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HIGHER ORDERS OF THE PERTURBATION THEORY AND SUMMATION OF PERTURBATIONAL SERIES IN QUANTUM MECHANICS

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Calculation of higher orders of the perturbation theory is considered for screened Coulomb potentials. Particular cases of such potentials are the Yukawa potential, a familiar object of nuclear physics, and the funnel-shaped potential, applied to analysis of heavy quark-antiquark systems. The calculation of higher perturbational orders is reduced to recursive relations, quite appropriate for computer. The Padé approximants and a modified Padé - Borel summation method are applied for calculation of sums of diverging PT series. A transformation of the variable, removing the nearest singularity of the Borel transform to infinity, is also used. The method enables one to calculate the energy eigen-value $E(g)$ with a good accuracy for all physical values of the coupling constant g, including the case $g \to \infty$. Thus we show that in the considered problems higher orders of the perturbation theory determine the behaviour of $E(g)$ in the region of strong coupling.

1. Introduction

In some recent works /1-3/ the perturbation theory (PT) was developed to high orders in the quantum-mechanical problem of screened Coulomb potential [1],

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

$$f(x) = \sum_{n=0}^{\infty} f_n (-x)^n , \quad f_0 = 1 ; \quad x = \mu r \qquad (1.2)$$

Treating μ as a small parameter, one can construct perturbational series for the energy eigen-values,

$$E^{(n,l)}(\mu) = \sum_{k=0}^{\infty} E_k^{(n,l)} \mu^k \qquad (1.3)$$

and for the wave functions. Here $n = 1, 2, \ldots$ is the principal quantum number, l is the orbital momentum, $0 \leqslant l \leqslant n-1$, and k is the PT order. To calculate E_k we use the logarithmic perturbation theory (LPT), for its use is quite suitable for nodeless states (see in /2-9/, and in the following Section). This method enables us, with account for the available computer facilities, to calculate easily 100 - 200 orders of PT for a number of problems: the anharmonical oscillator, $g(\vec{x}^2)^N$, in space of an arbitrary dimensionality D, N =2, 3,..., see the works /5,6/; the Stark /7/ and Zeeman /9/ effects in the hydrogen atom; the screened Coulomb

potential /2,3/, etc.

However, such calculations do not solve the important problem of determination of the energy eigen-values, since the real physical problems are relevant to the region of $\mu \sim 1$, or even $\mu \gg 1$ (like the region of strong coupling in quantum field theory). Meanwhile, the PT coefficients E_k, as a rule, have a factorial increase with $k \to \infty$,

$$\lim_{k\to\infty} E_k / \tilde{E}_k = 1, \qquad \tilde{E}_k = (k\alpha)!\, a^k k^\beta c_0 \tag{1.4}$$

where $z! \equiv \Gamma(z+1)$, and $\alpha > 0$, β, a and c_0 are some constants that can be calculated. The reason of this rise is that in the situation, typical in quantum mechanics and field theory, the perturbation operator has a stronger singularity than the unperturbed Hamiltonian H_0.

Because of the estimate (1.4), the PT series (1.3) have zero convergence radius; in other words, they are only asymptotical. Therefore, in order to reconstruct the eigen-value $E(\mu)$ with the PT coefficients E_k one has to apply the special methods of summation of diverging series /10/.

In the present work we consider calculation of higher PT orders E_k, their asymptotics $\tilde{E}_k$, and summation of diverging PT series for screened Coulomb potentials. The results of the summation are compared with the values of the energy obtained by means of other methods[2]. The comparison shows that in spite of the factorial rise of the PT coefficients E_k, the summation methods considered enable one to reconstruct the energy eigen-values with a fair accuracy even far beyond the region of the weak coupling. This fact excites a hope that the method can be applied successfully to other problems of quantum mechanics and field theory.

2. Logarithmic perturbation theory

Calculation of higher PT orders in quantum mechanics has been considerably advanced during the recent years as a result of the development of LPT (a few comments on the history are given in Appendix A). Using LPT one can reduce the calculation of higher PT orders for polynomial potentials to recursive relations, that are quite convenient for computer calculations.

Let us consider in brief the idea of this method, taking the screened Coulomb potential (1.1) as an example. Here we restrict ourselves to the states with l=n-1, the corresponding radial wave functions have no nodes[3]. The application of LPT to this case is especially simple.

The substitution

$$R(r) = const \cdot \rho^{n-1} \exp\left\{-\int_0^\rho y(\rho')\,d\rho'\right\}$$

$$\rho = r/n\,, \qquad E = -\varepsilon/2n^2$$

transforms the Schroedinger equation to the form

$$\frac{dy}{d\rho} = -\varepsilon + \frac{2n}{\rho}(f-y) + y^2 \tag{2.1}$$

where $f \equiv f(n\rho)$; R is the radial wave function. Expanding ε and y in formal power series,

$$\varepsilon = \sum_{k=0}^{\infty} (-\mu)^k \varepsilon_k\,, \qquad y(\rho,\mu) = 1 - \sum_{k=2}^{\infty} (-\mu)^k y_k(\rho) \tag{2.2}$$

one has the lowest orders of PT. $\varepsilon_0 = y_0 = 1$, $\varepsilon_1 = 2n^2 f_1$, $y_1 \equiv 0$, and for $k \geq 2$ one gets a differential equation for any $y_k(\rho)$, which is easily solvable by quadrature. It is easily seen that y_k is a polynomial of degree (k-1) :

$$y_k(\rho) = \sum_{j=1}^{k-1} c_j^{(k)} \rho^j \ , \quad k \geq 2 \qquad (2.3)$$

the highest coefficient here is $c_{k-1}^{(k)} = n^{k+1} f_k$, and other coefficients are determined by the recursive relations

$$c_j^{(k)} = (n + \frac{j+1}{2}) c_{j+1}^{(k)} + \frac{1}{2} \sum_{l=2}^{k-2} \sum_{\lambda+\varkappa=j} c_\lambda^{(l)} c_\varkappa^{(k-l)} \qquad (2.4)$$

$1 \leq j \leq k-2$. Lowering the subscript consecutively, at the last step, $j=1$, one gets the correction $\sim \mu^k$ to the energy eigen-value,

$$E_k = (-1)^{k+1} \frac{n+1/2}{n^2} c_1^{(k)} \qquad (2.5)$$

This completes the k-th order PT calculation.

A few comments are appropriate here.

1) Eqs.(2.4) hold for arbitrary screening function $f(\mu r)$. In order to get the formal PT series one has just to assume that Taylor's series (1.2) exists for $f(x)$ near the point $x=0$.

2) In the end, the quantities $c_j^{(k)}$ and E_k are expressed in terms of Taylor's coefficients f_k of the screening function. For instance,

$$c_{k-2}^{(k)} = \frac{1}{2} n^{k+1} \left[(2n+k-1) f_k + n \sum_{l=2}^{k-2} f_l f_{k-l} \right] ,$$

$$c_1^{(k)} = (n+1)\, c_2^{(k)} \qquad \text{at} \quad k \geq 3 .$$

3) The first two orders of the PT expansion are $E_1 = f_1$, $E_2 = -n(n+1) f_2$. The higher terms are

$$E_k = \frac{(n+1)(2n+1)}{2^{k-2}} (-n)^{k-1} Q_k \ , \quad k \geq 3 \qquad (2.6)$$

and Q_k is a polynomial of degree $k-3$ with respect to n. It con-

tains terms of the form $f_a f_b \dots f_c$, where $a+b+\dots+c=k$, and every subscript $a,b,\dots,c \geq 2$. For example,

$$Q_3 = f_3 \ , \quad Q_4 = (2n+3) f_4 + n f_2^2 \ ,$$

$$Q_5 = (2n+3)(2n+4) f_5 + 2n(4n+5) f_2 f_3 \ , \dots$$

It is not difficult to go on with these computations, using a routine for algebraic programming by means of computer. One should have in mind, however, that with increasing k the explicit expressions for Q_k in terms of f_n become too cumbersome rapidly (cf. also in /14,15/). A more suitable way is to calculate higher orders in PT for any particular screening function, using Eqs.(2.4), (2.5), substituting the corresponding coefficients f_k.

4) The above equations determine the perturbative expansion not only for the level energy, but also for the wave function. The relevant formulae are presented in Appendix B.

Let us consider some examples. Start from the Yukawa potential,

$$f(x) = e^{-x} \ , \quad f_k = (k!)^{-1} \qquad (2.7)$$

Replacing the coefficients in (2.3) by $c_j^{(k)} = 2^{j+1-k}(k!)^{-1} n^{k+1} A_j^{(k)}$, one has $A_{k-1}^{(k)} = 1$, and

$$A_j^{(k)} = (2n+j+1) A_{j+1}^{(k)} + n \sum_{l=2}^{k-2} \binom{l}{k} \sum_{\lambda+\varkappa=j} A_\varkappa^{(l)} A_\lambda^{(k-l)} \qquad (2.8)$$

Clearly, all $A_j^{(k)}$ are positive integers, so the computer calculations do not lead to a loss of the accuracy. The result is $E_1 = 1$, $E_2 = -\frac{1}{4} n(2n+1)$, and for $k \geq 3$,

$$E_k^{(n,n-1)} = (-1)^{k+1} \frac{(n+1)(2n+1) n^{k-1}}{2^{k-2} k!} A_2^{(k)} \qquad (2.9)$$

The quantity $A_2^{(k)}$ is a polynomial of degree k-3 with respect to n ,

$$A_2^{(4)} = 8n+3, \quad A_2^{(5)} = 84n^2+114n+12,$$

$$A_2^{(6)} = 1408n^3+2868n^2+1464n+60,$$

$$A_2^{(7)} = 28\,240n^4+85\,320n^3+78\,540n^2+$$

$$+19\,500n+360, \quad \ldots$$

We have calculated 25 PT orders using the algebraic programming system REDUCE-2. The results are in agreement with a previous paper /14/, where first 4 orders were calculated for states with l=n-1 (see Eq.(57) in /16/). Comparing our procedure here with that in Ref.16 , one sees to what extent LPT simplifies the calculations.

For the ground state, n=1 , the PT coefficients (2.9) are in agreement with those given in preceding works /1,2/; see Table 1 in Ref.1 , where 100 PT orders are presented [4].

