Logarithmic perturbation theory for a screened Coulomb potential and a charmonium potential

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Logarithmic perturbation theory (PT) for screened Coulomb potential is considered. Calculation of higher PT orders of the level energy E_k is reduced to recurrence relations that are valid for any type of screening and are very convenient for computer calculations. They are employed to calculate the PT coefficient of E_k up to $k = 100$ for a number of physically interesting cases such as the Yukawa potential, the quarkonium potential, etc. The approach of E_k as $k \to \infty$ to the asymptotic form of $\tilde{E}_k$, defined by the quasiclassical approximation, is discussed. The problem of summation of the divergent PT series is considered. By employing the Padé approximants and the asymptotic form of E_k it is possible to determine with a high accuracy the energy level $E(g)$ for the potentials mentioned above in a range that exceeds considerably the range of applicability of PT, including the strong coupling region.

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1. A "logarithmic perturbation theory"[1] was developed earlier[1-14] for the discrete-spectrum states in quantum mechanics. In this theory a transition is used from the Schrödinger equation to the Riccati equation for the logarithmic derivative of the wave function. With the anharmonic oscillator[3,4] and the Stark effect in the hydrogen atoms[5,6,11] as an example, it was shown that this modification of perturbation theory (PT) is very convenient for the calculation higher PT orders, especially in the case of the ground state. We continue here the study of this group of questions and consider the calculation of the higher orders and the summation of the diverging PT series for a screened Coulomb potential

$$H = \frac{1}{2}p^2 - \frac{1}{r}f(\mu r), \qquad (1.1)$$

where $\hbar = m = e = 1$ (atomic system of units),

$$f(x) = \sum_{n=0}^{\infty} f_n(-x)^n$$

is the screening function, with $f_0 = 1$ (the potential becomes pure Coulomb at short distances).

The class considered includes a number of physically important potentials. Thus, at $f(x) = e^{-x}$ we obtain the Yukawa potential, which is frequently encountered in nuclear physics, solid state theory, plasma physics (Debye screening), etc. The Thomas-Fermi model corresponds to $\mu = 2(4/3\pi)^{2/3}Z^{1/3}$, with $f(x)$ the solution of the equation $x^{1/2}f'' = f^{3/2}$. At $\mu = g^{1/2}$ and $f(x) = 1 - x^2$ we obtain a potential of the "funnel" type:

$$V(r) = -1/r + gr, \qquad (1.2)$$

which is a popular variant of the phenomenological description of the states of the heavy quarkonium.[15,16] The number of such examples can be easily increased.

The plan of the article is the following. In Sec. 2, the calculation of the higher PT orders for the level energy and for the wave function is reduced to recurrence relations that are much more convenient for calculations than the usual[17] PT scheme. In Sec. 3 is

discussed the asymptotic form of the coefficients E_k of the PT series as $k \to \infty$ and its connection with the quasiclassical theory. We proceed next (Sec. 4) to specific examples: the Hulthén and Yukawa potentials, the funnel, etc.

In quantum-mechanics and field-theory problems, the perturbation is as a rule[2] more singular than the initial potential V_0. As a result, the PT series coefficients increase factorially:

$$E_k \approx \tilde{E}_k(1 + c_1/k + c_2/k^2 + \ldots) \qquad k \to \infty,$$
$$\tilde{E}_k = (k\alpha)!(-a)^k k^\beta c_0, \qquad (1.3)$$

and the PT series itself is asymptotic and has a zero convergence radius. The question arises: what physical information is contained in this case in the higher PT orders?

To answer this question it is necessary to resort to methods of summing divergent series. In Sec. 5 is discussed the summation of the PT series for the ground-level energy with the aid of Padé approximants. Two examples are considered in detail: the Yukawa potential $V(r) = -e^{-\mu r}/r$ and the potential (1.2). It is shown that by this method it is possible to reconstruct with high accuracy the level energy in a wide range of values of μ and g, including the strong-coupling region (Sec. 6). Thus, the calculation of the higher PT orders, as well as their asymptotic forms as $k \to \infty$, makes it possible to obtain the energy $E(g)$ far beyond the limits of the region of applicability of standard PT. This conclusion is of interest, especially for quantum field theory, in view of the considerable progress made in recent years both in calculations of multiloop diagrams and of the asymptotic coefficients of the PT series,[19-21] and in summation of diverging PT series.[22-24]

2. Just as in the preceding papers,[3-6] we reduce the higher-order PT calculation to recurrence relations.[3] In the case of the ground state we make the substitution $R'/R + r^{-1} = -\xi$, where $R(r)$ is the radial wave function. The Schrödinger equation then goes over into the Riccati equation

$$\frac{d\xi}{dr}-\xi^2=2\left[\dot{E}+\frac{1}{r}f(\mu r)\right].\tag{2.1}$$

Expanding $\xi(r,\mu)$ and $E(\mu)$ in formal PT series in powers of the screening parameter μ:

$$\xi=\sum_{k=0}^{\infty}\xi_k(r)(-\mu)^k,\quad E=\sum_{k=0}^{\infty}E_k(-\mu)^k,\tag{2.2}$$

we obtain a chain of equations for the functions $\xi_k(r)$:

$$\xi_k'-2\left(1-\frac{1}{r}\right)\xi_k-\sum_{j=0}^{k}\xi_j\xi_{k-j}=2(E_k-f_kr^{k-1}).$$

