THE 1/n EXPANSION IN QUANTUM MECHANICS

V. M. Vainberg, V. D. Mur, V. S. Popov,
A. V. Sergeev, and A. V. Shcheblykin

The classical approximation ($\ell = n - 1 \to \infty$) for the energy $\varepsilon^{(0)}$ and the semiclassical expansion in problems of quantum mechanics are discussed. A recursive method is proposed for calculating the quantum corrections of arbitrary order to $\varepsilon^{(0)}$, this being valid for both bound and quasistationary states. The generalization of the method to states with an arbitrary number of nodes and the possibility of a more general choice of the parameter of the semiclassical expansion are considered. The method is illustrated by the example of the Yukawa and "funnel" potentials and for the Stark effect in the hydrogen atom. These examples demonstrate the rapid convergence of the 1/n expansion even for small quantum numbers.

1. An approximate method was recently proposed [1-3] for calculating the energy eigenvalues in quantum mechanics; it is valid both in the case of the discrete spectrum and for virtual and quasistationary levels.* The basic idea is as follows [4-9]. For highly excited ($\ell = n - 1 \gg 1$) states the effective potential $U(r) = V(r) + \ell(\ell + 1)/2r^2$ has a minimum at $r = r_0$. In the zeroth approximation, the energy is $E = U(r_0)$, this corresponding to a classical particle at rest at the bottom of the well. Allowance for the zero-point vibrations about the point r_0 and the effects of the anharmonicity in U(r) lead to the 1/n expansion

$$\varepsilon_{nl}=2n^2E_{nl}=\varepsilon^{(0)}+\varepsilon^{(1)}/n+\varepsilon^{(2)}/n+\ldots, \tag{1.1}$$

where $E_{n\ell}$ is the energy of the $n\ell$ level, with n = 1, 2, ... the principal quantum number. For the calculation of the coefficients $\varepsilon^{(k)}$ there is an algorithm convenient for computer implementation [2].

For the example of the Yukawa, Hulthén, and "funnel" potentials it was shown [1-3] that the 1/n expansion, theoretically valid in the case of highly excited ("Rydberg," cf. [10]) states, actually already works for small n (to calculate a level energy to an accuracy of order 10^{-3}—10^{-4} it is sufficient to take [2] the first three terms of the series (1.1)). The convergence of the 1/n expansion is determined by the fact that the amplitude of the quantum fluctuations of the particle around $r = r_0$ is of order $n^{-\frac{1}{2}}$, i.e., arbitrarily small as $n \to \infty$. We illustrate this by the example of the Coulomb potential, $V(r) = -r^{-1}$. The level with $\ell = n - 1$ has the wave function [11]

$$\chi_{n,\,n-1}(r)=\frac{(2r)^n e^{-r/n}}{n^{n+1}[(2n-1)!]^{1/2}}=(\pi n^3)^{-1/4}e^{-\rho^2/2}\left[1+\frac{\rho^3}{3n^{1/2}}+O\left(\frac{1}{n}\right)\right], \tag{1.2}$$

where $\chi(r)=rR(r)$, $r=r_0(1+\rho n^{-1/2})$, and $r_0 = n^2$ (the wave functions with $n_r = n - \ell - 1 > 0$ correspond in the region $r \sim r_0$ to excited oscillator states).

In the present paper, we present a method of recursion relations, which make it possible to calculate the corrections $\varepsilon^{(k)}$ of arbitrary order k. First (in Secs. 2 and 3) we shall consider nodeless states, for which the method is simplest. The generalization to the case of arbitrary n and ℓ is given in Sec. 4. Finally, we demonstrate the convergence of the 1/n expansion (Sec. 5) and consider some physical examples (Sec. 6).

*In the usual approach (numerical solution of the Schrödinger equation) this case encounters well-known difficulties related to the exponential growth of the Gamow wave function as $r \to \infty$.

Institute of Theoretical and Experimental Physics. Translated from Teoreticheskaya i Matematicheskaya Fizika, Vol. 74, No. 3, pp. 399-411, March, 1988. Original article submitted July 15, 1986.