The screening function for the Hulthen potential is

$$f(x) = x(e^x-1)^{-1}, \qquad f_k = (-1)^k B_k/k! \tag{2.10}$$

where B_k are the Bernoulli numbers /17/. Since $f(-x)-f(x) = x$, here $f_3 = f_5 = f_7 = \ldots = 0$, and all odd PT orders, starting from the third order, are zero. By means of Eqs.(2.4) we get at once:

$$E^{(n,n-1)}(\mu) = -\frac{1}{2n^2} + \frac{1}{2}\mu - \frac{1}{12}n(n+1/2)\mu^2 -$$

$$-\frac{1}{480}(n^2-1)(n+1/2)[\mu^4 + a_6\mu^6 + a_8\mu^8 + \ldots] \tag{2.11}$$

where

$$a_6 = \frac{1}{504}(64n^2+35n-60), \ldots$$

etc. For the ground level $E_k=0$ at $k\geq 3$, in agreement with the exact solution /18/ of the Schroedinger equation,

$$E_{10}(\mu) = -\frac{1}{2}(1-\mu/2)^2$$

The last example to be considered here is the potential[5]

$$V(r) = -\frac{1}{r} + g r^N, \quad N=1,2,\ldots \tag{2.12}$$

which fits the pattern (1.1) with $\mu = g^{1/(N+1)}$, $f(x) = 1-x^{N+1}$. Only integer powers of g are present in the expansion of E, so non-vanishing terms in the series $E = \sum \tilde{E}_k \mu^k$ are those with $k = N+1, 2(N+1), 3(N+1)$ etc. It is more reasonable to write the PT series directly in powers of g, not μ,

$$E = \sum_{k=0}^{\infty} E_k g^k,$$

$$y = -\frac{d}{dr}\ln[r^{1-n}R(r)] = \sum_{k=0}^{\infty} y_k(r)(-g)^k,$$

$$y_0 = \frac{1}{r},$$

$$y_k = -\sum_{j=1}^{kN} a_j^{(k)} r^j$$

for $k\geq 1$. Substituting these expansions in the Riccati equation

$$y' + \frac{2n}{r}y - y^2 = 2(E + \frac{1}{r} - g r^N)$$

we get the recursive relations

$$a_j^{(k)} = \frac{n}{2}\left[(2n+j+1)a_{j+1}^{(k)} + \sum_{l=1}^{k-1}\sum_{\lambda+\varkappa=j} a_\lambda^{(l)} a_\varkappa^{(k-l)}\right] \tag{2.13}$$

where $\lambda, \varkappa \geqslant 1$. With these relations one is able to decrease j at any fixed k , and $E_k=(-1)^k(n+\frac{1}{2})a_1^{(k)}$. However, one has first to find the higher coefficient in the polynomial $y_k(r)$with j=kN. With a provisional notation $\alpha_k = a_{kN}^{(k)}$, we obtain from (2.13) a closed equation

$$\alpha_k = \frac{n}{2} \sum_{\ell=1}^{k-1} \alpha_\ell \, \alpha_{k-\ell} \quad , \quad \alpha_1 = n$$

Because of this relation, the generating function for these numbers, $G(z) = \sum_{k=1}^{\infty} \alpha_k z^k$, satisfies the equation $G = \frac{1}{2}nG^2 + nz$. Its solution is $G(z) = \frac{1}{n}\left(1-(1-2n^2z)^{\frac{1}{2}}\right)$, so

$$\alpha_k = a_{kN}^{(k)} = \frac{n^{2k-1}}{2^{k-1}} C_k \tag{2.14}$$

where C_k are the Catalan numbers, used in the combinatorial analysis: $C_1 = C_2 = 1$, $C_3 = 2$, $C_4 = 5$, $C_5 = 14$ etc. As usual, we get the correction to the level energy at the last step j=1, $E_k=(-1)^k(n+\frac{1}{2})a_1^{(k)}$. The substitution

$$a_j^{(k)} = \frac{n^{(N+2)k-j-1}}{2^{(N+1)k-j-1}} \mathcal{Z}_j^{(k)} \tag{2.15}$$

reduces the problem to recursive equations with integers,

$$\mathcal{Z}_{kN}^{(k)} = C_k \equiv \frac{(2k-2)!}{k!\,(k-1)!} \quad ,$$

$$\mathcal{Z}_j^{(k)} = (2n+j+1)\,\mathcal{Z}_{j+1}^{(k)} + \sum_{\ell=1}^{k-1} \sum_{\lambda+\varkappa=j} \mathcal{Z}_\lambda^{(\ell)} \mathcal{Z}_\varkappa^{(k-\ell)} \tag{2.16}$$

$1 \leqslant j \leqslant kN-1$. The first-order PT correction to the energy of the (n,n-1) level is

$$E_1 = n^N\left(n+\frac{N}{2}\right)\left(n+\frac{N-1}{2}\right)\ldots\left(n+\frac{1}{2}\right) \quad , \tag{2.17}$$

and for $k \geq 2$,

$$E_k = (-1)^{k+1} \frac{n^{(N+2)k-2}}{2^{(N+1)k-3}} (n+1)(n+\tfrac{1}{2}) Z_2^{(k)} \qquad (2.18)$$

It is noteworthy that the nonlinearity N is not present explicitly in Eqs.(2.16). It determines the number of the recursive relations for a given order of PT, k. A similar situation takes place also in the case of the anharmonical oscillator /6/, that is the system with the Hamiltonian

$$H = \vec{p}^2 + \vec{r}^2 + g(\vec{r}^2)^N, \quad \vec{r}^2 = \sum_{i=1}^{D} x_i^2 \qquad (2.19)$$

Thus LPT is an effective method for calculation of higher orders in the PT expansions for the screened Coulomb potential, as well as in other quantum-mechanical problems /5-9/. Eqs.(2.16) were used already /2/ for calculation of the coefficients E_k for the cases N= 1, 2.

We do not concern here an interesting variant of LPT, introduced in Ref.4 (there it is called "perturbation theory in deviation from the asymptotics"). In that case the expansion is not in powers of the coupling constant g, but in more complicated functions of g. The choice of the zero approximation takes into account the behaviour of the exact wave function at singular points of the potential V(r), say at $r = 0, \infty$. The method leads to iterations converging rapidly, as it was shown in a number of examples: the anharmonical oscillator /4,21,22/, the Stark effect in the hydrogen atom /23/ etc. The fact essential for the calculations is that the k-th order in the perturbation theory is expressed by means of quadratures of the preceding order. Further details of the method are given in Refs.21,22.

3. WKB method and asymptotics of higher PT orders

Let us consider the Hamiltonian[6] $H = \frac{1}{2}p^2 - 1/r + gv(r)$. It is known /24/ that in order to calculate the $k \to \infty$ asymptotics of the PT coefficients E_k one has to find the discontinuity of the level energy at the cut $g<0$,

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

and to apply the dispersion relations:

$$E_k = \frac{(-1)^{k+1}}{2\pi}\int_0^\infty \frac{d\lambda}{\lambda^{k+1}}\gamma(\lambda), \quad k>k_0 \tag{3.1}$$

where $\lambda = -g$, and k_0 is the number of subtractions. At $g<0$ the potential barrier tunnelling becomes possible for the particle, see Figure 1, and the bound state is transformed into quasi-stationary, of a complex energy $E = \mathcal{E}_0 - i\gamma/2$. The asymptotics, $\widetilde{E}_k$, is determined by the behaviour of the level width γ at $g \to -0$, and the WKB method is quite appropriate for the problem. The result is

$$\gamma(\lambda) = \gamma_0 \exp\{-2\mathcal{J}(\lambda)\} \tag{3.2}$$

where

$$\mathcal{J}(\lambda) = \int_{r_-}^{r_+} |p|\,dr, \quad |p(r)| = \left\{-2E - \frac{2}{r} + \frac{\Lambda^2}{r^2} - 2\lambda v(r)\right\}^{1/2}$$

$$\gamma_0 = \frac{(n+\Lambda)^{n+\Lambda}(n-\Lambda)^{n-\Lambda}}{(n+l)!\,(n-l-1)!\,n^3}\,e^{-2n} \tag{3.3}$$

$\Lambda = l = 0$ for the S states, $\Lambda = l+\frac{1}{2}$ at $l \neq 0$, $r_\pm$ are the turning points. Some details on the derivation of these formulae may be found in Ref.2. One should have in mind that the accuracy of Eq.(3.2)

is asymptotical in the limit $\lambda \to 0$. The formula can be rewritten also in another form,

$$\gamma(\lambda) = A \frac{\omega_{cl}}{2\pi} \exp\left\{-2\int_{r_-}^{r_+} |p(r)|\,dr\right\} \qquad (3.4)$$

where

$$\omega_{cl} = n^{-3}, \qquad A = \begin{cases} [Q(n)]^2 , & l = 0 \\ q(n+\lambda)\,q(n-\lambda) , & l \geq 1 \end{cases}$$

$$Q(x) = \frac{\sqrt{2\pi x}\,(x/e)^x}{\Gamma(x+1)} , \qquad q(x) = \frac{\sqrt{2\pi}\,(x/e)^x}{\Gamma(x+1/2)}$$

and $e=2.71828\ldots$. The physical meaning of Eq.(3.4) is quite clear. Note that $\omega_{cl} = 2\pi/T$, where $T = \pi(2|E_0|^3)^{-\frac{1}{2}} = 2\pi n^3$ is the period of the classical particle motion on the Kepler ellipse, $E_0 = -1/2n^2$. So $\omega_{cl}/2\pi$ is the frequency of the particle impacts against the potential barrier at $r = r_-$, and the exponent in (3.4) is the probability of tunnelling at every impact. If the WKB approximation would be exact for arbitrary quantum numbers n and l, the coefficient A would be just 1. This is the case for large quantum numbers, since at $x \to \infty$ the expansions take place

$$Q(x) = 1 - \frac{1}{12x} + \frac{1}{288x^2} + \ldots ,$$

$$q(x) = 1 + \frac{1}{24x} + \frac{1}{1152x^2} + \ldots$$

However, the deviation of A from 1 is small also for n, l not very large, see Table 1. Even for the ground state $A = 2\pi e^{-2} = 0.8503\ldots$. Thus the domain of applicability of the WKB method is extended toward $n \sim 1$ (as it was observed in a number of other physical problems, see e.g. Refs.25,25a).

The function $gv(r)$, perturbation to the Coulomb potential, was not specified until now. Consider the potential (2.12). In this case, the integral $J(\lambda)$ is easily calculated for $l=0$, see Appendix B. Parameters of the asymptotics (1.4) are

$$\alpha = N, \quad \beta = 2n-1, \quad a = -A_N n^{N+2}, \tag{3.5}$$

where

$$A_N = 2\pi^{-N/2} \left\{ \Gamma\left(\frac{3N+2}{2N}\right) / \Gamma\left(\frac{N+1}{N}\right) \right\}^N$$

The coefficient c_0 in (1.4) for the funnel-shaped potential is

$$C_0 = -\frac{1}{2\pi (n \cdot n!)^2} \left(\frac{36}{e^3}\right)^n, \quad N=1 \tag{3.6}$$

For the ground state in the case of an arbitrary nonlinearity $N>1$ it is

$$C_0 = -2^{4/N-1} \left\{ \frac{(N+2)\Gamma\left(\frac{N+2}{2N}\right)}{\pi \Gamma\left(\frac{N+1}{N}\right)} \right\}^2 \tag{3.7}$$

Now we turn to the angular momentum dependence of the asymptotics $\tilde{E}_K$. The l-dependence of the pre-exponential factor in Eq.(3.2) is very slight, it is

$$\frac{\gamma_0(n,l)}{\gamma_0(n,0)} = \frac{q(n+\lambda)q(n-\lambda)}{[Q(n)]^2} = 1 + \frac{3n^2-2\lambda^2}{12n(n^2-\lambda^2)} + \dots \tag{3.8}$$

for $n \gg 1$, $l \neq 0$. The deviation from 1 is maximal for $l=n-1$, when

$$\frac{\gamma_0(n,n-1)}{\gamma_0(n,0)} = \begin{cases} 1.182, & n=2, \\ 1.145, & n=3, \\ (\pi/e)^{\frac{1}{2}} = 1.075\dots, & n \to \infty. \end{cases} \tag{3.9}$$

As to the integral $J(\lambda)$, its l-dependence for $N>1$ manifests

itself only in the terms, vanishing at $\lambda \to 0$, see Appendix B . If N=1, the constant b_3 in Eq.(C.7) depends on l. To conclude, the parameters α, β and a in the asymptotics (1.4) do not depend on l.

Finally, let us consider the Yukawa potential (2.7). Calculate the integral $J(\lambda)$ at $\lambda \to +0$, substitute it in the dispersion integral (3.1), and apply the steepest descent method to find the asymptotics for ns states /3/. The result is

$$E_k \sim (-1)^{k+1} k! \left(\frac{n}{2 \ln k}\right)^k , \quad k \to \infty \qquad (3.10)$$

(some details of the calculation are given in Appendix C). The obtained asymptotics is somewhat unusual, it is not $E_k \sim k! a^k$,as for a polynomial perturbation.

In the examples considered, higher orders of the perturbation theory rise as factorials at $k \to \infty$. Therefore to reconstruct the energy $E(g)$, having known the PT coefficients, one has to apply special methods of summation of divergent series.

4. Summation of PT series

The summation of the PT series will be applied to the Yukawa and funnel-shaped potentials[7]. We will show that, with a number of PT coefficients E_k calculated exactly, and with their asymptotics $\tilde{E}_k$, it is possible to reconstruct the energy $E(g)$ not only for $g \to 0$, but also in the strong coupling region, $g \gg 1$.