It follows from them that

$$\xi_0=1-r^{-1},\quad \xi_1=0,\quad \xi_2=-f_2r$$

and $\xi_k(r)$ is a polynomial of degree $k-1$ at $k\geq1$. We put therefore

$$\xi_k(r)=-\sum_{j=1}^{k-1}a_j^{(k)}r^j,\quad k>1\tag{2.3}$$

and arrive at recurrence relations for the coefficient $a_j^{(k)}$:

$$a_{k-1}^{(k)}=f_k,$$

$$a_j^{(k)}=\frac{1}{2}(j+3)a_{j+1}^{(k)}+\frac{1}{2}\sum_{l=2}^{k-2}\sum_{p+q=j}a_p^{(l)}a_q^{(k-l)},\quad j<k-1.\tag{2.4}$$

Decreasing the index j in succession, we calculate the k-th PT order for the level energy:

$$E_k=-3a_2^{(k)}=-\frac{3}{2}a_1^{(k)}.\tag{2.5}$$

The structure of the recurrence relations (2.4) does not depend at all on the actual form of the screening. These relations are convenient for computer calculations and make it possible to calculate quite high orders of PT (up to $k=150-200$ at our present computation capabilities). In principle it is possible to obtain with the aid of (2.4) also explicit expressions for E_k in terms of the first k coefficients of f_n, $1\leq n\leq k$, but such equations are quite cumbersome.[8] It is more convenient to use for the calculations Eqs. (2.4) directly in each concrete case.

Once the quantities ξ_k and E_k are calculated, it is easy to obtain[8] also a PT expansion for the wave function:

$$R(r)=Ce^{-r}\left[1-\sum_{k=2}^{\infty}R_k(r)(-\mu)^k\right],\tag{2.6}$$

where $R_2=(1/2)f_2r^3$, $R_3=f_3(1/3r^3+r^2)$, and at $k\geq4$ the polynomials R_k are determined from the recurrence relations

$$R_k=\eta_k+\frac{1}{k}\sum_{l=2}^{k-2}l\eta_lR_{k-l},\tag{2.7}$$

where

$$\eta_k(r)=-\int_0^r\xi_kdr=\sum_{n=2}^{k}a_{n-1}^{(k)}n^{-1}r^n.$$

The constant C in (2.6) in k-th PT order is determined from the normalization condition

$$\int_0^{\infty}R^2(r)r^2dr=1+O(\mu^{k+1}).$$

We note that $\xi_1(r)$ and $R_1(r)$ vanish identically at an arbitrary form of the screening $f(\mu r)$. This is seen even from the fact that

$$V(r)=-r^{-1}+f_1\mu+O(\mu^2).$$

Thus, the first-order correction in μ yields a constant energy shift that does not alter the wave functions.

We have confined ourselves above to the ground state. The presence of a node of the radial wave function at the point $r=r_0(0<r_0<\infty)$ raises a certain difficulty in the considered method, since $\xi(r)\to\infty$ as $r\to r_0$. It was shown in Ref. 6 how to use the Riccati equation and the method of recurrence relations in the case of states with nodes.

3. Asymptotics of the higher PT orders and the quasiclassical approximation.

Let

$$H=-\tfrac{1}{2}\Delta-1/r+gv(r),\tag{3.1}$$

where $v(0)=0$ and $v(r)\to\infty$ as $r\to\infty$ [we assume for simplicity that $v(r)$ is a monotonically increasing function of r, although this is not obligatory]. As is known,[18,21] to calculate the asymptotics of the coefficients E_k as $k\to\infty$ it is necessary to find the jump in the level energy[4)]

$$\Delta E=\frac{1}{2i}[E(g+i0)-E(g-i0)]=\frac{1}{2}\gamma(\lambda)$$

on the cut $g\equiv-\lambda<0$. At $g<0$ tunneling of a particle through the potential barrier becomes possible, i.e., the bound level turns into a quasistationary one.

As $\lambda\to+0$, the WKB method can be used to calculate its width γ. The quasiclassical momentum

$$p(r)=i\left[\varepsilon-\frac{2}{r}+\frac{\Lambda^2}{r^2}-2\lambda v(r)\right]^{1/2}\tag{3.2}$$

has three turning points: r_0, r_- and r_+. The region $r_0<r<r_-$ is allowed for classical motion, and the region $r_-<r<r_+$ is forbidden. At small λ, the first two turning points are almost independent of λ:

$$r_0=n^2[1-(1-\Lambda^2/n^2)^{1/2}]+O(\lambda),\quad r_-=n^2\left[1+\left(1-\frac{\Lambda^2}{n^2}\right)^{1/2}\right]+O(\lambda),$$

whereas the point r_+ goes off to infinity as $\lambda\to0$. Thus, for $v(r)=r^N$ we have

$$r_+=(2n^2\lambda)^{-1/N}-c+O(\lambda^{1/N}),$$

$$c=\begin{cases}2n^2-\dfrac{1}{2}\varepsilon_1, & N=1\\[2mm]2n^2/N, & N>1\end{cases}\tag{3.3}$$

Here $\varepsilon=-2E$ and E is the level energy (at $g=0$, $\varepsilon=\varepsilon_0=1/n^2$); $\Lambda=0$ for s-levels, $\Lambda=l+1/2$ at $l\neq0$ (Langer correction), ε_1 is the level shift in first order in g:

$$\varepsilon(g)=\varepsilon_0-\varepsilon_1g+O(g^2).\tag{3.4}$$

We note that for the ground level $\varepsilon_0=1$, $\varepsilon_1=2^{-N}(N+2)!$, and in the case $N=1$ (funnel) $\varepsilon_i=3n^2-l(l+1)$ for a level with arbitrary quantum numbers n and l.

