Asymptotic form of higher orders of the $1/n$ expansion

V. S. Popov and A. V. Sergeev[1)]

Institute of Theoretical and Experimental Physics, Russian Academy of Sciences, 117259, Moscow

(Submitted 29 January 1993)

Pis'ma Zh. Eksp. Teor. Fiz. **57**, No. 5, 273–276 (10 March 1993)

The asymptotic form of higher orders of the $1/n$ expansion in quantum mechanics is factorial. The Yukawa potential and the hydrogen atom in electric and magnetic fields are discussed.

The $1/n$ expansion, a new method in quantum mechanics and field theory, has already found numerous applications (see, for example, the review article by Chatterjee[1]). In particular, it has been applied successfully to the hydrogen atom in strong electric and magnetic fields[2–5] and to the problem of two Coulomb centers.[6,7] A topic which has been taken up recently[7,8] is the asymptotic form of higher orders of the $1/n$ expansion. This topic is of theoretical interest and also important to calculations of atomic states with spectroscopic accuracy. In this letter we report results on spherically symmetric potentials and on the problem of the hydrogen atom in parallel electric and magnetic fields.

The energy eigenvalues (which are complex in the case of quasistationary states) are given by power series in the "small parameter" $1/n$:

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

where $n=n_r+1+1$ is the main quantum number ($n_r=0,1,...$ is fixed; $l\to\infty$), and k is the order of the $1/n$ expansion. In the cases of interest in this paper the asymptotic form of the coefficients $\epsilon^{(k)}$ is factorial:

$$\epsilon^{(k)}\approx k!a^kk^\beta\left(c_0+\frac{c_1}{k}+\frac{c_2}{k^2}+\cdots\right),\quad k\to\infty, \tag{2}$$

or

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

where $a,\beta,...$ are constants which can be calculated. For example we have[2)]

$$a^{-1}=2^{3/2}\int_{r_0}^{r_2}\left[U(r)-\frac{1}{2}\epsilon^{(0)}\right]^{1/2}dr, \tag{3}$$

where $U(r)=n^2V(n^2r)+1/2r^2$ is an effective potential which incorporates a centrifugal energy, and $V(r)$ is the original potential which appears in the Schrödinger equation. For bound states, the turning point r_2 goes off into the complex plane, and the constants a and c_0 are generally complex. Consequently, the coefficients of the

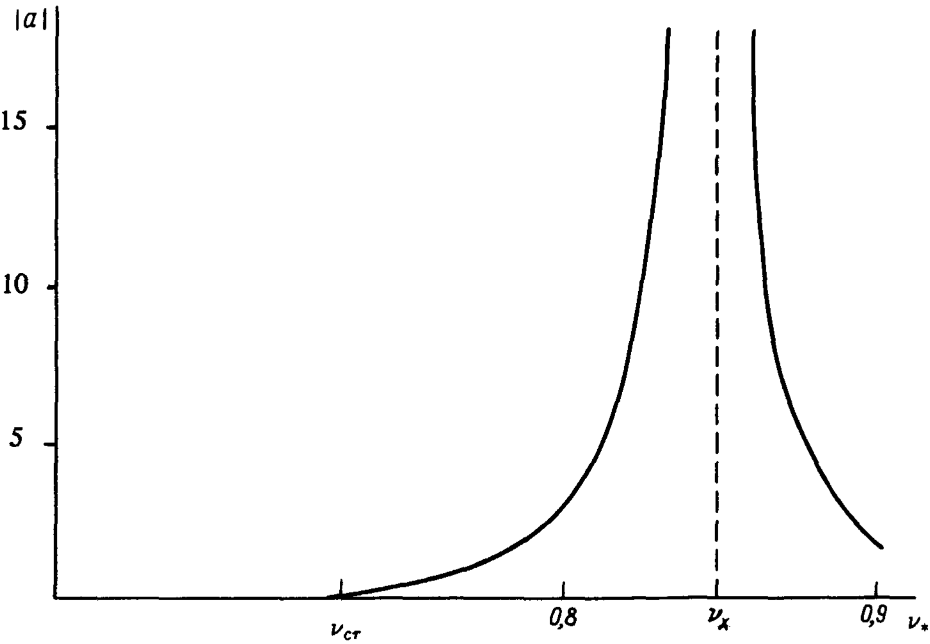

FIG. 1. The parameter of the asymptotic behavior, a, vs $\nu = n^2\mu$ (μ is a screening parameter) for a Yukawa potential.

$1/n$ expansion oscillate at large values of k: $\epsilon^{(k)} \propto k! \cos(k\delta + \varphi)$, where $\delta = \arg a$. For quasistationary states, a and c_0 are real, with $a > 0$; in other words, series (1) is of constant sign.