Start from the Yukawa potential (2.7). This is an example of especial physical importance, as it is involved very often in atomic and nuclear physics, theory of solid state, plasma physics (the Debye screening) etc. As it is seen from (3.10), the PT series

in this case is asymptotical, not converging. For the summation we use the Padé approximants (PA), $[M/N](\mu) = P_M(\mu)/Q_N(\mu)$. Here P_M and Q_N are polynomials of orders M and N, respectively, that are determined unambiguously from first M+N+1 coefficients of the PT expansion, by means of the condition

$$E(\mu) = \sum_k E_k \mu^k = [M/N](\mu) + O(\mu^{M+N+1}) \qquad (4.1)$$

(explicit expressions for P_M and Q_N are presented, say, in Ref. 28). We use diagonal PA , i.e. M=N.

The results of summation of PT series are shown in Figures 2 and 3, respectively, for the cases l=0 (the ground state) and l= =n-1, n≥2. A rapid convergence of PA $[N/N](\mu)$ with increase in N is seen in Figure 2 (more details can be found in Table 2). With rising μ , the bound energy is increased, and λ falls. At certain value of $\mu = \mu_{cr}$ the quantities E and λ are equal to zero, and the real bound state disappears. As it is seen from Figure 2 , PA provide with the sum of the PT series not only for $\lambda > 0$, but also for $\lambda < 0$ (this region corresponds to a virtual level in the case l=0). It is interesting to compare Figure 2 with a problem having an exact solution. In the case of the Hulthen potential /18/ one has for ns states

$$\lambda = \frac{1}{n} - \frac{n}{2}\mu , \qquad \mu_{cr}(ns) = 2n^{-2} \qquad (4.2)$$

Thus $\lambda = (-2E_{ns})^{\frac{1}{2}}$ is a linear function of the screening parameter μ in this case. For the Yukawa potential the μ-dependence of λ is also close to linear for $\mu \gtrsim \mu_{cr}$, see Figure 2 . Besides, the n-dependence of $\mu_{cr}(ns)$ is also similar to (4.2), see Figure 4.

As for the states with l≠0, all curves corresponding to $2 < l < 10$ in Figure 3 lie between the curves for l=2 and l=10. Thus the angular momentum dependence of $\mathcal{E}$ is rather slow, in the reduced va-

riables $\mathcal{E} = 2n^2 E^{(nl)}$ and μ/μ_{cr}.

The calculated magnitudes of μ_{cr} are given in Table 3. There is a slight loss of the accuracy in calculation of μ_{cr} by means of PA when we go from l=0 to l=1, then the accuracy is improved again. The agreement between the summation of the PT series and the numerical solution of the Schroedinger equation for this case/11/ is perfect.

If $l \neq 0$, then for $\mu > \mu_{cr}$ the bound state is replaced by the Breit-Wigner resonance: $E = E_0 - i\Gamma/2$,

$$E_0 \sim \mu - \mu_{cr}, \quad \Gamma \sim (\mu - \mu_{cr})^{l+1/2} \qquad (4.3)$$

Meanwhile, for s states one has for μ near the critical value μ_{cr}

$$\lambda \sim \mu_{cr} - \mu, \quad E \sim -(\mu - \mu_{cr})^2 \qquad (4.4)$$

This is an effect of a qualitative difference between the states with l=0 and $l \geq 1$ that is due to a presence of a centrifugal barrier in the latter case, which is essential for slow particles.

For the funnel-shaped potential (2.12), the problem of reconstruction of the energy E(g) from the PT coefficients is reasonable in the whole region $0 < g < \infty$, but its solution requires more powerful methods than PA. Such a method, and very suitable for physical applications, is the Padé - Borel method (see e.g. Refs.29, 30). If at $k \to \infty$ the asymptotics is $E_k \sim (k\alpha)!$, we put

$$E(g) \equiv \sum_k E_k g^k = \alpha^{-1} g^{-1/\alpha} \int_0^\infty \exp\left\{-\left(\frac{x}{g}\right)^{1/\alpha}\right\} x^{\frac{1-\alpha}{\alpha}} B(x)\,dx, \qquad (4.5)$$

where

$$B(x)=\sum_k b_k x^k \quad , \quad b_k = E_k/\Gamma(k\alpha+1) \qquad (4.6)$$

Because of (1.4), the nearest singularity of the Borel transform B(x) is situated at the point $x_0=a^{-1}$, and $B(x)\sim(x-x_0)^{-2}$ at $x\to x_0$. Substituting in the integral (4.5) the function B(x) by a PA $[M/N](x)$, constructed with the coefficients b_k, we get an approximate for the energy E(g). As it is well known /28/, a use of PA enables one to reconstruct B(x) outside the circle of convergence.

Note that the behaviours of the functions E(g) and B(x) at infinity are essentially identical. Actually, the asymptotics

$$E(g)\approx c_\infty g^\nu(1+b_1 g^{-\nu_1}+\ldots), \quad g\to\infty \qquad (4.7)$$

corresponds to

$$B(x)\underset{x\to\infty}{\approx} c_\infty x^\nu\left[\frac{1}{\Gamma(\alpha\nu+1)}+\frac{b_1}{\Gamma(\alpha(\nu-\nu_1)+1)}x^{-\nu_1}+\ldots\right], \qquad (4.8)$$

(here $\nu>-1$, $0<\nu_1<\nu+1$). Taking this fact into account one can use the following equality in order to find the index of the asymptotics ν in Eq.(4.7):

$$\nu=\lim_{x\to\infty} x\,B'(x)/B(x) \qquad (4.9)$$

as well as the following identity, for $\nu>-1$,

$$\nu=-1+\lim_{x\to\infty} x\,B(x)/\int_0^x B(x')dx' \qquad (4.10)$$

Numerators and denominators in these fractions were replaced with the diagonal PA's $[L/L](x)$. To calculate the index ν one has to find the limit of $\nu_N(x)$ at $N\to\infty$ and fixed x, and then let x tend to infinity. For illustration, the corresponding quantities at $x=100$, calculated by means of (4.10), are given in Table 4. For $L>10$ the convergence of ν_L is rapid enough. The averaged value $\overline{\nu}$, calculated over the last five iterations ν_L, deviates from the exact quantity $\nu=\frac{2}{3}$ by a small number of 0.5 %. Thus this simple method enables one to determine the index of the asymptotics of the energy eigen-value $E(g)$ at $g\to\infty$, basing on the coefficients E_L of the diverging PT series. Eq.(4.9) leads to similar results, though the convergence of ν_L with rising L is somewhat slower. The result is $\overline{\nu}=0.70\pm0.02$ for $L = 10$-14. /26/

More sophisticated methods are necessary to calculate the coefficient c_∞. We use the substitution

$$y = x/(1-ax)^{1-\nu} \qquad (4.11)$$

where a is the same parameter, as in Eq.(1.4). The substitution (4.11) removes the nearest singularity of the Borel transform $B(x)$ to infinity: $y\to\infty$ when $x\to x_0 = a^{-1}$. Besides, $B(x)\sim x^\nu\sim y$ at $x\to\infty$, and such a behaviour is easily reproduced by means of PA[8] $[N+1/N](y)$ for any ν. These Pade approximants are determined from the coefficients β_k of the series rearranged in terms of powers of the new variable y,

$$B(x)=\sum_k b_k x^k = \sum_k \beta_k y^k \qquad (4.12)$$

(see Appendix D). As one should expect, the transformation (4.11) leads to a sharp decrease in the coefficients. For instance, for $N=1$ we have $E_{10}=-3.281\cdot10^8$, $b_{10}=-90.4$ and $\beta_{10}=0.0883$, and for $N=2$; $E_{10}=8.581\cdot10^{18}$, $b_{10}=-3.53$ and $\beta_{10}=-0.00187$. For higher PT

orders the decrease in the coefficients is even more manifest, see Figure 5. Therefore the series $\sum \beta_k y^k$ is summed up easily. It follows from Eqs.(4.8) and (4.11) that

$$c_\infty^{(N)} = \Gamma(\alpha\nu+1)(-a)^{\nu-1} \lim_{y\to\infty} y^{-1}\,[N+1/N](y) \qquad (4.13)$$

For the funnel potential, Eq.(2.12) with N=1, we get $c_\infty = 1.764$ at M=15, to be compared with the exact quantity $c_\infty = 1.855\,756...$ (see Appendix D).

Now we turn to calculation of the energy E(g) at finite values of the coupling constant g. In the case N=1 we have $E_k \sim k!$, i.e. $\alpha=1$ in (4.5). Substituting B(x) in (4.5) by its PA $[L+1/M](y)$ and calculating the integral numerically, one obtains E(g). As it is seen from Table 5, at M = 15 and $g \sim 1000$, the error in E(g) does not exceed 2 %, and the accuracy is sharply improved for lower g. The method used here to sum up the diverging PT series, enables one to obtain the ground state energy with a good accuracy for all physical magnitudes of the coupling constant, $0 < g < \infty$.

The summation of the PT series for the oscillator well, Eq.(2.12) with N=2, was carried out in the same manner. In this case $E_k \sim (2k)!$ and the divergence of the PT series is even worse, so the reconstruction of the energy E(g) in the strong coupling region basing on the coefficients E_k is more difficult. In particular the index of the asymptotics ν is found with a poorer accuracy than in the preceding case (see Table 4). Since $\alpha=2$, the Borel integral (4.5) at $g \gg 1$ converges slower than in the case $\alpha=1$. This fact, in turn, requires a calculation of the Borel transform B(x) for higher values of the variable x.

The results of calculation[10] of the energy E(g) are given in Table 6, and it is seen that the usual PA $[L/L+1](g)$ are invalid even for $g \sim 0.15$. Using the Pade - Borel approximants one gets E(g)

at $g \sim 0.1$ with a high accuracy and the results are satisfactory up to $g \sim 5$. In the examples considered the diagonal approximants $[L/L]$ converge to the limit most rapidly, a similar situation was found also in a number of other problems /27/.

The effectiveness of the Pade - Borel summation method can be appreciated properly comparing it with the conventional perturbation theory. The PT polynomials

$$P_L(g) = \sum_{k=0}^{L} E_k g^k \qquad (4.14)$$

for N=1 and 2 are shown in Figure 5. The boundaries of the domain of applicability for PT are at $g \sim 0.1$ and $g \sim 0.01$, respectively. The estimate is in agreement with the formula /31/

$$g \lesssim \frac{1}{a}\left(\frac{e}{La}\right)^{a} = \begin{cases} 1.84\, L^{-1}, & \text{for } N=1 \\ 2.28\, L^{-2}, & \text{for } N=2 . \end{cases} \qquad (4.15)$$

With rising L, the number of terms in the PT series, taken into account in (4.14), the domain of the approximation of $E(g)$ by means of the polynomials $P_L(g)$ is contracted, so it is necessary to abandon the usual PT and to apply the special summation methods. The behaviour of the PT polynomials in other problems is analoguous. See e.g. Figure 6, relevant to the Yukawa potential (the comparison to Figure 2 illustrates the effectiveness of the use of PA instead of the standard PT polynomials).

Note that for the potentials of the type (2.12) the PT series is summable by means of the Borel method /32/. In this case higher PT orders contain an information on the behaviour of the exact solutions in the region of strong coupling, in spite of the factorial increase in the coefficients E_k. An effective method for the reconstruction of $E(g)$ for $g \gg 1$ was considered above. From the examples

considered it is evident , however, that to apply the method successfully one needs a sufficiently high number of PT coefficients calculated exactly[11].