The level width γ is determined by the penetrability of the barrier. As $\lambda \to 0$ there exists a region of values of r, $r_- \ll r \ll r_+$, in which the quasiclassical wave function

$$\chi_{nl}^{cl} = C|p(r)|^{-\frac{1}{2}} \exp\left(\int_r^{r_+} |p(r')| dr'\right)$$

is matched to the tail of the exact wave function of the free atom[17]:

$$\chi_{nl}(r) = rR_{nl}(r) \approx \frac{(-1)^{n-l-1} 2^n}{n^{n+1}[(n+l)!(n-l-1)!]^{\frac{1}{2}}} e^{-r/n} r^n,$$

and this determines the constant C. Going next around the turning point r_+, we continue the solution into the region $r > r_+$, where it takes the form of a divergent wave. The flux of particles that go off to infinity determines the width of the level

$$\gamma(\lambda) = |C|^2 = \gamma_0 \exp\{-2J(\lambda)\},$$

$$\gamma_0 = \frac{(n+\Lambda)^{n+\Delta}(n-\Lambda)^{n-\Delta}}{(n+l)!(n-l-1)!n^3} e^{-2n}, \quad J(\lambda) = \int_{r_-}^{r_+} |p(r)| dr. \tag{3.5}$$

We emphasize that Eq. (3.5) is asymptotically exact in the limit as $\lambda \to 0$. The reason is that the quasiclassical approximation was used only in the region $r \gg r_-$, where the conditions of its applicability are satisfied.

We rewrite the preceding equation in a more illustrative form

$$\gamma = A \frac{\omega_{cl}}{2\pi} \exp\left\{-2\int_{r_-}^{r_+} |p(r)| dr\right\}, \tag{3.6}$$

where $\omega_{cl} = 2\pi/T = n^{-3}$ is the frequency of the revolution of the particle along the Keppler ellipse [period $T = \pi(2|E|^3)^{-1/2} = 2\pi n^3$],

$$A = \begin{cases} [Q(n)]^2, & l=0 \\ q(n+\Lambda)q(n-\Lambda), & l \geqslant 1, \end{cases}$$

$$Q(x) = \frac{(2\pi x)^{\frac{1}{2}}(x/e)^x}{\Gamma(x+1)}, \quad q(x) = \frac{(2\pi)^{\frac{1}{2}}(x/e)^x}{\Gamma(x+\frac{1}{2})}. \tag{3.7}$$

Equation (3.6) has a lucid physical meaning. The factor $\omega_{cl}/2\pi$ is equal to the frequency of the impacts of classical particle (localized in the region $r_0 < r < r_-$) against the wall of the potential barrier $r = r_-$, while the exponential corresponds to the probability of tunneling at each impact. If the quasiclassical approximation were exact for all n and l, the coefficient A would be equal to unity. This is satisfied when $n \to \infty$:

$$A = \begin{cases} 1-1/6n+\ldots, & l=0 \\ 1+1/12n(1-\Lambda^2/n^2)+\ldots, & l \neq 0. \end{cases} \tag{3.8}$$

Even for small quantum numbers, however, the difference between A and unity is small. Thus, for the ground state $\gamma_0 = e^{-2}$ and $A = 2\pi e^{-2} = 0.85033\ldots$. The region of applicability of the WKB method is seen to stretch out all the way to $n \sim 1$ (this takes place also in other physical problems, see, e.g., Ref. 25).

Thus, the determination of the asymptotic form of $\gamma(\lambda)$ as $\lambda \to 0$ reduces to a calculation of the integral $J(\lambda)$. Subsequent calculations will be made for a power-law potential $v(r) = r^N$. This corresponds to Eq. (1.1) with

$$\mu = g^{1/(N+1)}, \quad f(x) = 1-x^{N+1}.$$

The scale transformation $r = (\varepsilon/2\lambda)^{1/N} x$ yields

$$J(\lambda) = \varepsilon^{(N+2)/2N}(2\lambda)^{-1/N} f(\nu) \tag{3.9}$$

for the ground state, where

$$\nu = \left(\frac{2}{\varepsilon}\right)^{(N+1)/N} \lambda^{1/N}, \quad f(\nu) = \int_{x_-}^{x_+} \left(1 - \frac{\nu}{x} - x^N\right)^{\frac{1}{2}} dx. \tag{3.10}$$

We are interested in the expansion $f(\nu)$ as $\nu \to 0$. In this case

$$x_- = \nu[1 + \nu^N + (N+1)\nu^{2N} + \ldots],$$
$$x_+ = 1 - \frac{\nu}{N} - \frac{N+1}{2N^2}\nu^2 + \ldots,$$

and it is easy to show that

$$J(\lambda) = b_1 \lambda^{-1/N} + b_2 \ln \lambda + b_3 + O(\lambda^{1/N} \ln \lambda), \tag{3.11}$$

where

$$b_1 = 2^{-1/N}\pi^{\frac{1}{2}}\Gamma\left(\frac{1}{N}\right) \Big/ (N+2)\Gamma\left(\frac{N+2}{2N}\right), \quad b_2 = 1/N,$$

$$b_3 = \begin{cases} \frac{1}{2} - 2\ln 2, & N=1 \\ -\left(1 + \frac{N+1}{N}\ln 2\right), & N > 1. \end{cases}$$

At $k > k_0$ we have

$$E_k = -\frac{1}{2\pi} \int_0^\infty \gamma(\lambda)\lambda^{-(k+1)} d\lambda. \tag{3.12}$$