0040-5779/88/7403-0269$12.50

2. Recursion Relations. To calculate the corrections $\varepsilon^{(k)}$, we use logarithmic perturbation theory [12-14]. Assuming $\ell = n - 1 \gg 1$, we go over from the Schrödinger equation to the nonlinear Riccati equation

$$\frac{1}{n}\left(\frac{dy}{d\rho} - y^2\right) - \frac{2}{\nu} v(x) + \left(1 - \frac{1}{n}\right) x^{-2} - \frac{\varepsilon}{\nu^2} = 0, \tag{2.1}$$

where $y = -\frac{d}{d\rho}\ln\chi$, $v(x) = f(x)/x$,

$$\nu = n^2\mu, \quad x = \mu r = x_0 - n^{-1/3}\rho \tag{2.2}$$

and we consider the screened Coulomb potential*

$$V(r) = -r^{-1} f(\mu r) \tag{2.3}$$

($\hbar = m = e = 1$). It can be seen from (1.2) that $\Delta r/r_0 \to 0$ and the variable ρ remains constant in the limit $n \to \infty$; this is the justification of the substitution (2.2). Substituting in (2.1) the expansions

$$y = \sum_{k=0}^{\infty} n^{-k/2} y_k(\rho), \quad v(x) = \sum_{k=0}^{\infty} n^{-k/2} \frac{v^{(k)}(x_0)}{k!}\rho^k, \quad x^{-2} = x_0^{-2}\sum_{k=0}^{\infty} n^{-k/2}(-1)^k (k+1)(\rho/x_0)^k, \tag{2.4}$$

we arrive at the chain of equations

$$-\frac{dy_k}{d\rho} + \sum_{i=0}^{k} y_i y_{k-i} + \frac{1 + (-1)^k}{2\nu^2}\varepsilon^{((k+2)/2)} + a_k\rho^{k+2} + b_k\rho^k = 0, \tag{2.5}$$

where

$$a_k = \frac{2}{(k+2)!\,\nu} v^{(k+2)}(x_0) + (-1)^{k+1}(k+3)\,x_0^{-(k+4)}, \quad b_k = (-1)^k (k+1)\,x_0^{-(k+2)},$$

and $x_0 = x_0(\nu)$ is determined from the condition

$$x^3 v'(x) = -\nu \tag{2.6}$$

(or $\nu = xf - x^2 f'$; cf. [1]). Thus, x_0 is the point of equilibrium in the effective potential $U(r)$.

The solution of Eq. (2.5) has the form of a polynomial of degree $k + 1$ and a definite parity:

$$y_k(\rho) = \sum_{j=0}^{\left[\frac{k+1}{2}\right]} A_j^{(k)} \rho^{k+1-2j}, \tag{2.7}$$

where $[\varkappa]$ is the integral part of the number $\varkappa$. Note that the expansion of the "energy" ε is with respect to not only integral powers $1/n$ but also other quantities — half-integral powers. This follows directly from the relations

$$y(-x, -n^{-1/3}) = -y(x, n^{-1/3}), \quad \varepsilon(-n^{-1/3}) = \varepsilon(n^{1/3}). \tag{2.8}$$

We calculate the coefficients $A_j^{(k)}$, raising the index j successively:

$$A_0^{(k)} = -\frac{1}{2\omega}\left[a_k + \sum_{l=1}^{k-1} A_0^{(k-l)} A_0^{(l)}\right], \quad A_1^{(k)} = -\frac{1}{2\omega}\left[b_k - (k+1)A_0^{(k)} + 2\sum_{l=1}^{k-1} A_1^{(k-l)} A_0^{(l)}\right] \tag{2.9}$$

and for $j \geq 2$

$$A_j^{(k)} = \frac{1}{2\omega}\left[(k + 3 - 2j)A_{j-1}^{(k)} - \sum_{l=1}^{k-1}\sum_{i=0}^{j} A_{j-i}^{(k-l)} A_i^{(l)}\right]. \tag{2.10}$$

*This formula encompasses many physically important examples. Thus, $f(x) = \exp(-x)$ and $x/(e^x - 1)$ correspond to the Yukawa and Hulthén potentials, which are frequently used in nuclear physics, $f(x) = 1 - x^2$ corresponds to the "funnel" potential, which is used to calculate the spectra of quarkonium and multiquark systems [15,16], etc.