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Appendix A

There is an increasing interest in calculations of higher perturbational orders during the past few years. The structure of PT series was investigated thoroughly for energy levels in one-dimensional /24/ and multidimensional /4,6/ anharmonical oscillators and for a number of other quantum-mechanical problems /1-9/. Bender and Wu /24/ established a relation between the asymptotics of the energy coefficients E_k, for $k \to \infty$, and the width of the unstable state, appearing when the coupling constant g gets the opposite sign; they have also shown that the WKB method is applicable to the calculation. Extension of these methods to quantum field theory was originated by Lipatov /34/, who developed a semiclassical method for calculation of the functional integral and applied this technique to a renormalizable scalar field theory with the interaction

$$H_{int} = \frac{g}{n!} \int \varphi^n d^D x \quad , \qquad D = \frac{2n}{n-2}$$

(in particular, for D=4 we have the φ^4 field theory). Further this region was elaborated intensively by a number of authors; see for example Refs.30, 35-37 and the reviews /38,39/.

The standard quantum-mechanical PT methods require a knowledge of the whole spectrum of the unperturbed Hamiltonian, for the PT orders higher than the first one. The main difficulty in such calculations lies usually in calculation of spectral sums that are involved in formulae of the Rayleigh - Schroedinger perturbation theory. One of the possible ways to avoid the difficulty is to formulate the PT expansion in terms of the logarithmic derivative of the wave function, that is a solution of the Riccati equation.

It is for a long time that this method has been applied to one-dimensional problems . Zeldovich /40/ (see also in the book, /41/,p.143) was first who has indicated that the whole perturbation theory for a state belonging to the discrete spectrum can be constructed with the unperturbed wave function for only the level, corrections to which are to be found. The following expression was obtained for the second correction to the energy of the bound state, by means of the Lagrange method,

$$E_2 = \int\int [E_0 - \chi_0^2(x)]\,[E_0 - \chi_0^2(x')]\,dx\,dx'$$

The calculation of higher PT orders based on the Riccati equation was considered exhaustively by Polikanov /42/. The author has shown that any PT order for the energy eigen-value in the discrete spectrum can be calculated, in principle, in terms of the wave function of the zeroth approximation. The method was applied to the Dirac equation in Ref.43 . The particular scheme for calculation of k-th order of the perturbation theory, developed in Refs.42,43, is rather cumbersome for $k>2$. For instance, one has to normalize the wave function with the accuracy up to μ^{2k} for the k-th PT order, to exponentiate power series etc. In Ref.42 seven lower PT orders were calculated for the ground state energy in the Yukawa potential. The coefficients E_6 and E_7 in that work do not coincide with those in Eq.(2.9) and are wrong.

The method of construction of the perturbation theory basing on the Riccati equation, instead of the Schroedinger equation, was rediscovered recently /4,8,9/. For the one-dimensional problems it was shown that the k-th PT order is expressed in terms of the lower corrections by means of quadratures in a closed form. For the potentials of the type

$$V(x) = \sum_{k=-2}^{n} c_k x^k$$

(in particular, for polynomial potentials) the method is further simplified. The calculation of higher PT orders is reduced to simple recursive relations. This approach to PT is rather effective, as it was shown in Section 2. The same method was applied to higher PT corrections for anharmonical oscillator, the perturbation is $g(x^2)^N$ N=2, 3,..., in space of arbitrary dimensionality/4-6/, for the Stark effect /7/, Zeeman effect /9/ in hydrogen atom, the atom in crossed fields /9/ etc. The use of the recursive relations enables one to calculate easily a great number of PT orders, that are inaccessible for the standard variant /13/ of PT.

The application of LPT is especially successful for nodeless states. If the wave function has a node the problem is somewhat more complicated. The logarithmic derivative of a function $R(r) \sim (r-r_0)^n$ has the pole,

$$R'/R = \frac{n}{r-r_0} + O(1), \quad r \to r_0 ,$$

and the singularity is present in the Riccati equation. Various methods to overcome this difficulty, and an extension of LPT to excited states with nodes, are considered in Refs.7-9 . In particular, it is shown in Ref.7 for the example of the Stark effect for excited states of hydrogen atom that the calculation of higher PT orders is reduced to recursive relations also in this case. It was also shown there that the summation of the PT series enables one to determine the Stark shift and the width of the atomic levels in strong electric fields.

Note, finally, that the LPT method can be extended to multidimensional problems/8,9,22/. Introducing the vector $\vec{y}(r) = -\nabla\psi/\psi$,

for the wave function $\phi(r)$, one gets a chain of equations similar to those for the one-dimensional case, but with partial derivatives. These equations are identical to the equations of electrostatics in a medium with a variable dielectric permeability. However, unlike the one-dimensional case, the solution of the equations is not reduced to quadratures. Development of effective numerical methods for solution of such equations is rather interesting, it would enable one to solve an ample class of physical problems.

Appendix B

Eqs.(2.3)-(2.6) determine an iterative procedure for expansion of the quantities $y(\rho,\mu)$ and $E(\mu)$ in PT series. Hence one easily gets the corresponding expansion for the wave function.

From (2.1),(2.4) we obtain

$$R = const\cdot\rho^{n-1}\exp\Big\{-\rho+\sum_{k=2}^{\infty}(-\mu)^k\sum_{j=1}^{k-1}c_j^{(k)}\frac{\rho^{j+1}}{j+1}\Big\} \qquad (B.1)$$

$\rho = r/n$. The following method is appropriate for exponentiating the power series. Let $f(z) = \exp[g(z)]$,

$$f(z)=\sum_{k=0}^{\infty}a_k z^k, \qquad g(z)=\sum_{k=1}^{\infty}b_k z^k$$

Evidently, $f' = fg'$; so $a_0=1$, $a_k = k^{-1}\sum_{l=1}^{k} l a_{k-l} b_l$, $k\geqslant 1$. Aplying this formula to Eq.(B.1), one gets

$$R(r)=const\cdot e^{-r/n}r^{n-1}\Big\{1+\sum_{k=2}^{\infty}u_k(r)(-\mu)^k\Big\} \qquad (B.2)$$

where

$$u_2(r) = \frac{1}{2} n f_2 r^2, \quad u_3(r) = \frac{n}{3} f_3 r^3 + \frac{1}{2} n^2 (n+1) f_2^2 r^2 \qquad (B.3)$$

and for $k \geq 4$ the polynomials $u_k(r)$ are determined easily from the recursive relations

$$u_k = p_k + \frac{1}{k} \sum_{\ell=2}^{k-2} \ell p_\ell u_{k-\ell}$$

$$p_k(r) = \sum_{j=2}^{k} \frac{1}{j} c_{j-1}^{(k)} r^j \qquad (B.4)$$

For example,

$$u_4 = \frac{1}{4} n^4 (n f_4 + \frac{1}{2} f_2^2) r^4 + [n^5 (n + \frac{3}{2}) f_4 + \frac{1}{2} n^6 f_2^2] (\frac{1}{3} r^3 + \frac{n+1}{2} r^2),$$

etc. Note that the principal quantum number n is not present explicitly in these equations. For $n=1$ we reconstruct the formulae of Ref.1.

The PT expansion for the wave function starts from the terms $\sim \mu^2$, because at $\mu \to 0$

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

so the first-order perturbation in μ results just in a shift of the level spectrum and does not change the wave functions.

Appendix C.

Here we present a derivation of the asymptotics $\tilde{E}_k$. For the potential (2.12), the change of the integration variable, $r = (\mathcal{E}/2)^{-1/2} x$, results in the expression

$$\mathcal{J}(\lambda) = \mathcal{E}^{\frac{N+2}{2N}} \cdot (2\lambda)^{-1/N} \cdot I \ , \qquad (C.1)$$

where

$$I = \int_{x_-}^{x_+} dx \left(1 - x^N - \frac{\nu}{x} + \frac{\sigma}{x^2}\right)^{1/2} \qquad (C.2)$$

$$\nu = \left(\frac{2}{\mathcal{E}}\right)^{\frac{N+1}{N}} \lambda^{1/N} \ , \quad \mathcal{E} = -2E \ , \quad \sigma = \Lambda^2 \mathcal{E}^{-\frac{N+2}{N}} (2\lambda)^{2/N}$$

Below we list the results for some particular cases.

1. For the s-levels $\sigma = 0$,

$$\gamma_0 = n^{2n-2} e^{-2n} (n!)^{-2} \qquad (C.3)$$

$$I = \int_{x_-}^{x_+} dx \left(1 - x^N - \frac{\nu}{x}\right)^{1/2} = \begin{cases} C_N \ , & \nu = 0 \\ 0 \ , & \nu = \nu_0 \end{cases} \qquad (C.4)$$

where

$$C_N = \frac{\pi^{1/2} \Gamma(1/N)}{(N+2)\Gamma\left(\frac{N+2}{2N}\right)} \ , \qquad \nu_0 = N (N+1)^{-\frac{N+1}{N}}$$

We are interested in the behaviour of the integral $\mathcal{J}(\lambda)$ for $\lambda \to 0$, i.e. $I = I(\nu)$ for $\nu \to 0$. Divide the integration region in $I(\nu)$ in two parts: $I(\nu) = I_1 + I_2$. Here I_1 is the integral from x_- up to x, and I_2 - from x up to x_+, and x is an intermediate point, $x_- \ll x \ll x_+$. Then

$$I_1 = \sqrt{x(x-\nu)} - \nu \operatorname{Arch} (x/\nu)^{1/2} = x - \frac{\nu}{2} \ln x + \frac{\nu}{2} (\ln \nu - 1 - 2\ln 2) + \ldots$$

In order to calculate I_2 it is helpful to expand the integrand in powers of ν,

$$\left(1-x^N-\frac{\nu}{x}\right)^{1/2}=(1-x^N)^{1/2}-\frac{\nu}{2x(1-x^N)^{1/2}}+\dots$$

Discarding the terms $\sim\nu^2$ and replacing x_+ by 1, one makes a negligible error $\sim\nu^{3/2}$. With account for

$$\int_x^1\frac{dx}{x(1-x^N)^{1/2}}=-\ln x+\frac{2\ln 2}{N}+\dots\ ,\ x\to 0$$

one has

$$I(\nu)=C_N+\frac{\nu}{2}\ln\nu-\left(\frac{1}{2}+\frac{N+1}{N}\ln 2\right)\nu+\dots \qquad (C.5)$$

$$C_N=\begin{cases}2/3, & \text{for } N=1,\\ \pi/4, & \text{for } N=2,\\ 1, & \text{for } N\to\infty.\end{cases}$$

At $N>1$, one may put $\varepsilon\approx\varepsilon_0=n^{-2}$ in Eq.(C.1). If $N=1$, one must take into account the shift of nl-level in the first order in the coupling $g=-\lambda$,

$$\varepsilon=\frac{1}{n^2}\left\{1+[3n^2-l(l+1)]n^2\lambda+O(\lambda^2)\right\}$$

$$\frac{\varepsilon^{3/2}}{2\lambda}=\frac{1}{2n^3\lambda}+\frac{3}{4n}\left[3n^2-l(l+1)\right]+\dots\ ,\ \lambda\to 0 \qquad (C.6)$$

Finally, we have

$$J(\lambda)=b_1\lambda^{-1/N}+b_2\ln\lambda+b_3+\dots\ ,\lambda\to 0 \qquad (C.7)$$

where

$$b_1=\frac{2^{-1/N}\pi^{1/2}\Gamma(1/N)}{(N+2)\Gamma((N+2)/2N)}n^{-\frac{N+2}{N}}\ ,\qquad b_2=\frac{n}{N}\ ,$$

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

Putting (C.7) and (3.2) into the dispersion integral (3.1) and calculating it by means of the steepest descent method , one gets the parameters of the asymptotics α, β, a, c_0 given in Eqs.(3.5)-(3.7).

2. Dependence on the angular momentum l. The calculation of the integral (C.2) is substantially more complicated if $l \neq 0$. At $\lambda \to 0$, however, $\nu \sim \lambda^{1/N}$ and $\sigma \sim \lambda^{2/N}$, so the account of the term σx^{-2} in (C.2) contributes a correction $\sim \lambda^{2/N}$ to I , i.e. proportional to $\lambda^{1/N}$ to $\mathcal{J}(\lambda)$. In the limit $\lambda \to 0$ these terms vanish, so the coefficients b_1, b_2 and b_3 in the expansion (C.7) are independent of l in the case $N>1$. Thus the l-dependence of the level width $\gamma(\lambda)$ is completely due to the pre-exponential factor γ_0 , and is rather slow (see Section 3).