Here k_0 is the number of subtractions in the dispersion relations for $E(g)$. Substituting here expressions (3.5) and (3.11), we obtain the asymptotic form of the coefficients of the PT series. For the ground level it takes the form (1.3), where

$$\alpha = N, \quad \beta = 1,$$
$$a = 2^{1-N}\pi^{-N/2}\left[(N+2)\Gamma\left(\frac{N+2}{2N}\right)\Big/\Gamma\left(\frac{1}{N}\right)\right]^N \tag{3.13}$$

and at $N > 1$

$$c_0 = -\frac{1}{\pi^2} 2^{(4-N)/N}\left[N(N+2)\Gamma\left(\frac{N+2}{2N}\right)\Big/\Gamma\left(\frac{1}{N}\right)\right]^2. \tag{3.14}$$

We consider now the Yukawa potential. When the sign of the screening parameter μ is reversed, this potential takes the form

$$V(r) = -\frac{1}{r} e^{\lambda r}, \quad \lambda = |\mu| > 0. \tag{3.15}$$

Since now $V(r) \to \infty$ as $r \to \infty$, a barrier is present and tunneling takes place. At any positive λ, the level has a width, i.e., the energy $E = E(\mu)$ has a discontinuity at $\mu < 0$. The asymptotic form of the coefficient of the PT series is in this case

$$E_k \sim k!(2\ln k)^{-k}, \quad k \to \infty \tag{3.16}$$

This asymptotic form is somewhat unusual and differs from expression (1.3) for perturbations of the polynomial type.

Finally, in the case of a Hulthén potential the reversal of the sign of μ leads to the potential

$$V(r) = -\lambda/(1-e^{\lambda r}).$$

Since

$$V(\infty) = -\lambda > E_0 = -\frac{1}{2},$$

tunneling is impossible in such a potential, therefore $\gamma(\lambda)=0$ at sufficiently small λ. From the dispersion relations (3.12) it follows that the PT-series coefficients do not grow factorially. In this case $E_k = 0$, starting with $k = 3$ (see below).

4. Higher PT orders.

The equations obtained in Secs. 2 and 3 make it possible to calculate high PT orders for the level energy and consider the question of their acquiring an asymptotic value $\bar{E}_k$ as $k \to \infty$. We present several results.

a) in Eq. (1.1), the Hulthén potential corresponds to

$$f(x) = \frac{x}{e^x - 1}, \quad f_n = \frac{(-1)^n}{n!} B_n, \tag{4.1}$$

where B_n are Bernoulli numbers. From (2.4) we obtain $E_0 = E_1 = -1/2$, $E_2 = -1/8$, and $E_k = 0$ at $k > 2$, which coincides with the exact solution of the Schrödinger equation for the ground level:

$$E(\mu) = -\frac{1}{2}\left(1 - \frac{\mu}{2}\right)^2, \quad \xi = 1 - \frac{\mu}{2}\operatorname{cth}\frac{\mu r}{2}.$$

b) Yukawa potential

$$f(x) = e^{-x}, \quad f_n = 1/n!. \tag{4.2}$$

It follows from (2.4) that in this case all the E_k are negative and are rational fractions. We calculated 100 PT coefficients for the ground level:

$$E(\mu) = -\frac{1}{2} + \mu - \frac{3}{4}\mu^2 + \frac{1}{2}\mu^3 - \frac{11}{16}\mu^4$$
$$+ \frac{21}{16}\mu^5 - \frac{145}{48}\mu^6 + \frac{757}{96}\mu^7 - \frac{69\,433}{3072}\mu^8 + \frac{321\,449}{4608}\mu^9 - \ldots \tag{4.3}$$

and, for example,

$$E_{10} = -\frac{2343967}{10240} = -228.9\ldots, \quad E_{100} = -7.665892 \cdot 10^{84}.$$

(for more details see Table 1 of Ref. 8).

We note that the higher PT orders in this problem were first considered by Polikanov[1] who suggested the transition from the Schrödinger to the Riccati equation. He, however, constructed the PT in a somewhat different manner than in Refs. 3–8 and in the present paper. In the k-th approximation the wave function was determined accurate to μ^{2k}, but in each PT order it is necessary to normalize the wave function to unity accurate to terms $\sim\mu^{2k}$, take exponentials of the power series, etc. In the upshot, the calculation procedure turned out to be quite cumbersome. In Ref. 1 were calculated the seven first PT orders for the ground-level energy; the coefficients E_6 and E_7 differ from (4.3) and are in error. Recently[14] the coefficients E_k were calculated (by another method) up to $k = 40$. The results of Refs. 8 and 14 are in full agreement.[5]

c) The screened Coulomb potential

$$f(x) = e^{-x}\cos x, \quad f_n = \frac{2^{1/2}}{n!}\cos\frac{n\pi}{4} \tag{4.4}$$

is encountered in solid state physics when it comes to describing the potential of an impurity ion in metals and semiconductors (see, e.g., Refs. 26–28). The method
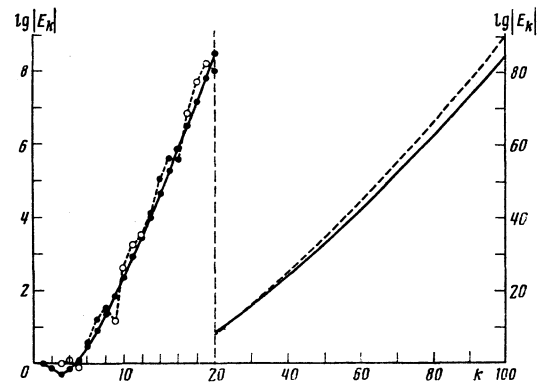