As an example we consider a Yukawa potential, which is frequently used in atomic and nuclear physics: $V(r) = -r^{-1}\exp(-\mu r)$, $\hbar = m = 1$ (Fig. 1). The value $\nu = \nu_{cr} = 0.7358$ corresponds to the situation in which level $nl (n = l + 1 \gg 1)$ goes off into the continuum ($\nu = n^2\mu$), and the value $\nu_* = 0.8400$ corresponds to the collision of two classical equilibrium points. The effective potential thereafter no longer has a minimum at $0 < r < \infty$. In the interval $0 < \nu < \nu_{cr}$, which corresponds to the discrete spectrum, the coefficients $\epsilon^{(k)}(\nu)$ oscillate at large values of k. With $\nu = 0.526$ we have $\delta = \pi/2$, and the period of the oscillations in the sign of $\epsilon^{(k)}$ is 4. For $\nu_{cr} < \nu < \nu_*$ the parameter of the asymptotic behavior satisfies $a(\nu) > 0$ and has a power-law singularity as $\nu \to \nu_*$:

$$a(\nu) = A(1 - \nu/\nu_*)^{-5/4}[1 + O((\nu_* - \nu)^{1/2})], \tag{4}$$

where $A = 0.1116$. An analytic continuation into the region $\nu > \nu_*$ leads to complex values of $a(\nu)$. This situation corresponds to the case in which the coefficients $\epsilon^{(k)}(\nu)$ become complex, so that (by summing the first few terms of the $1/n$ expansion) one can describe not only a shift but also the width of the level.[3,5]

The problem of the hydrogen atom in external fields $\mathscr{E}$ and $\mathscr{H}$ is more compli-

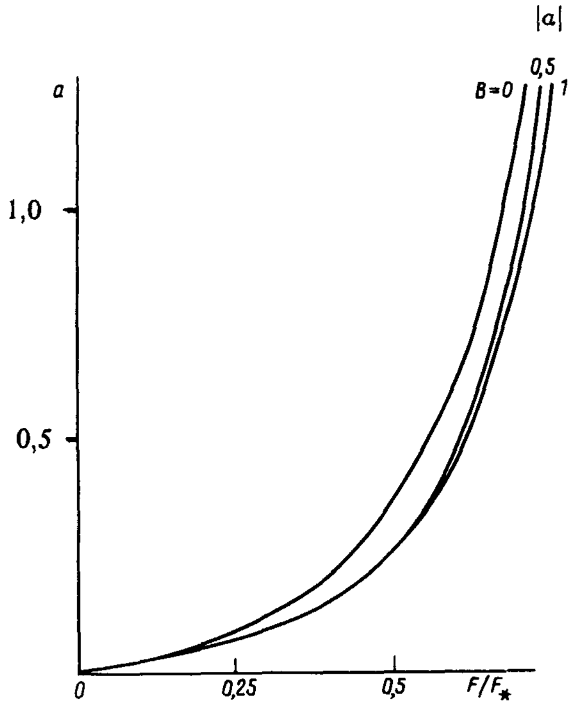

FIG. 2. The same as in Fig. 1 for the problem of the hydrogen atom in electric and magnetic fields ($F=n^4\mathscr{E}$; the curves are labeled by the values of B).

cated. We consider the case of uniform, parallel fields and states with magnetic quantum number $m=n-1$, which corresponds to circular electron orbits. The $1/n$ expansion is constructed around the classical orbit, whose radius, $r_0=r_0(F,B)$, is found from the equation

$$r(1-F^2r^4)^2\left(1+\frac{1}{4}B^2r^3\right)=1 \tag{5}$$

($\hbar=m_c=e=1$, $F=n^4\mathscr{E}$ and $B=n^3\mathscr{H}$ are "reduced" variables).

Let us briefly describe the calculation of the parameter of the asymptotic behavior, a. Through a numerical integration we find the classical trajectory $\mathbf{r}(t)$, which connects the point of the maximum, $\mathbf{r}_0=(\rho_0,z_0)$, of the effective potential

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

(taken with the opposite sign, in accordance with the description of the below-barrier motion of a particle in the imaginary-time method[9]) with the turning point $\mathbf{r}_2$, which lies on the constant-energy surface[3] $U(\mathbf{r})=U(\mathbf{r}_0)$. The parameter a in (2) is then calculated from (t is the imaginary time)

$$a=(2\mathrm{Im}S)^{-1}, \quad S=\int_{\mathbf{r}_0}^{\mathbf{r}_2}\mathbf{p}d\mathbf{r}=\int_0^{\infty}\dot{\mathbf{r}}^2dt. \tag{6}$$