For k = 0 we have $A_0^{(0)}=\omega$, $y_0=\omega\rho$, where

$$\omega=x_0^{-2}[h(x_0)/g(x_0)]^{1/3} \tag{2.11}$$

and, by definition,

$$g(x)=f-xf', \quad h(x)=f-xf'-x^2f''. \tag{2.12}$$

The first coefficients in (1.1) are

$$\varepsilon^{(0)}=x^2(f')^2-f^2\equiv g^2-2fg, \quad \varepsilon^{(1)}=g^{1/3}h^{1/3}-g^2 \tag{2.13}$$

(see [2] for the formula for $\varepsilon^{(2)}$), the values of the functions f, g, and h being taken at the point $x = x_0$. Using the recursion relations (2.10) and considering even $k = 2q - 2 = 2, 4, \ldots$ we obtain in the last step the correction to the energy

$$\varepsilon^{(q)}=\nu^2\left[A_{k/2}^{(\cdot)}-\sum_{i=0}^{k/2-1}A_{k/2-i}^{(k-1-2i)}A_{i+1}^{(2i+1)}\right] \tag{2.14}$$

(thus, $\varepsilon^{(2)}=\nu^2\{A_1^{(2)}-[A_1^{(1)}]^2\}$). These equations are very convenient for computer calculations (all the numerical calculations in [1-3] and the present work were made using them). Note that the quantity ω that occurs above has a simple physical meaning – it is the frequency of small vibrations about the equilibrium point $x_0(\nu)$. Indeed, $y_0(\rho) = \omega\rho$ corresponds in an obvious manner to the oscillator wave function: $\chi_0(\rho) = \text{const}\cdot\exp(-\frac{1}{2}\omega\rho^2)$.

3. The 1/n Expansion in the Problem of the Stark Effect. We now use the 1/n expansion to calculate quasistationary states in a system that does not possess spherical symmetry. For the hydrogen atom in a homogeneous electric field $\mathscr{E}$, the variables separate:

$$\psi_{n_1n_2m}(\mathbf{r})=(\xi\eta)^{-1/2}\chi_1(\xi)\chi_2(\eta)\exp(im\varphi),$$

where $\xi = r + z$, $\eta = r - z$; n_1, n_2, m are parabolic quantum numbers, $n = n_1 + n_2 + |m| + 1$. The functions χ_1 and χ_2 satisfy one-dimensional Schrödinger equations [11], in which E/4 plays the part of an energy, and the potentials are $U_1(\xi)$ and $U_2(\eta)$:

$$U_1(\xi)=-\frac{\beta_1}{2\xi}+\frac{m^2-1}{8\xi^2}+\frac{1}{8}\mathscr{E}\xi, \quad U_2(\eta)=-\frac{\beta_2}{2\eta}+\frac{m^2-1}{8\eta^2}-\frac{1}{8}\mathscr{E}\eta. \tag{3.1}$$

We consider the nodeless states with $n_1 = n_2 = 0$, $|m| = n - 1$, for which there are no "radial" excitations (with respect to the variables ξ and η). In the limit $n \to \infty$, the classical equilibrium point (ξ_0, η_0) and the energy E are determined from the system of equations

$$\frac{d}{d\xi}U_1(\xi)=\frac{d}{d\eta}U_2(\eta)=0, \quad U_1(\xi_0)=U_2(\eta_0)=\tfrac{1}{4}E, \quad \beta_1+\beta_2=1 \tag{3.2}$$

(β_1 and β_2 are separation constants).

The direct analysis of this system is rather complicated. We simplify it by using the fact that for $n \gg 1$ Bohr's model of the atom is valid. In the absence of an external electric field, the state (0, 0, m) corresponds to a circular orbit of the electron perpendicular to the z axis. Since the force $F=-\mathscr{E}$ is perpendicular to the velocity, application of an electric field displaces the orbit and changes its radius, but the orbit remains circular. Hence

$$\mathscr{E}=-zr^{-3}, \quad \rho r^{-3}=v^2\rho^{-1}, \quad E=\frac{1}{2}v^2-\frac{1}{r}+\mathscr{E}z, \quad \rho v=m\approx n, \quad \rho=(r^2-z^2)^{1/2} \tag{3.3}$$