FIG. 1. Coefficients of the PT series for the ground-level energy: solid curve—Yukawa potential, dashed curves—the potential (4.4). The points $\bigcirc$ and $\bullet$ correspond to positive and negative E_k. The scales of both axes change at $k = 20$.

described above works successfully also in this case [see Table 2 of Ref. 8, where the coefficients of the expansion (2.2) are given up to $k = 100$]. The growth of $|E_k|$ is not so regular here as for the Yukawa potential, and the E_k do not maintain a constant sign. As seen from Fig. 1, the sequence of the alternation of the signs in them is quite complicated.

d) In the case of the potential (1.2) $f_0 = -f_2 = 1$, and the remaining f_n are equal to zero. The coefficients E_k were calculated with the aid of (2.4) and are given in Table I. For $k > 10$ they are approximate and only a small fraction of the result is given, but this fraction does given an idea of the growth rate of the PT coefficients as $k \to \infty$. Their asymptotic form is determined by Eqs. (3.13) and (3.14). In particular, at $N = 1$ [funnel, see (1.2)] it is necessary to put in Eq. (1.3) for $\bar{E}_k$

$$\alpha = 1, \quad a = 3/2, \quad \beta = 1, \quad c_0 = -18/\pi e^3, \tag{4.5}$$

and at $N = 2$ (a potential equal to the sum of the Coulomb and oscillator potentials) we have

$$\alpha = 2, \quad a = 8/\pi^2, \quad \beta = 1, \quad c_0 = -128/\pi^3. \tag{4.6}$$

The ratio $E_k/\bar{E}_k$, as a function of the PT order k, is shown in Fig. 2. Just as in other quantum-mechanics problems,[4-6] the asymptotic value of E_k, which is determined by the discontinuity of the energy $E(g)$ on the

TABLE I.

k	$-E_k$	k	$-E_k$
0	1/2	25	$2.295 \cdot 10^{30}$
1	3/2	30	$3.708 \cdot 10^{38}$
2	3/2	35	$1.312 \cdot 10^{47}$
3	$27/2^2$	40	$9.152 \cdot 10^{55}$
4	$795/2^4$	45	$1.162 \cdot 10^{65}$
5	$3\,845/2^3$	50	$2.521 \cdot 10^{74}$
6	$11\,166/2$	55	$8.867 \cdot 10^{83}$
7	$9\,543\,339/2^7$	60	$4.849 \cdot 10^{93}$
8	$1\,141\,062\,999/2^{10}$	65	$3.979 \cdot 10^{103}$
9	$18\,769\,071\,555/2^{19}$	70	$4.750 \cdot 10^{113}$
10	$1\,343\,699\,301\,873/2^{12}$	75	$8.040 \cdot 10^{123}$
15	$1.703 \cdot 10^{15}$	80	$1.886 \cdot 10^{134}$
20	$3.578 \cdot 10^{22}$		

Note. It can be shown with the aid of the recurrence relations (2.4) that E_k are rational fractions of the form $E_k = -M_k/2^{n_k}$. Here M_k and n_k are positive integers, with $n_k \leq 3k - 3$ at $k > 1$.
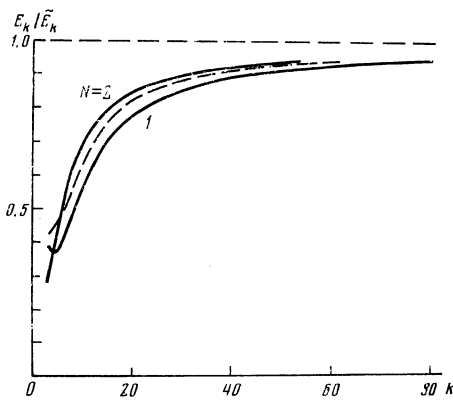
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FIG. 2. Approach of the PT coefficients to the asymptotic values $\bar{E}_k$ for the ground level in the potential $V(r) = -r^{-1} + gr^N$. Marked on the curves are the values of N. Dashed curve—the ratio $a_k/\bar{a}_k$ in the case $N = 1$, see Eq. (5.4).

cut $g < 0$, is quite slow. This indicates that the power-law corrections to $\bar{E}_k$ [i.e., the terms c_1/k, c_2/k^2, ... in the expansion (1.3)] are not small.

5. *Summation of the* PT *series.* We consider now a question that is perhaps the most interesting from the point of view of the use of methods of summing asymptotic series in quantum field theory (see Refs. 19–24): what information on the properties of the exact solution $E(g)$ can be obtained if one knows in exact form the first few PT orders and the asymptotic value of $\bar{E}_k$ as $k \to \infty$. To sum diverging PT series we use the method of Padé approximants.

From the coefficients E_k we can construct the rational fractions

$$[N, M]\,(\mu) = P_M(\mu)/Q_N(\mu). \tag{5.1}$$

Here P_M and Q_N are respectively polynomials of degree M and N; they are determined completely from the condition that the first $M + N + 1$ terms of the Taylor series for (5.1) coincide with the corresponding terms of the asymptotic series (2.2) for the level energy. The func-
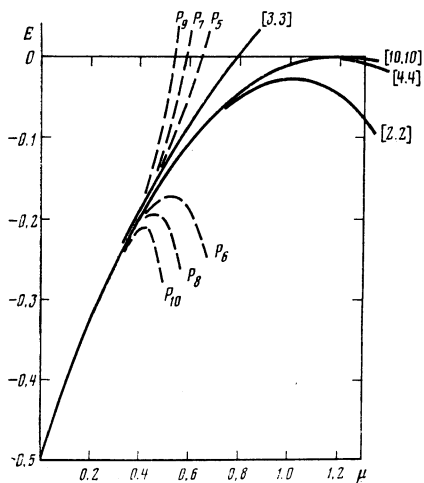
tions (5.1) are called Padé approximants. Explicit forms for the calculations of $P_M(\mu)$ and $Q_N(\mu)$ are given, for example, in Ref. 29.