If $N=1$, then $\mathcal{J}(\lambda) = \varepsilon^{3/2} I / \lambda$, and one has to take into account the first term in the expansion (C.6). Now $\nu = 4n^4\lambda + O(\lambda^2)$,

$$\mathcal{J}(\lambda) = \frac{1}{3n^3\lambda} + n\ln\lambda + b_3 + O(\lambda\ln\lambda)$$

$$b_3 = 2n\left[2\ln n - \ln 2 + \frac{1}{4}\left(1 - \frac{l(l+1)}{n^2}\right)\right] \qquad \text{(C.8)}$$

In this case the constants α, β and a are still independent of l. However, $\exp(-2\mathcal{J}(\lambda))$ contains the factor $\exp[l(l+1)/n]$, the variation of which is from 1 up to $\exp(n-1)$, when $0 \leq l \leq n-1$. The same l-dependence is present in the constant c_0 and in the asymptotics $\tilde{E}_k$.

3. The cases N = 1 and 2 (funnel-shaped and oscillator potentials) are most interesting from the physical point of view. For l=0 the function $I(\nu)$ can be calculated in a closed form. We will use this opportunity to test the above approximations*). For N=1, $x_{\pm} = \frac{1}{2}(1 \pm \sqrt{1-4\nu})$. Using the formula 3.141 (35) of the handbook by Gradshteyn and Ryzhik /11/, one gets

$$I(\nu) = \frac{2k^2}{3(1+k'^2)^{3/2}}\left\{E(k) - 2k'^2 D(k)\right\} \qquad (C.9)$$

where

$$k^2 = 1 - x_-/x_+ , \quad k'^2 = 1 - k^2 = \frac{1-\sqrt{1-4\nu}}{1+\sqrt{1-4\nu}}$$

In the limit $\nu \to 0$, we obtain

$$k'^2 = \nu + 2\nu^2 + \dots$$

$$I(\nu) = \frac{2}{3} - \left(\ln\frac{4}{k'} + \frac{1}{2}\right)k'^2 + \dots =$$

$$= \frac{2}{3} + \frac{1}{2}\nu\ln\nu - \left(\frac{1}{2} + 2\ln 2\right)\nu + O(\nu^2 \ln\nu) ,$$

in agreement with Eq.(C.5).

For N=2, we use the notation

$$I_n = \int_{x_-}^{x_+} \frac{x^n}{\sqrt{x\, q(x)}}\, dx$$

$$q(x) = x - x^3 - \nu = (x_+ - x)(x - x_-)(x + x_+ + x_-)$$

It follows from (C.4) that $I(\nu) = I_1 - \nu I_0 - I_3$. Integration by parts with account for $q(x_{\pm}) = 0$, leads to the identity

$$\int_{x_-}^{x_+} (q/x)^{1/2} dx = -\int_{x_-}^{x_+} q'\, q^{-1/2}\, x^{1/2}\, dx ,$$

hence $I(\nu) = 3I_3 - I_1$. Excluding I_3 from two above equalities, one gets

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*) We are grateful to V.L.Eletsky for verification of the subsequent formulae.

$$I(\nu) = \int_{x_-}^{x_+} \sqrt{\frac{2\varphi(x)}{x}}\, dx = \frac{1}{2} I_1 - \frac{3}{4}\nu I_0 \qquad (C.10)$$

where

$$x_+ I_0 = \int_\rho^1 \frac{dx}{\sqrt{x(x-\rho)(1-x^2+\rho(1-x))}} = \frac{2}{\sqrt{1+2\rho}} K(k)$$

$$I_1 = \int_\rho^1 dx \sqrt{\frac{x}{(x-\rho)(1-x^2+\rho(1-x))}} = \frac{2\rho}{\sqrt{1+2\rho}} \Pi\left(\frac{\pi}{2}, n, k\right)$$

$$\rho = x_-/x_+ \,, \quad n = 1-\rho \,, \quad k = \left[(1-\rho^2)/(1+2\rho)\right]^{1/2}$$

K and Π are the complete elliptic integrals of the first and third kind, respectively /17/. In the limit $\nu \to 0$ the parameters n and k are close to 1 :

$$\rho = \nu + \tfrac{1}{2}\nu^2 + \dots \,, \quad n = 1 - \nu - \tfrac{1}{2}\nu^2 + \dots \,,$$

$$k = 1 - \nu + \tfrac{1}{2}\nu^2 + \dots$$

Hence

$$I_0 = -\ln \nu + 3\ln 2 + \dots \,, \quad I_1 = \frac{\pi}{4\nu} - \frac{1}{4}\ln\nu + \dots \,,$$

$$\mathcal{J}(\lambda) = 2^{-5/2}\pi\lambda^{-1/2} + \tfrac{1}{2}\ln\lambda + O(1) \,, \qquad (C.11)$$

$$\gamma(\lambda) = \frac{8}{\lambda} \exp\left\{-\pi(8\lambda)^{-1/2}\right\} \,, \quad \lambda \to 0$$

and one gets the asymptotics (1.4) with the following parameters

$$\alpha = 2 \,, \quad \beta = 1 \,, \quad a = -\frac{8}{\pi^2} \,, \quad c_0 = -\frac{128}{\pi^3}$$

(cf. (3.5) for the case N=2, n=1).

We have shown thus , that the exact calculation of the function $\mathcal{J}(\lambda)$, possible for N = 1 and 2, confirms the result of the approximate method of § 1.

4. Consider, finally, the Yukawa potential. Inversion of the sign of the screening parameter μ produces a potential with a barrier,

$$V(r) = -\frac{1}{r} e^{\varkappa r}, \quad \varkappa = -\mu > 0$$

where the bound state decays by means of the tunnelling. For the s states,

$$\mathcal{J}(\lambda) = \frac{1}{n\lambda} \int_{x_-}^{x_+} q(x)\,dx , \quad q = (1 - \eta \frac{e^x}{x})^{1/2} ,$$

where $\eta = 2\lambda/\varepsilon = 2n^2\lambda + \ldots$, $x_\pm$ are the turning points, determined from the equation $\varkappa \exp(-\varkappa) = \eta$:

$$x_- = \eta + \eta^2 + \frac{3}{2}\eta^3 + \ldots$$
$$x_+ = \Lambda + \ln\Lambda + O((\ln\Lambda)/\Lambda) , \quad \Lambda = \ln\frac{1}{\eta} >> 1 \qquad (C.12)$$

The function e^x/x has a minimum at the point x=1, and is monotonous in the intervals $(0,1)$ and $(1,\infty)$. Therefore, $\mathcal{J}(\lambda) = (\mathcal{J}_1 + \mathcal{J}_2)/n\lambda$

$$\mathcal{J}_1 = \int_{x_-}^{1} q\,dx = 1 + \frac{1}{2}\eta\ln\eta + O(\eta) ,$$

and $\mathcal{J}_2$ is the integral from 1 up to x_+ . Since $x_+ \gg 1$ at $\eta \to 0$, we introduce an intermediate point $\varkappa$, such that $1 \ll \varkappa \ll x_+$. Then

$$\int_1^{x} q\,dx = \int_1^{x} (1 - \frac{\eta}{2x} e^x + \ldots)\,dx = x - 1 - \frac{1}{2}\eta \int_1^{x} e^y \frac{dy}{y} + O(\eta^2) ,$$

$$\int_{x}^{x_+} q\,dx = x_+ - x - \bar{Q}(x) ,$$

$$\bar{Q}(x) = \int_{x}^{x_+} dy \left[1 - \left(1 - \eta \frac{e^y}{y}\right)^{1/2}\right]$$

Next, we change the integration variable, $t = \eta e^y/y$,

$$\bar{Q}(x) = \int_{\xi(x)}^{1} dt \, \frac{1-\sqrt{1-t}}{t(1-w)}$$

where $\xi = \eta e^x/x$, and w is a function of t , determined by the equation $w\exp(1/w) = t/\eta$. Since $w \ll 1$, we write the expansion of Q(x) in powers of w. The result is $\gamma(\lambda) = \frac{1}{n\lambda}\left[x_+ - 2(1-\ln 2) + \ldots\right]$ and , with account for Eq.(C.12):

$$\gamma(\lambda) \sim \exp\left\{-\frac{2}{n\lambda}\left[\ln\frac{1}{\lambda} + \ln\ln\frac{1}{\lambda} - \right.\right.$$

$$\left.\left. - (2 - \ln 2 + 2\ln n) + \ldots\right]\right\} \qquad (C.13)$$

Put this expression into Eq.(3.1) and calculate the integral by means of the steepest descent method. The saddle point, $\lambda = \lambda_0$, is determined from the equation $\ln(1/\lambda) + \ln\ln(1/\lambda) + O(1) = \frac{1}{2}nk\lambda$, hence

$$\lambda_0 = \frac{2}{n}\left[\frac{\ln k}{k} + O\left(\frac{\ln\ln k}{k}\right)\right] , \quad k \to \infty \qquad (C.14)$$

The result is Eq.(3.10) of Section 3.

Appendix D

Behaviour of the energy eigen-values $E(g)$ for the Hamiltonian

$$\mathcal{H} = \tfrac{1}{2}p^2 - \frac{\Sigma}{r} + g r^N \qquad (D.1)$$

in the strong coupling limit can be found by means of a scaling transformation[12]. Performing a change of the variable in (D.1), $x_i \to (2g)^{-1/(N+2)} x_i$, one gets

$$\mathcal{H}(\Sigma, g) = 2^{-\frac{N}{N+2}} g^{\frac{2}{N+2}} H(\alpha)$$

where

$$H(\alpha) = p^2 + r^N - \alpha r^{-1} \quad \text{and} \quad \alpha = 2^{\frac{N+1}{N+2}} g^{-\frac{1}{N+2}} \Sigma \qquad (D.2)$$

As $\alpha \to 0$ at $g \to \infty$, we obtain Eq.(4.7), where

$$\nu = 2\nu_1 = \frac{2}{N+2}, \quad c_\infty = 2^{-\frac{N}{N+2}} \mathcal{E} \qquad (D.3)$$

and $\mathcal{E}$ is the eigen-value of a simple Hamiltonian $H(0) = p^2 + r^N$. In some cases $\mathcal{E}$ and c_∞ are determined without numerical calculations.

1. For the s-states in the funnel potential, $N=1$, the solution falling at infinity, is expressed in terms of the Airy function: $\chi(r) = \text{const}\cdot \mathrm{Ai}(r - \mathcal{E})$. The energy spectrum is determined from the condition $\chi(0)=0$. Let $-z_n$ be the n-th zero of the function $\mathrm{Ai}(z)$, then

$$\nu = \frac{2}{3}, \quad \nu_1 = \frac{1}{3}, \quad c_\infty = 2^{-1/3} z_n \qquad (D.4)$$

There is a table of the roots /33/. For instance, at $n=1$ (the ground state) $z_1 = 2.338107$ and $c_\infty = 1.855756$, and for $n \gg 1$ we have $c_\infty \approx \frac{1}{2}(3\pi n)^{\frac{2}{3}}$.