(the first two equations correspond to the condition of equilibrium of the forces that act on the electron in its rest frame). Making the scaling

$$\mathbf{r}\to n^2\mathbf{r}, \quad v\to v/n, \quad \varepsilon=2n^2E, \quad F=n^4\mathscr{E} \tag{3.4}$$

and setting $r = u^{-2}$, we arrive at the equation

$$u^4(1-u)^{1/2}=F, \tag{3.5}$$

and

$$\varepsilon^{(0)}=3u^3-4u^2, \quad \varepsilon^{(1)}=u^3[(1+3\sqrt{1-u})^{1/2}+(1-3\sqrt{1-u})^{1/2}-2] \tag{3.6}$$

($u \to 1$ as $F \to 0$).

We obtain the following corrections $\varepsilon^{(k)}$ by means of recursion relations. After the scale transformation (3.4) we obtain the equations

$$\begin{aligned}&\frac{d^2\chi_1}{dx^2}+\frac{n^2}{4}\left(\varepsilon+\frac{4\beta_1}{x}-\frac{1-2/n}{x^2}-Fx\right)\chi_1(x)=0,\\ &\frac{d^2\chi_2}{dy^2}+\frac{n^2}{4}\left(\varepsilon+\frac{4\beta_2}{y}-\frac{1-2/n}{y^2}+Fy\right)\chi_2(y)=0\end{aligned} \tag{3.7}$$

($\xi=n^2x$, $\eta=n^2y$). Setting with allowance for (1.2) $x=x_0(1+\rho n^{-1/2})$ and $y=y_0(1+\sigma n^{-1/2})$ (so that $\langle\rho^2\rangle\sim\langle\sigma^2\rangle\sim 1$ as $n \to \infty$), we obtain

$$\frac{d\varphi_1}{d\rho}-\varphi_1^2=\frac{nx_0}{4}\left(\varepsilon+\frac{4\beta_1}{x}-\frac{1-2/n}{x^2}-Fx\right), \quad \frac{d\varphi_2}{d\sigma}-\varphi_2^2=\frac{ny_0}{4}\left(\varepsilon+\frac{4\beta_2}{y}-\frac{1-2/n}{y^2}+Fy\right), \tag{3.8}$$

where $\varphi_1(\rho)=-\frac{d}{d\rho}\ln\chi_1$, $\varphi_2(\sigma)=-\frac{d}{d\sigma}\ln\chi_2$. We expand the solution of this system in powers of the small parameter $n^{-\frac{1}{2}}$:

$$\varphi_1=\sum_{k=0}^{\infty}n^{-k/2}\varphi_1^{(k)}(\rho), \quad \varphi_2=\sum_{k=0}^{\infty}n^{-k/2}\varphi_2^{(k)}(\sigma), \quad \varepsilon=\sum_{k=0}^{\infty}\varepsilon^{(k)}n^{-k}, \quad \beta_i=\sum_{k=0}^{\infty}\beta_i^{(k)}n^{-k} \quad (i=1,2) \tag{3.9}$$

Substituting these series in (3.8), we obtain in the lowest approximation Eqs. (3.5) and (3.6). From the condition of vanishing of the coefficient of $n^{-k/2}$ we arrive at the chain of equations

$$\frac{d\varphi_1^{(k)}}{d\rho}-\sum_{l=0}^{k}\varphi_1^{(k-l)}\varphi_1^{(l)}=a_1^{(k)}\rho^{k+2}+b_1^{(k)}\rho^k+c_1^{(k)}+(-1)^k x_0\sum_{l=2}^{\left[\frac{k+1}{2}\right]}\beta_1^{(l)}\rho^{k-2l+2}, \tag{3.10}$$

where

$$a_1^{(k)}=(-1)^{k+1}\left(\frac{k+3}{4}-x_0\beta_1^{(0)}\right), \quad b_1^{(k)}=(-1)^k\left(\frac{k+1}{2}+x_0\beta_1^{(1)}\right),$$

$$c_1^{(k)}=\frac{1+(-1)^k}{2}\left(\frac{x_0^2}{4}\varepsilon^{((k+2)/2)}+x_0\beta_1^{((k+2)/2)}\right),$$