The results of the calculation in the case of a Yukawa potential are shown in Fig. 3. The sequence of the approximants $[N, N](\mu)$ converges rapidly with increasing N, in contrast to the PT polynomials

$$p_N(\mu) = \sum_{k=0}^{N} E_k(-\mu)^k.$$

The employed approximants $[10, 10]$, i.e., the first 20 coefficients E_k, determine with sufficient accuracy the energy $E(\mu)$ in the entire interval $0 < \mu < \mu_{cr}$, in which the level is bound. At least nine significant figures of $E(\mu)$ are determined at $\mu \leqslant 0.5$, and six figures at $\mu = 1$. With increasing μ, the accuracy with which the energy is determined decreases, but even at $\mu \sim \mu_{cr}$ it remains high enough. At the same time, ordinary PT is not suitable at all at $\mu \sim \mu_{cr}$ (see the dashed curves in Fig. 3). At $\mu = \mu_{cr} = 1.190612$ the level goes off to the continuous spectrum. This value of μ_{cr} refines the value obtained earlier[30] in a numerical solu-
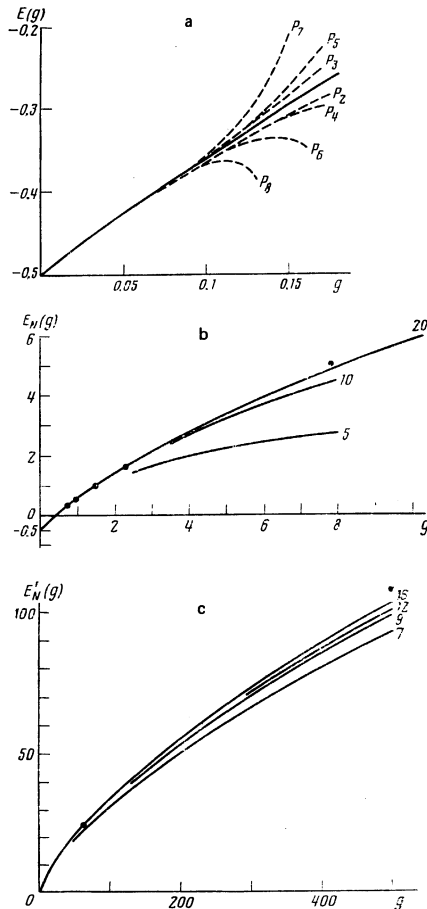

FIG. 4. Summation of the PT series for the ground-level energy in the potential (1.2): a) region of small g; solid curve—exact solution, dashed curve—PT polynomials $p_N(g)$; b) Padé approximants (5.2); c) the approximants (5.5). The points on the Figs. b and c denote the values of $E(g)$ taken from Ref. 15; the values of N are indicated on the curves.

FIG. 3. Diagonal Padé approximants (solid curves) and PT polynomials (dashed curves) for the ground-level energy in a Yukawa potential.

tion of the Schrödinger equation. Similar results were obtained[8] also for the oscillating potential (4.4).

In the case of the funnel (1.2), the PT polynomials yield a good approximation to the energy $E(g)$ only at small $g < 0.1$ (see Fig. 4a). Advance into the region of larger g is possible with the aid of the Padé approximants. We consider the functions

$$E_N(g) = \tilde{E}(g) + [N, N](g), \quad \tilde{E}(g) = \sum_{k=0}^{\infty} \tilde{E}_k(-g)^k, \quad (5.2)$$

where $\tilde{E}(g)$ is the Borel sum[6] of the series with the asymptotic coefficients $\tilde{E}_k$, and $\tilde{E}_k$, a $[N, N](g)$ is the approximant (5.1) for the series

$$\sum_k (E_k - \tilde{E}_k)(-g)^k,$$

constructed from the differences $E_k - \tilde{E}_k$.

The first $2N + 1$ coefficients of $E_N(g)$ coincide with the exact ones, and in addition correct account is taken of the asymptotic form of the far tail of the PT as $k \to \infty$. Therefore the function (5.2), in contrast to the PT polynomials, has a correct analytic behavior at the point $g = 0$.

The results of the calculation for the ground level are shown in Fig. 4b. At $N > 17$ the $E_N(g)$ curves are practically indistinguishable from one another and are in good agreement with the results of a numerical solution of the Schrödinger equation.[7]

The convergence can be further improved by taking into account the asymptotic value of the correct solution as $g \to \infty$, which in this case can be easily obtained [see the next section, Eq. (6.3)]. The function $E(g) \sim g^{2/3}$ cannot be described exactly with the aid of Padé approximants, i.e., in the class of rational fractions $P_M(g)/Q_N(g)$. This, however, can be done by changing over from g to a new variable g'; for example, the simplest variant is

$$g' = g(1 + Kg)^{-1/3}, \quad K > 0. \quad (5.3)$$

Rearranging the PT series in powers of g':

$$E(g) = \sum_{k=0}^{\infty} E_k(-g)^k = \sum_{k=0}^{\infty} a_k(-g')^k, \quad (5.4)$$

it is easy to find the connection between the coefficients a_k and E_k (see Appendix B), after which we determine functions similar to (5.2):

$$E_{N'} = \tilde{A}(g') + [N, N+1](g'). \quad (5.5)$$

Here $\tilde{A}(g')$ is the Borel sum of the series

$$\sum_{k=0}^{\infty} \tilde{a}_k(-g')^k,$$

and the Padé approximants $N, N+1 (g')$ are constructed from the differences $a_k - \tilde{a}_k$. It is easy to see that

$$[N, N+1](g') = c_N g^{1/3} + O(1)$$

as $g \to \infty$; the correct asymptotic form of E_N' at infinity is ensured by the same token.

