E=U(q_1)-U(q_0)=\frac{2N-2}{N}\alpha^{N/N-1}\beta^{-1/N-1}.$$

Using $\alpha\propto\nu_*-\nu$ and $\epsilon^{(0)}<\epsilon^{(1)}$, we then find Eq. (6.6).

We now consider potential (6.7). If $\nu>\nu_*$, it has a unique minimum at $q=0$, and the turning point migrates into the complex plane:

$$q_{0,2}=\pm i\left(-\frac{N\alpha}{2\beta}\right)^{1/N-2}, \quad \alpha<0.$$

Hence

$$\frac{1}{a}=2\int_0^{q_0}\sqrt{-p^2}dq=\text{const}\cdot\sqrt{-\alpha}q_0^2.$$

At $\nu<\nu_*$, the appropriate expression follows from (6.2). As a result we find

$$a(\nu)\approx A_\pm|\nu-\nu_*|^{-\sigma}, \quad \sigma=\frac{N+2}{2(N-2)}, \tag{C5}$$

$$\frac{A_+}{A_-}=-2^{-(\sigma+2)}N^\sigma\frac{J_+}{J_-}, \tag{C6}$$

where $\nu\to\nu_*$,

$$J_+=\int_0^1\sqrt{(1-t^{N-1/2})}$$

$$dt=\frac{2\sqrt{\pi}\Gamma[2/(N-2)]}{(N+2)\Gamma[(N+2)/2(N-2)]}),$$

$$J_-=\int_0^1\sqrt{\left(t^N-\frac{N}{2}t^2+\frac{N-2}{2}\right)}dt.$$

In this case, $a(\nu)$ has a power-law singularity, and it changes sign when the point $\nu=\nu_*$ is crossed. For the problem of two centers with $Z_1=Z_2$ we have $N=4$, $J_+=J_-=2/3$, and

$$\sigma=3/2, \quad A_+/A_-=-2^{-1/2}, \tag{C7}$$

in complete agreement with Eq. (3.13), which was derived through an analysis of the exact solutions (the role of ν is played in this case by the distance R). It follows that as we pass through $R=R_*$ the series in (2.1) changes from a constant-sign series to a variable-sign series, in agreement with numerical calculations.[11,13]

Note added in proof (7 February 1994). One of the present authors (A.S.) has developed an alternative method, based on the solution of the Hamilton–Jacobi equation, to calculate the asymptotic parameter a in multidimensional problems. The time $t=i\tau$ (which is complex for tunneling motion) does not appear explicitly in the equation, and such an approach is therefore probably also applicable when $F>F_*$. Based on the problem discussed in Sec. 4 of the present paper, we have shown that one obtains the same value of ImS as when the imaginary-time method is used to calculate tunneling trajectories.

[1)]See Refs. 24–26, where this question is discussed in the example of an expansion of the energy in inverse powers of R. The energy $\epsilon(R)$ is real in this problem. The imaginary part of the Borel sum of the series $\Gamma/2\propto\exp(-2R/n)$ cancels out with exponentially small imaginary terms in the complete asymptotic expansion of $\epsilon(R)$, which was found in Ref. 26.

[2)]There are two classical orbits, which correspond to a localization of the electron at one nucleus or the other as $R\to\infty$ (Fig. 2a).

[3)]These equations were given in Ref. 14, but no derivation of them has been published previously.

[4)]See Appendix B and also Ref. 7. The electric field is expressed in units of $m^2e^5\hbar^{-4}=5.14\cdot10^9$ V/cm, and the magnetic field in units of $m^2e^3c\hbar^{-3}=2.35\cdot10^9$ G. The results derived below were discussed briefly in Ref. 29.

[5)]See also the paper by Schmid,[32] in which the method of characteristics is used to calculate semiclassical wave functions and tunneling probabilities in multidimensional problems. That approach is equivalent to a calculation of classical trajectories in an "inverted" potential on the basis of the Hamilton–Jacobi equation.

[6)]Compare this situation with the case $R<R_*$ in the two-center problem, in which the turning points $\pm\eta_1$ become complex. In that case, it is possible to calculate $a(R)$ analytically [see Eq. (3.9)], but not numerically.

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