and a similar chain for $\varphi_2^{(k)}(\sigma)$, in which $a_2^{(k)}=(-1)^{k+1}\left(\frac{k+3}{4}-y_0\beta_2^{(0)}\right)$, etc. The solutions have the form of the polynomials

$$\varphi_1^{(k)}(\rho)=\sum_{j=0}^{\left[\frac{k+1}{2}\right]}A_j^{(k)}\rho^{k+1-2j}, \quad \varphi_2^{(k)}(\sigma)=\sum_{j=0}^{\left[\frac{k+1}{2}\right]}B_j^{(k)}\sigma^{k+1-2j},$$

where $A_0^{(0)}=\omega_1$ and $B_0^{(0)}=\omega_2$. We finally arrive at the recursion relations

$$\begin{aligned}&A_0^{(k)}=-\frac{1}{2\omega_1}\left[a_1^{(k)}+\sum_{l=1}^{k-1}A_0^{(k-l)}A_0^{(l)}\right], \quad A_1^{(k)}=-\frac{1}{2\omega_1}\left[b_1^{(k)}-(k+1)A_0^{(k)}+2\sum_{l=1}^{k-1}A_1^{(k-l)}A_0^{(l)}\right],\\ &A_j^{(k)}=-\frac{1}{2\omega_1}\left[(-1)^k\beta_1^{(j)}x_0-(k+3-2j)A_{j-1}^{(k)}+\sum_{l=1}^{k-1}\sum_{i=0}^{j}A_{j-i}^{(k-l)}A_i^{(l)}\right]\end{aligned} \tag{3.11}$$

($1 < j \leq (k+1)/2$) and similar relations for $B_j^{(k)}$. If $k = 2q-2$ is even, then the terms in (3.10) that do not contain the variables ρ and σ determine the correction of order n^{-q} in (1.1) and in the corresponding expansion for the separation constant

$$\varepsilon^{(q)}=\frac{4}{x_0y_0(x_0+y_0)}(y_0\tilde{A}_q+x_0\tilde{B}_q), \quad \beta_1^{(q)}=\frac{1}{x_0y_0(x_0-y_0)}(y_0^2\tilde{A}_q-x_0^2\tilde{B}_q), \tag{3.12}$$

where for $q = (k+2)/2 = 2, 3, \ldots$

$$A_q = A_{k/2}^{(k)} - \sum_{j=0}^{k/2-1} A_{k/2-j}^{(k-1-2j)} A_{j+1}^{(2j+1)}, \tag{3.13}$$

and there is a similar formula for $\bar{B}_q$. This completes the calculation of the coefficient $\varepsilon^{(q)}$ in the 1/n expansion.

It remains for us to give the definition of some of the quantities that occur in the previous equations*:

$$x_0 = \frac{1}{u^2}(1-\sqrt{1-u}), \quad y_0 = \frac{1}{u^2}(1+\sqrt{1-u}),$$

$$\omega_1 = (1+3\tau)^{1/2}/2(1+\tau), \quad \omega_2 = (1-3\tau)^{1/2}/2(1-\tau), \quad \beta_{1,2}^{(0)} = {}^1/_2 \pm {}^1/_4(\tau - 3\tau^3), \tag{3.14}$$

$$\beta_1^{(1)} = -\beta_2^{(1)} = {}^1/_4(1-\tau^2)[(1+\tau)(1+3\tau)^{1/2} - (1-\tau)(1-3\tau)^{1/2} - 4\tau],$$

where $\tau = \sqrt{1-u}$. The variable τ is somewhat more convenient than u, and the substitution $\tau \to -\tau$ corresponds to the index interchange $1 \rightleftarrows 2$ in Eqs. (3.7). At the same time, the formulas simplify; thus, Eq. (3.5) takes the form $\tau(1-\tau^2)^4 = F$.

Hitherto we have assumed $n_1 = n_2 = 0$. Expansions of the type (1.1) can also be obtained for other states if $n_1, n_2 \ll n$. For example, the first-order correction is

$$\varepsilon^{(1)} = (1-\tau^2)^3[(2n_1+1)(1+3\tau)^{1/2} + (2n_2+1)(1-3\tau)^{1/2} - 2], \tag{3.15}$$

and for spherically symmetric potentials

$$\varepsilon^{(1)} = [(2n-2l-1)(h/g)^{1/2} - 1]g^2 \tag{3.16}$$

(cf. (2.13)). It is convenient to calculate $\varepsilon^{(k)}$ for $k \geq 2$ for states with arbitrary quantum numbers in a somewhat different way.