The parameter K in (5.3) can be chosen in principle

from the condition of the fastest convergence of the approximants E_N' with increasing N. We, however, did not carry out such an optimization, and simply fixed K from the condition $a_2 = 0$, which yields $K = 3E_2/E_1 = 3$. This choice, obviously, improves the convergence in the region of small g, but offers no special advantages as $g \to \infty$.

We consider now the calculation results. It is seen from Fig. 2 that the rate at which the coefficients a_k reach the asymptotic values $\tilde{a}_k$ is approximately the same as for the coefficients E_k. Summation of the PT series with the aid of the approximants (5.5) is shown in Fig. 4c. The transition to the functions (5.5) ensures good agreement with the numerical solution[15] up to values $g \sim 500$, i.e., it expands the region of applicability of PT by 3–4 orders of magnitude.

6. *The strong coupling limit:* $g \to \infty$. We consider the Hamiltonian $\mathcal{H}(\alpha, g) = (1/2)p^2 - \alpha/r + gr^N$.

Using a procedure proposed by Symanzik (cited in Ref. 31), we carry out the scale transformation $r \to g^{-1/(N+2)}r$, which yields

$$\mathcal{H}(\alpha, g) = g^{2/(N+2)} \mathcal{H}(\alpha g^{-1/(N+2)}, 1). \quad (6.1)$$

It follows that as $g \to \infty$ the eigenvalues take the asymptotic form

$$E_{nl}(g) = E_{nl}(1, g) \approx c_\infty^{(nl)} g^{2/(N+2)}, \quad (6.2)$$

where the constant $c_\infty^{(nl)}$ coincides with the corresponding eigenvalue of the simpler Hamiltonian

$$H = \tfrac{1}{2}p^2 + r^N.$$

At $N = 1$ and $l = 0$ we obtain the Airy equation. In this case we have for the ns level $c_\infty^{(n)} = 2^{-1/2}\xi_n$, where $-\xi_n$ denotes the n-th zero of the Airy function $Ai(\xi)$, $\xi_n > 0$. In particular, the ground level in the potential (1.2) we have

$$E(g) = c_\infty g^{1/3}[1 + O(g^{-1/3})], \quad c_\infty = 1.8557\ldots \quad (6.3)$$

this determines the behavior of the energy $E(g)$ in the region $g \to \infty$, where PT is certainly not applicable.

We consider now the approximants (5.5). In this case we have at infinity

$$[N, N+1](g') \sim g' \sim g^{1/3}, \quad \tilde{A}(g') \sim g^{-1/3} \ln g \to 0$$

[see Eq. (A.3)]. Therefore $E_N' \approx c_N g^{2/3}$ as $g \to \infty$, i.e., the E_N' account correctly for the functional dependence of E on g in the strong-coupling region. The coefficient c_N is easily expressed in terms of the ratio of the lowest-order coefficients of the numerator and denominator of the fraction $[N, N+1](g')$. It turns out that c_N is numerically close enough to the exact value (6.3) even at $N \sim 10$: $c_{10} = 1.61$, $c_{20} = 1.68$, etc.

We note that the coefficient c_N depends on the choice of the parameter K that enters in the definition of the new variable g'. Variation of this parameter in the interval $1 \leq K \leq 4$ has shown that the character of the convergence of c_N to the limit c_∞ as $N \to \infty$ depends little on the choice of K. Thus, for example, $c_{10} = 1.62$ and $c_{20} = 1.73$ at $K = 2.5$, $c_{10} = 1.28$ and $c_{20} = 1.67$ at $K - 3.5$, etc.

Comparison of these results with Fig. 4b leads to the following conclusion. If we use in the calculations, besides the first PT orders and the asymptotic values of $\bar{E}_k$, also information on the behavior of the exact solution $E(g)$ as $g \to \infty$, we can reconstruct $E(g)$ in a substantially larger region of g (in our example, for practically all $0 < g < \infty$). A similar situation obtains also in the calculation of the Gell-Mann–Low function[8] in field theory with the interaction $g\varphi^4$ (cf. Refs. 22 and 24 in this connection).

The examples considered above show, however, that for a reliable advance into the strong-coupling region the number of exact coefficients of the PT series must be sufficiently large (for example, 42 coefficients E_k of the PT series are used in the calculation of c_{20}).

APPENDIX A

If $\alpha = 1$ in (1.3) and β is a non-negative integer, then the Borel sum of the series with the asymptotic coefficients $\bar{E}_k$ is calculated in finite form

$$S_n(x) = \sum_{k=0}^{\infty} k! k^n (-x)^k = (-1)^{n+1} \{ U_n(x^{-1}) e^{1/x} \text{Ei}(-x^{-1}) + V_n(x^{-1}) \}, \quad (A.1)$$

where Ei is the integral exponential function

$$\text{Ei}(-z) = -\int_z^{\infty} e^{-t} \frac{dt}{t},$$

and U_n and V_n are polynomials defined in Ref. 22. In particular,

$$U_0(z) = z, \quad V_0(z) = 0, \quad U_1(z) = z^2 + z, \quad V_1(z) = z \text{ , etc.}$$