2. If $N=2$, then

$$\nu = \tfrac{1}{2}; \quad c_\infty^{(n\ell)} = 2^{1/2}\left(n + \tfrac{3}{2}\right), \quad n - \ell = 0, 2, 4, \ldots \qquad (D.5)$$

3. For $n \gg 1$ the quantities $\mathcal{E}_{nl}$ and c_∞ can be found approximately from the Bohr - Sommerfeld quantization condition. In particular, for ns-states we have

$$c_\infty^{(n0)} \approx A \cdot n^{\frac{2N}{N+2}}$$

$$A = \left\{ \sqrt{\frac{\pi}{2}} \cdot \frac{(N+2)\Gamma\left(\frac{N+2}{2N}\right)}{\Gamma(1/N)} \right\}^{\frac{2N}{N+2}} \qquad (D.6)$$

For example, $A = \frac{1}{2}(3\pi)^{\frac{2}{3}}$, $A = 2^{3/2}$ and $A = \frac{1}{2}\pi^2$ for $N=1$, $N=2$ and $N \to \infty$, respectively.

Footnotes

1) Here and in the following we put $\hbar = m = e = 1$ (the atomic units). For a more general potential, $V(r) = -Zr^{-1}f(\mu r)$, the scale transformation $r \to Zr$ in the Schroedinger equation leads to the corresponding transformation of the energy eigen-value $E^{(nl)}(Z,\mu) = Z^2 \cdot E^{(nl)}(1, \mu/Z)$. Here Z is the nuclear charge, μ^{-1} is the screening radius of the Coulomb field. So we put throughout the paper Z=1. Note that the PT series (1.3) corresponds to the expansion in 1/Z in the atomic physics.

2) Numerical calculations of the Schroedinger equation for the Yukawa [11] and funnel-shaped[12] potentials.

3) For instance, for $\mu=0$ one has[13] $R_{n,n-1}(r) = C_n \rho^{n-1} e^{-\rho}$, where $\rho = r/n$, and $C_n = 2^n n^{-2} [(2n-1)!]^{-\frac{1}{2}}$ is the normalization constant. The case l=n-1 corresponds to the deepest level with the angular momentum l.

4) By means of a somewhat different method, Privman[3] has calculated 40 PT orders for the Yukawa potential and 20 PT orders for the funnel-shaped potential (2.12). Note that the normalization of the Hamiltonian in his work was not identical to the ours. The relations are as follows: $E'_k = 2^{k-1} E_k$ in the case of the Yukawa potential, $E'_k = 2^{(N+1)k-1} E_k$ for the potential in (2.12), where E'_k are Privman's coefficients, and E_k are defined above. With account for these relations the results of the cited works[1-3] are in a complete agreement.

5) Such a potential with N=1 is used in the phenomenological calculation of the level spectrum for heavy quarkonium[12]. Cf. also in recent reviews on potentials for heavy quark-antiquark

systems[19,20]. For N=2 one has a model potential, which is rather like the potential for the Zeeman problem for hydrogen.

6) For example, $v(r) = r^N$ for the funnel-shaped potential (2.12). In the case of the screened Coulomb potential (1.1) the screening parameter μ stands for g, and $v = [1-f(x)]/x$, $x = \mu r$.

7) A brief presentation of the results given in this Section was published in the previous papers[2,26].

8) On the other hand, $[M/N](x) \sim x^{M-N}$ at $x \to \infty$. Therefore, PA without a transformation of the type (4.12) can not reproduce correctly the Borel transform $B(x)$ for large x, unless the index of the asymptotics ν is an integer.

9) The recent work by Sergeev and Shirstyuk[28] contains tables analogous to our tables 2 and 3.

10) Let us make a few technical remarks. In the case of $\alpha=2$ it is convenient to rewrite eq.(4.5) as

$$E(g) = g^{-1/2} \int_0^\infty \exp(-g^{-1/2}x) B(x^2)\, dx$$

with the power singularity at $X \to 0$ excluded. The Borel transform $B(x^2)$ replaced here by PA $[L/L+j]$ which results in the values of $E(g)$, presented in table 6.

We used the $[L/L+j]$ approximants with $j = 0, \pm 1$. The sequence of diagonal approximants (j=0) exhibits the fastest convergence to $E(g)$ which is the case for ordinary PA. The values of PA $[L/L+1]$ are unstable at $X \gtrsim 0.2$ due to influence of neighbouring poles.

In our attempt to use the transformation (4.12) for the potential $V(r) = -r^{-1} + g r^2$ we encountered with a technical restriction: the accuracy of computation of β_k decreases

rapidly with increasing k. This fact is connected with large range of β_k values. For instance, $\beta_1 = 1.5$, $\beta_{20} = -2.156.10^{-7}$ and $\beta_{40} = 1.382.10^{-14}$ for N=2. On the other hand, $\beta_1 = 1.5$, $\beta_{20} = -0.0434$ and $\beta_{40} = 0.0013$ for N=1.

As a result, the summation of divergent PT series for the funnel-shaped potential (2.12) with N=2 determines $E(g)$ in a considerably smaller region of g, as compared to that with N=1, see tables 5 and 6. We guess that this fact is connected with the faster increase of higher PT orders in the N=2 case.

11) To compute the PA $[L/M]$ one should know L+M+1 orders of PT. In particular, determination of index ν with a per cent precision in the N=1 case requires about 25 exact coefficients B_k, see table 4.

12) This trick is effective for power potentials and was originally demonctrated for the anharmonic oscillator by K.Symanzik, see ref. in [44] p.85.

Table 1

x	$Q(x)$	$q(x)$
I.0	0.922I	I.0405
I.5	0.9467	I.0275
2.0	0.9595	I.0208
2.5	0.9674	I.0I67
3.0	0.9727	I.0I39
4.0	0.9794	I.0I04
5.0	0.9835	I.00835
I0	0.99I7	I.004I7

Table 2

Convergence of diagonal PA $N/N(\mu)$ for states with $l=n-1$ in Yukawa potential.

$l = 0$			$l = 1$			
N	$\mu = 0.5$	$\mu = 1.0$	N	$\mu = 0.10$	N	$\mu = 0.15$ $\mu = 0.20$
6	14.811721 8	1.0318	6	4.653442434	6	2.11076858 0.4182
7	14.811704 1	1.02911	7	4.653438968	8	2.11045816 0.4076
8	14.81117024	1.02866	8	4.653438936	10	2.11048937 0.4101
9	14.811 7022	1.02859	9	4.653439088	12	2.11048846 0.4099
10	14.811 7022	1.02858	10	4.653439049	15	2.11048889 0.4101
15	14.811 7022	1.02858	15	4.653439049	18	2.11048889 0.4102
18	14.811 7022	1.02858	20	4.653439049	20	2.11048889 0.4102

Footnote. The presented values are $100 \cdot E(\mu)$.

Table 3

Determination of μ_{cr} by means of diagonal PA.

N \ ℓ	0	I	2	5	I0
6	I.I896	0.2220	$9.II8 \cdot I0^{-2}$	$2.I505 \cdot I0^{-2}$	$6.24644 \cdot I0^{-3}$
8	I.I906	0.2I89	9.I08	2.I532	6.24988
I0	I.I906II	0.2I98	9.I27	2.I52I	6.24924
I2	I.I906I2	0.2I97	9.I40	2.I524	6.24997
I4	I.I906I2	0.2200	9.I32	2.I525	6.25004
I6	I.I906I2	0.2I99	9.I34	2.I524	6.2500I
I8	I.I906I2	0.220I	9.I33	2.I524	6.25005
20	I.I906I2	0.220I	9.I34	2.I525	6.25005
according to ref./11/	I.I906I	0.2202	$9.I35 \cdot I0^{-2}$	$0.02I525 \cdot I0^{-2}$	—
according to ref./28/	1.1906214	0.220	0.0913	—	—

Table 4

The index ν of asymptotic (4.7) for the ground state.

$V(r) =$	$-\frac{1}{r}+gr$	$-\frac{1}{r}+gr^2$	
L	ν_L according eq. (4.10)	ν_L according eq. (4.9)	ν_L according eq. (4.10)
6	0.915	—	—
8	0.560	0.453	0.298
10	0.585	0.336	0.855
11	0.670	0.471	0.390
12	0.670	0.400	0.582
13	0.662	—	—
14	0.667	0.423	0.669
15	0.666	0.508	0.415
16	—	0.479	0.503
$\bar{\nu}$	0.667 ± 0.003	0.46 ± 0.04	0.51 ± 0.10
exact value	$\nu=2/3=0.6666\ldots$	$\nu = 0.5$	

Table 5

Summation of PT series for the funnel-shaped potential by Padé-Borel method.

M \ g	0.976 562 ...	4.0	62.5	100	300	500	1000
3	0.554 641	-	-	32.75	69.85	98.9	157.9
5	0.556 523	-	-	33.56	71.76	101.7	162.5
7	0.556 744	2.79384	24.503	34.25	73.59	104.4	167.1
9	0.556 761	2.79515	24.634	34.47	74.21	105.4	168.7
11	0.556 763	2.79556	24.716	34.61	74.66	106.1	170.0
13	0.556 764	2.79566	24.763	34.70	74.95	106.6	170.8
15	0.556 764	2.79573	24.792	34.75	75.15	106.9	171.4
according to ref.[8]	0.556 767	2.795754	24.8563	-	-	108.366	-

Footnote. The enclosed values are refered to the ground state energy for $V=-r^{-1}+gr$. The last row represents results of numerical solution[12] of the Schrödinger equation with $\lambda = 2^{2/3} g^{-1/3} = 1.6$, 1.0, 0.4 and 0.2 .

Table 6

PT series summation for the ground state energy in $V=-1/r+gr^2$ potential.

Padé approximants

L	$g = 0.1$			$g = 0.2$		
	[L/L]	[L/L-1]	[L/L+1]	[L/L]	[L/L-1]	[L/L+1]
8	-0.2984	-0.2986	-0.2740	-0.168	-0.184	-0.886
10	-0.2976	-0.2945	-0.2883	-0.163	-0.189	-0.652
12	-0.2971	-0.2950	-0.2920	-0.161	-0.142	0.008
14	-0.2968	-0.2958	-0.2936	-0.159	-0.144	-0.082
15	-0.2967	-0.2954	-0.2940	-0.158	-0.144	-0.099
16	-0.2966	-0.2955	-0.2944	-0.157	-0.145	-0.109
17	-0.2966	-0.2956	-0.2946	-0.157	-0.146	-0.117

Padé-Borel approximants

L	$g = 0.1$		$g = 0.2$		$g = 0.5$		$g = 1.0$		$g = 3.0$
	[L/L]	[L/L+1]	[L/L]	[L/L+1]	[L/L]	[L/L+1]	[L/L]	[L/L+1]	[L/L]
8	-0.296 098	-0.296 078	-0.151 26	-0.150 81	0.1767	0.1848	0.577	0.618	1.50
10	-0.296 087	-0.296 070	-0.151 08	-0.150 71	0.1802	0.216	0.597	0.643	1.75
12	-0.296 088	-0.296 087	-0.151 11	-0.151 08	0.1794	0.1809	0.592	0.604	1.70
14	-0.296 088	-0.296 086	-0.151 10	-0.151 01	0.1797	0.182	0.594	0.621	1.73
15	-0.296 088	-0.296 087	-0.151 10	-0.151 08	0.1795	0.1806	0.592	0.605	1.70
16	-0.296 088	-0.296 088	-0.151 10	-0.151 10	0.1796	0.1798	0.593	0.596	1.71
17	-0.296 088	-0.296 088	-0.151 10	-0.151 10	0.1795	0.1798	0.592	0.595	1.70