4. The 1/n Expansion for States with Nodes. We obtain the recursion relation for the components $C_p^{(k)}$ of the wave function in the basis of eigenfunctions of the harmonic oscillator. As expansion parameter, we choose in place of $1/n = (l+1)^{-1}$ the more general quantity $1/\Lambda$, and

$$l(l+1) = \Lambda^2 + A\Lambda + B, \tag{4.1}$$

where A and B are certain constants.†

We make a linear change of the variable $x = \mu r = x_0 + \Lambda^{-1/2}\rho$ and write the Schrödinger equation in the form

$$\left[-\frac{1}{2\Lambda}\frac{d^2}{d\rho^2} + v^{-1}v(x) - \frac{1}{2x^2}\left(1 + \frac{A}{\Lambda} + \frac{B}{\Lambda^2}\right) + \frac{\varepsilon}{2v^2}\right]\chi = 0, \tag{4.2}$$

where $\varepsilon = 2\Lambda^2 E$, $v = \Lambda^2\mu$, and v(x) and x_0 are determined in the same way as in Sec. 2.

Substituting in (4.1) the expansions (2.4) for v(x) and x^{-2}, we obtain the equation

$$\left[-\frac{1}{2}\frac{d^2}{d\rho^2} + \frac{\omega^2}{2}\rho^2 + \sum_{k=1}^{\infty} V^{(k)}(\rho)\Lambda^{-k/2} - W\right]\chi = 0, \tag{4.2a}$$

where

$$V^{(k)}(\rho) = -{}^1/_2 a_k \rho^{k+2} + {}^1/_2 A b_k \rho^k + {}^1/_2 B b_{k-2}\rho^{k-2}, \quad W = \frac{\varepsilon\Lambda}{2v^2} + \frac{\Lambda}{2}a_{-2} - \frac{1}{2}Ab_0, \tag{4.2b}$$

and ω, a_k, and b_k are determined by the same formulas as in Sec. 2.

In the limit $\Lambda \to \infty$, (4.2a) reduces to the equation for a harmonic oscillator with frequency ω. In this limit, $W = W^{(0)} = (n_r + {}^1/_2)\omega$, where $n_r = n - l - 1$ is the number of nodes of the radial wave function; this number is assumed to be fixed.

---

*Note that ω_1 and ω_2 are the frequencies of small vibrations about the equilibrium points x_0 and y_0 in the effective potentials (3.1).

†This relation is satisfied, for example, in the cases $\Lambda = l + c$ ($A = 1 - 2c$, $B = c^2 - c$) and $\Lambda = [l(l+1)]^{1/2}$ ($A = B = 0$).

To solve (4.2a) by perturbation theory, we expand W and χ in powers of the parameter $\Lambda^{-\frac{1}{2}}$:

$$W=\sum_{k=0}^{\infty}\Lambda^{-k/2}W^{(k)},\quad \chi=\sum_{k=0}^{\infty}\Lambda^{-k/2}\chi^{(k)}. \tag{4.3}$$

Substituting the expansions (4.3) in (4.2) and equating to zero the coefficients of equal powers of $\Lambda^{-\frac{1}{2}}$, we obtain an inhomogeneous equation for determining $\chi^{(k)}$:

$$\left(-\frac{1}{2}\frac{d^2}{d\rho^2}+\frac{\omega^2}{2}\rho^2-W^{(0)}\right)\chi^{(k)}=\sum_{i=1}^{k}(W^{(i)}-V^{(k)})\chi^{(k-i)}. \tag{4.4}$$

We shall seek the correction to the wave function in the form of an expansion with respect to the complete system of eigenfunctions χ_p of the harmonic oscillator:

$$\chi^{(k)}=\sum_{p=0}^{\infty}C_p^{(k)}\chi_p \tag{4.5}$$

(the normalization condition is $C_p^{(0)}=\delta_{p,\,n_r}$, $C_{n_r}^{(k)}=\delta_{k0}$).