In the case (4.5) we have

$$E(g) = c_0 [(t^2 + t) e^t \text{Ei}(-t) + t], \quad t = 2/3g. \quad (A.2)$$

Let $a_k = k! k^\beta$, $\beta > 0$. The asymptotic form of the sum (A.1) as $x \to$ can be easily obtained with the aid of the Sommerfeld-Watson transformation:

$$S_\beta(x) = \sum_{k=0}^{\infty} a_k (-x)^k$$

$$= (-2i)^{-1} \int_{\sigma-i\infty}^{\sigma+i\infty} \frac{dk}{\sin \pi k} a_k x^k, \quad 0 < \sigma < 1.$$

The singularity of a_k farthest to the right on the complex k-plane is $k = 0$ (if β is not an integer) or $k = -1$ (at $\beta = n = 1, 2, \ldots$). Bending the integration contour to the left, we obtain

$$S_\beta(x) \underset{x \to \infty}{\approx} \begin{cases} -\dfrac{1}{\Gamma(1-\beta)} (\ln x)^{-\beta}, & \beta \neq n \\ \dfrac{(-1)^\beta}{x} [\ln x - (\beta + C) + \ldots], & \beta = n \end{cases}, \quad (A.3)$$

where $C = 0.5772\ldots$. The last equation can be easily obtained also from (A.1), recognizing that

$$U_n(z) = z + O(z^2), \quad V_n(z) = nz + O(z^2), \quad z \to 0.$$

We note that (A.3) remains valid also at $\beta = 0$, as can be verified from the explicit result:

$$S_0(x) = \sum k! (-x)^k = -\frac{1}{x} e^{1/x} \text{Ei}(-x^{-1}). \quad (A.4)$$

APPENDIX B

We indicate the connection between the coefficients E_k and a_k. Let

$$w = g(1 + Kg)^{-\nu}, \quad K > 0 \quad (B.1)$$

[in (5.3), $\nu = 1/3$ and $w = g'$]. Using the binomial series

$$w^k = \sum_{n=0}^{\infty} \frac{\Gamma(k\nu + n)}{\Gamma(k\nu) n!} (-K)^n g^{k+n}$$

and equating in (5.4) the coefficient of like powers of g, we obtain

$$a_0 = E_0, \quad a_1 = E_1, \quad a_2 = E_2 - \nu K E_1$$

and at $k \geq 2$

$$a_k = E_k - \sum_{l=1}^{k-1} \frac{\Gamma(k + (\nu-1)l)}{\Gamma(\nu l)(k-l)!} K^{k-l} a_l. \quad (B.2)$$

These recurrence relations make it possible to calculate a_k in succession from the already known PT coefficients E_k. We obtain now the asymptotic value of a_k as $k \to \infty$. The factorial relation

$$E_k \approx \bar{E}_k = c_0 k! (-a)^k k^\beta, \quad k \to \infty,$$

determines the discontinuity of $E(g)$ on the cut $g = -\xi < 0$:

$$\Delta E(g) = -\pi c_0 (a\xi)^{-(\beta+1)} \exp(-1/a\xi), \quad \xi = -\to +0. \quad (B.3)$$

In the vicinity of point $g = 0$

$$g = w + \nu K w^2 + \ldots, \quad g^{-1} = w^{-1} - \nu K + O(w).$$

It follows therefore that on going from g to a new variable w the coefficient c_0 in (B.3) is multiplied by $\exp(-\nu K/a)$, while the remaining parameters remain unchanged. Therefore the asymptotic forms of the coefficients E_k and a_k differ by the same numerical factor. In particular, for the ground state in the potential (1.2) we obtain

$$\bar{a}_k = A_0 k! \left(\frac{3}{2}\right)^k k, \quad A_0 = -\frac{18}{\pi} \exp\left\{ -\left(3 + \frac{2}{9}K\right)\right\}. \quad (B.4)$$

[1] This name was proposed in Ref. 9.

[2] It suffices to mention such known problems as the anharmonic oscillator,[18] the Stark and Zeeman effects in the hydrogen atom.[17] Also included are most screened-Coulomb-potential variants considered below.

[3] A more detailed exposition of the content of this section is given in Ref. 8.

[4] The quasistationary level $E = E_0 - i\gamma/2$ is located on the lower edge of the cut $g < 0$. This is seen from the following considerations. At $g > 0$ the quasiclassical asymptotic form of the wave function of the bound state is

$$\psi(r) \sim \exp\left(-\int^r |p| dr\right) \sim \exp\left[-(2g)^{1/2} \int^r [v(r)]^{1/2} dr\right], \quad r \to \infty.$$

Corresponding to the quasistationary state is a solution of the type of "diverging wave at infinity," which is obtained from this at $g = \lambda e^{-i\pi}$, $\lambda > 0$.

[5] With account taken of the different normalization of the Hamiltonian, which leads to the relation $E_k' = (-1)^k 2^{k-1} E_k$, where E_k' are the Privman's coefficients,[14] and the E_k were defined above.

[6] In the case (4.5) this sum is calculated explicity—see Appendix A, Eq. (A.2).

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[7] See Ref. 15. We note that $g = 4/\lambda^3$, $E = 2\zeta/\lambda^2$, and λ and ζ are the Schrödinger-equation parameters used in Ref. 15.

[8] A number of workers have shown[32-34] that when the sign of the coupling constant g is reversed in the functional integral for the Green's function, the latter acquire an imaginary part $\propto \exp(-c/|g|)$, $c > 0$. The analogy of this result with the results of Sec. 3 is obvious. When the function integral is analytically continued to complex values of g, a number of subtle problems arise dealing with regularization and renormalization. These problems are considered in particular detail in Ref. 34 for the $g\varphi^4$ scalar field theory.

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