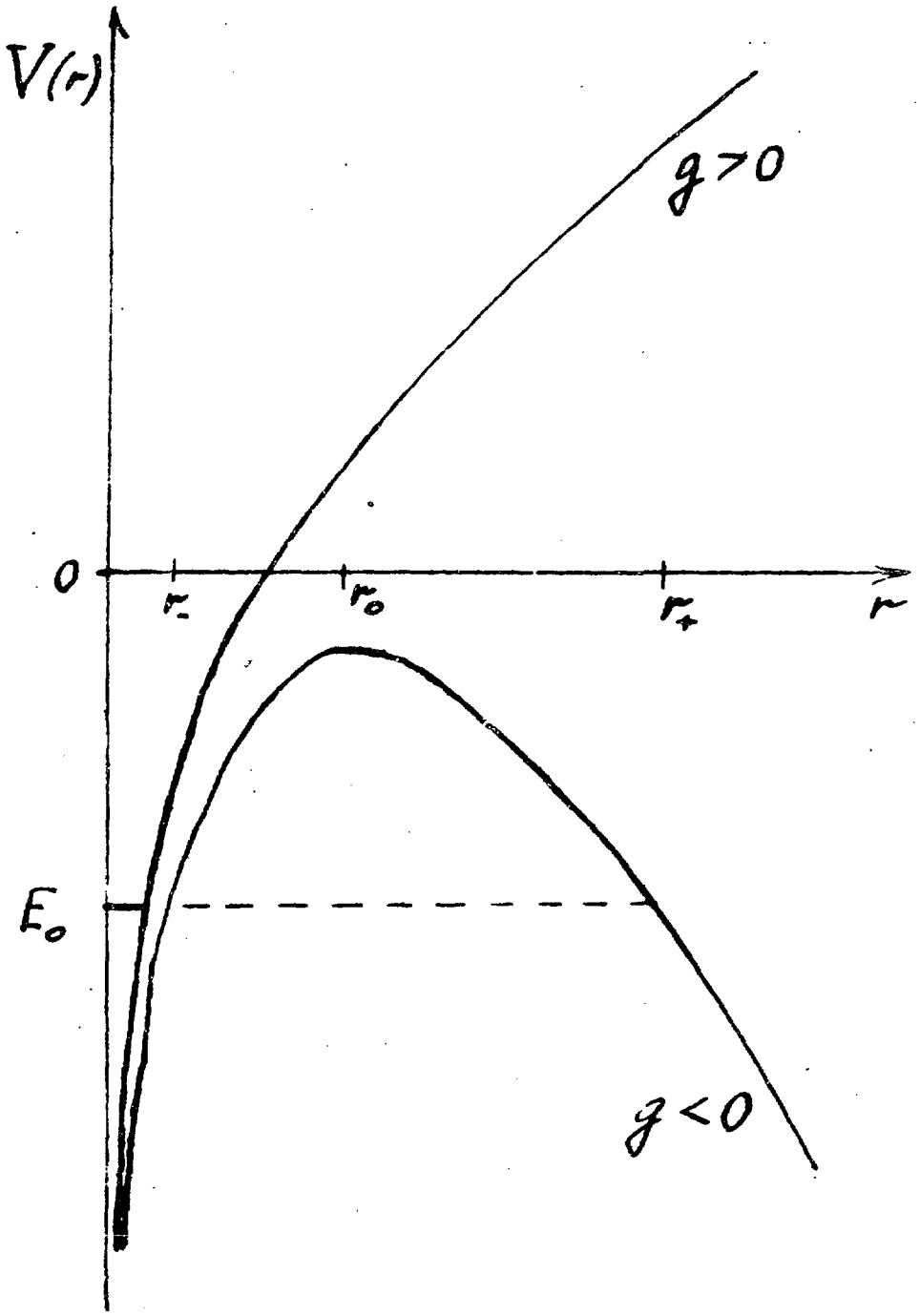

Figure 1. Shape of the potential in (2.12). For $g<0$ the potential has a maximum at the point $r_0=(-Ng)^{-1/(N+1)}$, and $V(r_0) \sim (-g)^{1/(N+1)}$; $r_\pm$ are the turning points for the S states.

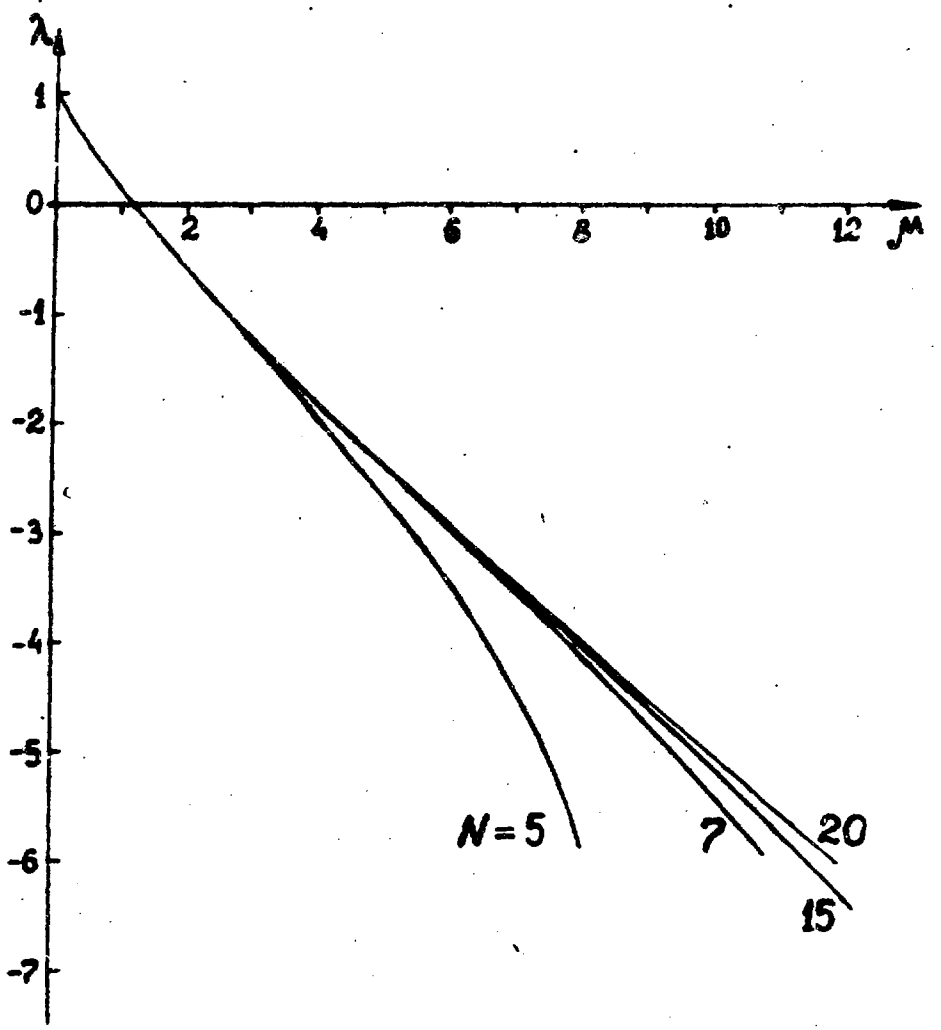

Figure 2. Screening parameter (μ) dependence of $\lambda=(-2E)^{\frac{1}{2}}$ for the ground state in the Yukawa potential. Numbers at the curves indicate the values of N. The curves with N = 18 - 22 coincide within the accuracy of the drawing.

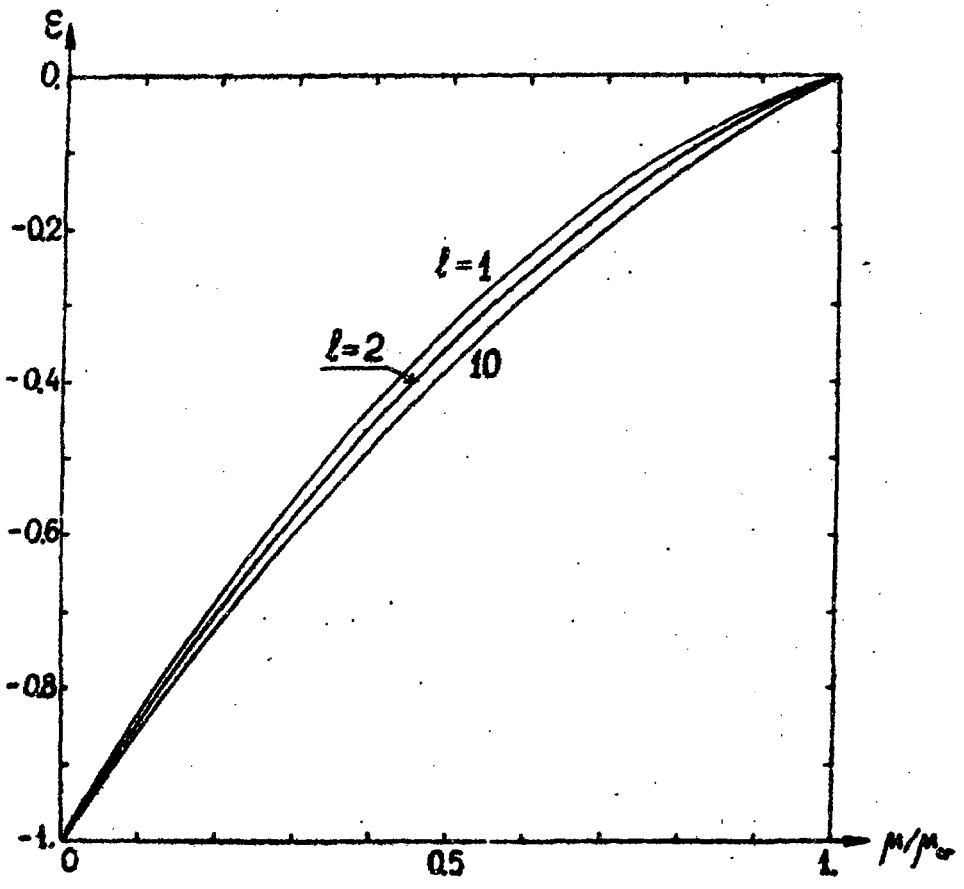

Figure 3. Screening parameter (μ) dependence of the binding energy for the state with l=n-1. The variables are $\varepsilon=2n^2E^{(n,n-1)}$ and μ/μ_{cr}. The curves are calculated by means of PA with N=15.

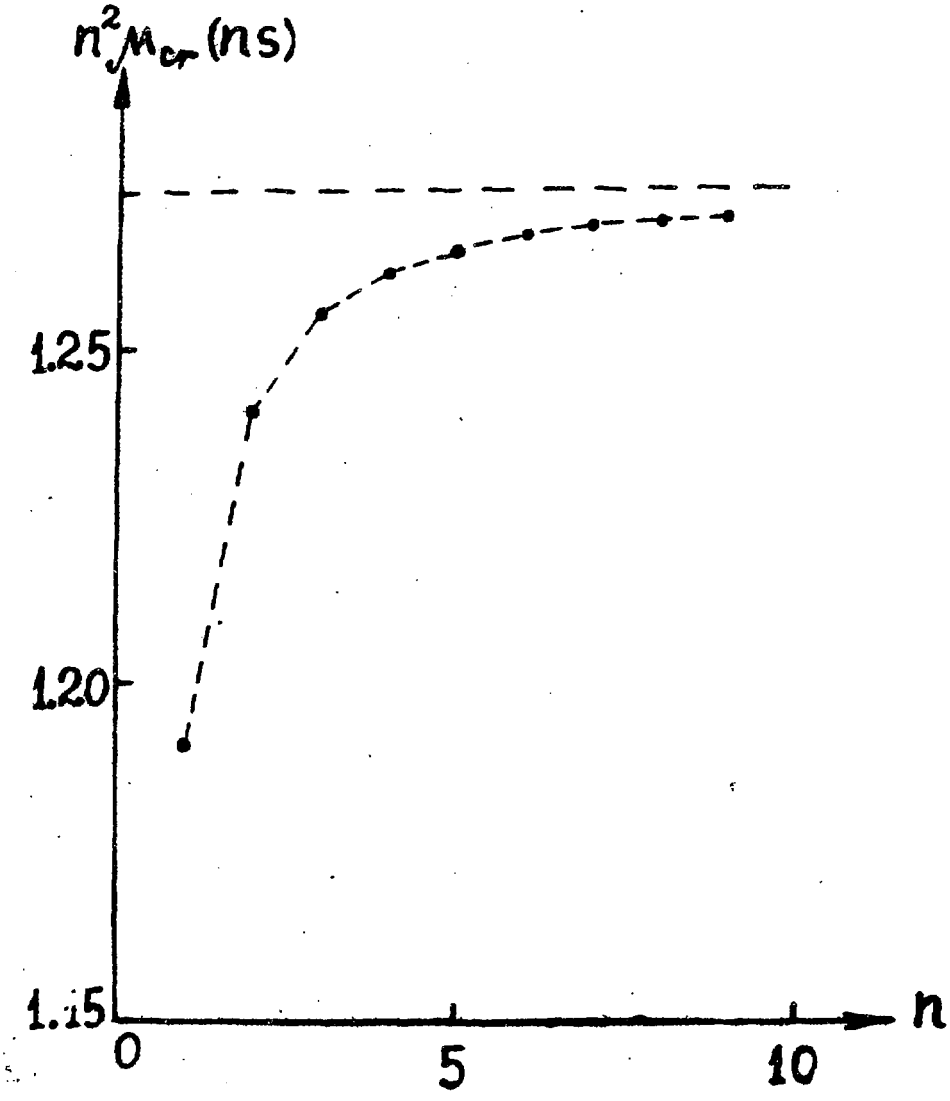

Figure 4. Values of $n^2\mu_{cr}$ for ns states in the Yukawa potential.