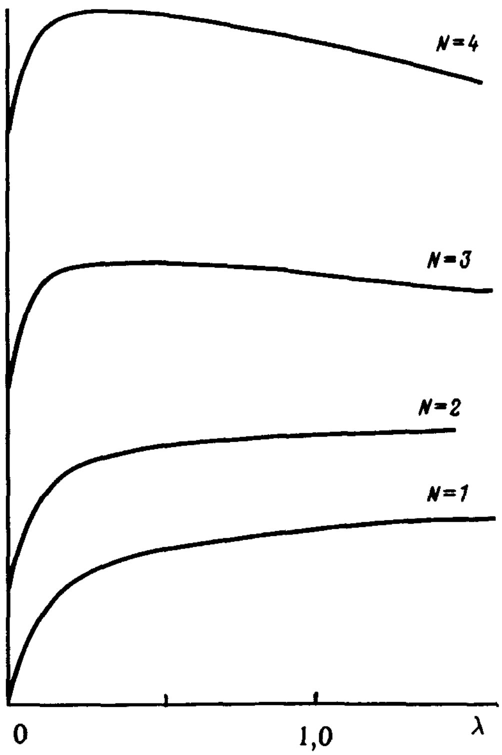

FIG. 3. The parameter of the asymptotic behavior, from (2′), for the potentials in (7). The case $N=1$ corresponds to a funnel potential.

The results are shown in Fig. 2, which corresponds to fields $F<F_*$. Here $F_*(B)$ is the classical ionization threshold,[3,4] which is analogous to $\nu=\nu_*$ in the case of the Yukawa potential. The values of F_* are 0.2081, 0.2532, and 0.3449 for B values of 0, 0.5, and 1.0. As in the preceding case, a becomes infinite as $F\to F_*$.

For the generalized funnel potential

$$V(r)=-1/r+g(r^N/N), \quad N>0, \tag{7}$$

the spectrum is discrete, the point of a minimum, $r_0(g)$, exists for all $0<g<\infty$, and there are no collisions of the classical solutions. Figure 3 shows $|a|$ as a function of the effective coupling constant $\lambda=n^{2N+2}g$.

The asymptotic form of the higher orders of the $1/n$ expansion is thus factorial (cf. "Dyson's phenomenon"[10] for ordinary perturbation theory). In many cases the parameters of asymptotic expression (2) can be found analytically.

We are indebted to V. D. Mur for a useful discussion.

[1)]S. I. Vavilov State Optics Institute, 199164, St. Petersburg, Russia.

[2)]A corresponding expression (although more complicated) can be derived for the preexponential factor c_0. The reduced energy $\epsilon^{(0)}$ corresponds to the minimum of the potential $U(r)$, so the two turning points coincide: $r_0=r_1$. The classically allowed region contracts to a point, and $r_0<r<r_2$ is the below-barrier region.

[3)]This surface is the boundary of the classically allowed region, and the electron trajectory involved here is analogous to a below-barrier trajectory of the instanton type, which connects points r_0 and r_2 in (3).

[1]A. Chatterjee, Phys. Rep. **186**, 249 (1990).
[2]C. M. Bender, L. D. Mlodinow, and N. Papanicolaou, Phys. Rev. A **25**, 1305 (1982).
[3]V. S. Popov, V. D. Mur, A. V. Scheblykin *et al.*, Phys. Lett. A **124**, 77 (1987); A **149**, 418, 425 (1990).
[4]V. M. Vaĭnberg, V. S. Popov, and A. V. Sergeev, Zh. Eksp. Teor. Fiz. **98**, 847 (1990).
[5]V. S. Popov, in *Dimensional Scaling in Chemical Physics* (ed. D. R. Herschbach), Kluwer Acad. Publ., Dordrecht, 1993, pp. 179, 217.
[6]V. D. Mur, V. S. Popov, and A. V. Sergeev, Zh. Eksp. Teor. Fiz. **97**, 32 (1990) [Sov. Phys. JETP **70**, 16 (1990)].
[7]M. Lopez-Cabrera, D. Z. Goodson, D. R. Herschbach *et al.*, Phys. Rev. Lett. **68**, 1992 (1992).
[8]V. S. Popov and A. V. Scheblykin, Yad. Fiz. **54**, 1582 (1991) [Sov. J. Nucl. Phys. **54**, 968 (1991)].
[9]A. M. Perelomov, V. S. Popov, and M. V. Terent'ev, Zh. Eksp. Teor. Fiz. **51**, 309 (1966) [Sov. Phys. JETP **24**, 207 (1966)].
[10]F. J. Dyson, Phys. Rev. **85**, 631 (1952).

Translated by D. Parsons