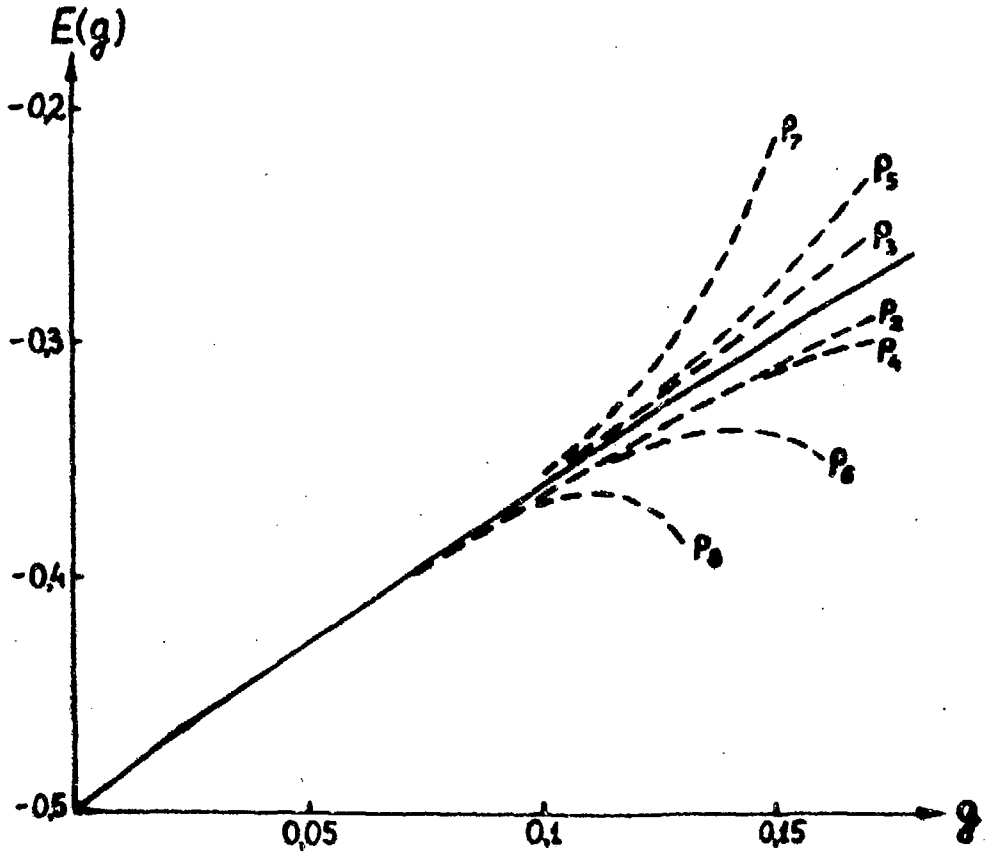

Figure 5. PT polynomials for the ground level energy in the funnel-shaped potential, a) N=1, and b) N=2. Curves are labeled by k, see eq.(4.14).

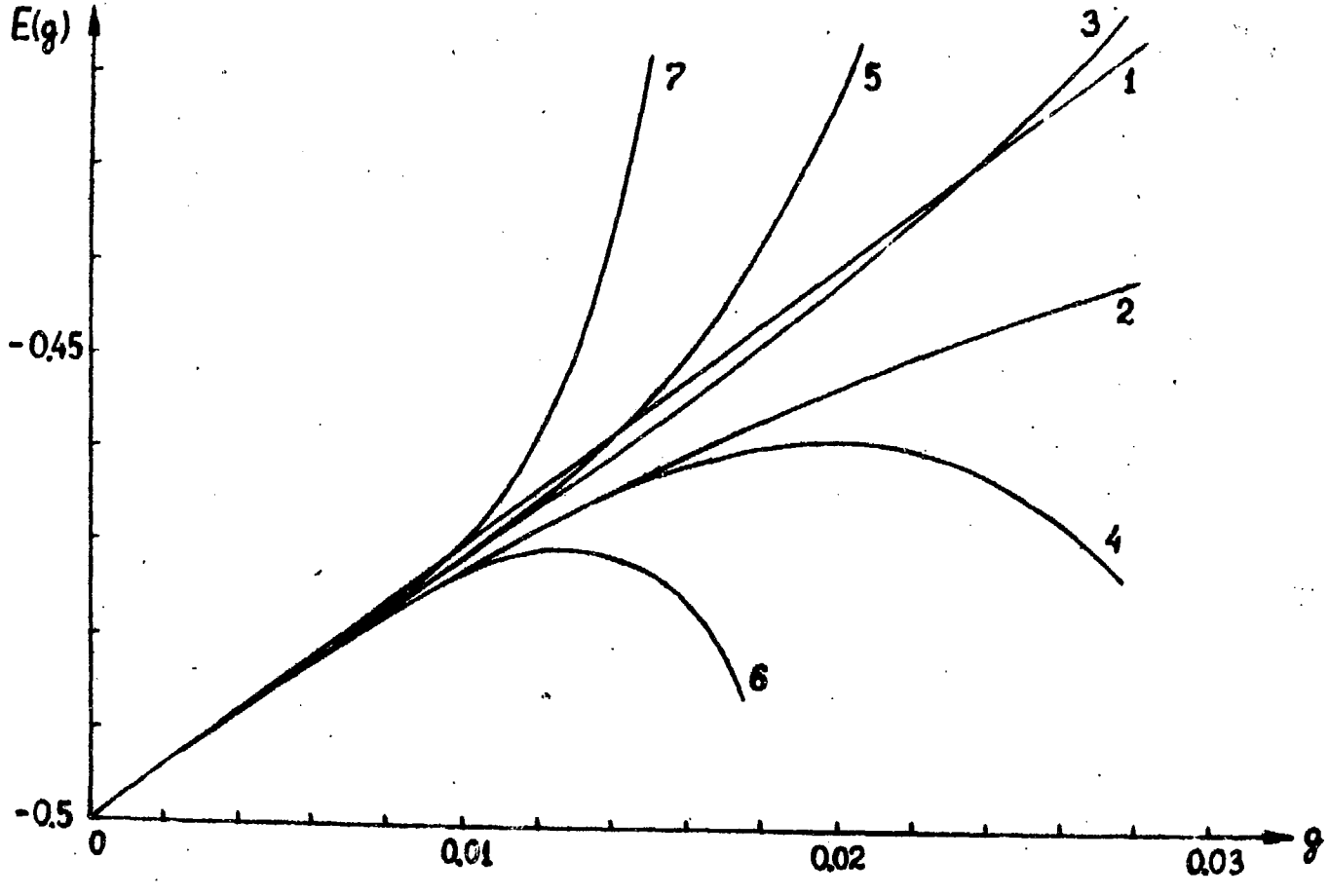

Fig. 5b

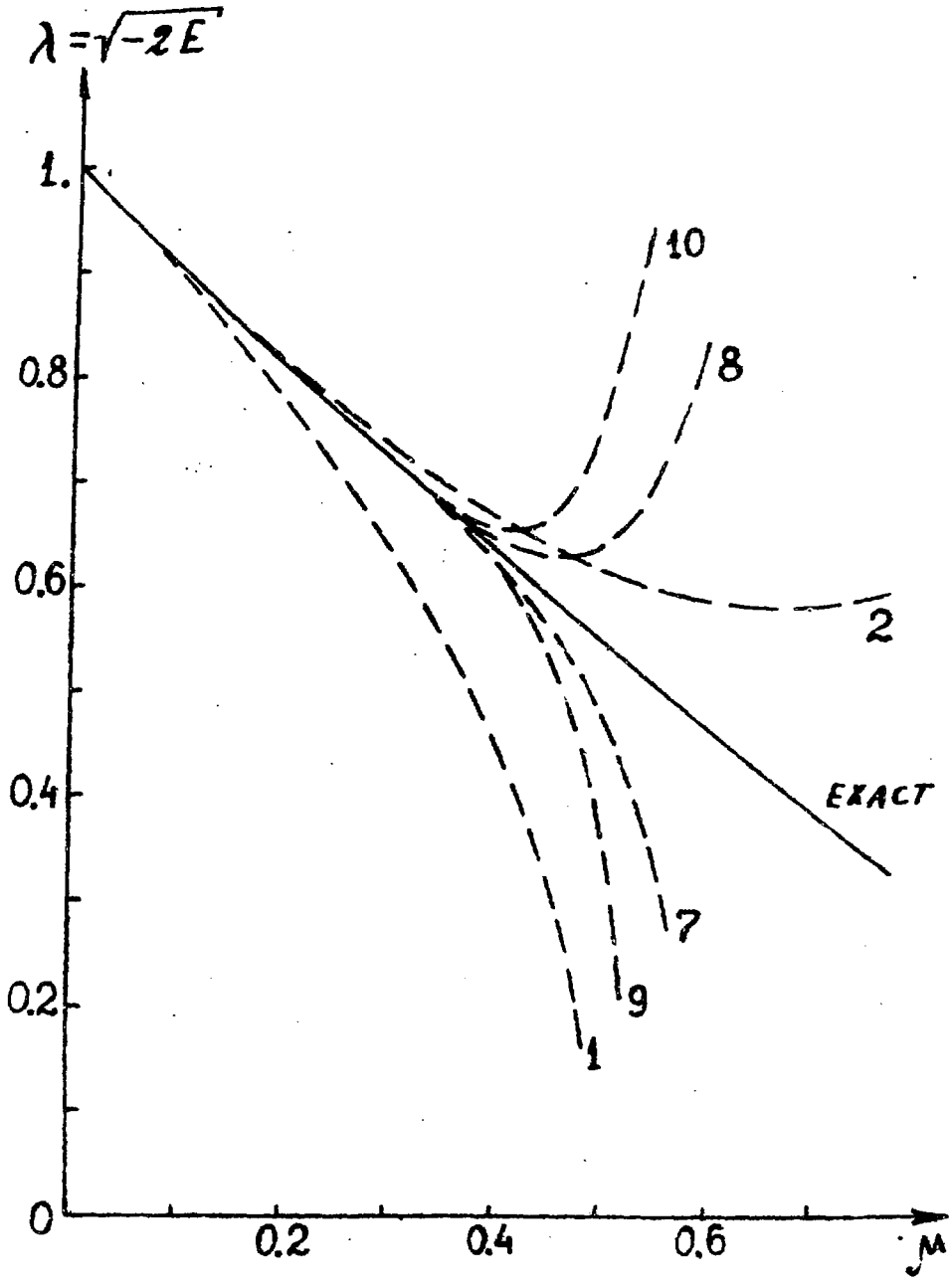

Figure 6. PT polynomials for the ground state in the Yukawa potential. The comparison of this figure with fig.2 demonstrates the advantage of PA.

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