We describe the algorithm for finding $W^{(k)}$ and $C_p{}^{(k)}$. To find the coefficients $C_p{}^{(k)}$, we write Eq. (4.4) in matrix form in the basis $\{\chi_p\}$:

$$(p-n_r)\,\omega C_p^{(k)}=\sum_{i=1}^{k}\sum_{q=0}^{\infty}(\delta_{pq}W^{(i)}-V_{pq}^{(i)})\,C_q^{(k-i)}, \tag{4.6}$$

where by $V_{pq}^{(i)}$ we denote the matrix elements of the operator $V^{(i)}$.

The right-hand side of Eq. (4.6) contains the already known quantities $W^{(k')}$, $C_q^{(k')}$ with $k' < k$ and the matrix elements $V_{pq}^{(i)}$ for $i \leq k$, which can be expressed in accordance with (4.2b) in terms of the matrix elements of the coordinate operator. To determine the unknown quantity $W^{(k)}$, which occurs on the right-hand side of (4.6), we use the equation obtained from (4.6) for $p = n_r$,

$$W^{(k)}-V_{n_r,\,n_r}^{(k)}+\sum_{i=0}^{k-1}\sum_{q=0}^{\infty}(\delta_{n_r,\,q}W^{(i)}-V_{n_r,\,q}^{(i)})\,C_q^{(k-i)}=0. \tag{4.7}$$

With allowance for (4.7), $W^{(k)}$ can be expressed in terms of the coefficients $W^{(i)}$ and $C_q{}^{(i)}$ of lower order. Since $V_{pq}^{(i)}=0$ under the condition $|p-q| > i+2$, the sum over q in (4.6) and (4.7) is finite. By induction, using (4.6), we can also show that $C_p{}^{(k)}=0$ for $|p-n_r| > 3k$, and therefore the sum (4.5) is also finite. Thus, the perturbation-theory corrections of any order can be expressed in the form of analytic expressions containing a finite number of terms.

Note that Eq. (4.2) goes over after simultaneous replacement of the parameter $\Lambda^{-\frac{1}{2}}$ by $-\Lambda^{-\frac{1}{2}}$ and $\chi(\rho)$ by $\chi(-\rho)$ into an equation equivalent to (4.2), this being obtained from (4.2) after the substitution $\rho \to -\rho$. Therefore, on the substitution $\Lambda^{-\frac{1}{2}} \to -\Lambda^{-\frac{1}{2}}$ the wave function $\chi(\rho)$ goes over into $\chi(-\rho)$, while the eigenvalue W remains unchanged, i.e., is an even function of the parameter $\Lambda^{-\frac{1}{2}}$. Therefore, the expansion of the energy contains only even powers of Λ:

$$\varepsilon=\sum_{k=0}^{\infty}\tilde{\varepsilon}^{(k)}\Lambda^{-k}, \tag{4.8}$$

where $\tilde{\varepsilon}^{(0)}=-\nu^2a_{-2}$, $\tilde{\varepsilon}^{(1)}=2\nu^2W^{(0)}+\nu^2Ab_0$, $\tilde{\varepsilon}^{(k)}=2\nu^2W^{(k-2)}$ for $k \geq 2$.

5. Turning to definite examples, we begin with the Yukawa potential, for which $f(x) = \exp(-x)$ in (2.3). In this case [3]

$$\varepsilon^{(0)}=(x^2-1)e^{-2x},\quad \nu=(x^2+x)e^{-x},\quad \varepsilon^{(1)}=-(x+1)^2\left[1-\left(1-\frac{x^2}{x+1}\right)^{1/2}\right]e^{-2x}, \tag{5.1}$$

$$\varepsilon^{(2)}=\left(1-\frac{x^2}{x+1}\right)^{-2}\left[\frac{1}{2}(3+3x-x^3)(1+x)^{1/2}(1+x-x^2)^{1/2}-\right.$$

TABLE 1

ν	$l=3$	$l=10$	$l=30$
0,5	−0,243206 то же	−0,230412 −0,2304119	−0,225541 −0,225542
ν_{cr}	−0,036872 −0,036871	−0,014040 −0,0140396	−0,00507 −0,0050673
1,25	0,10917−i0.12189 то же	0,1541−i0,1343 0,154112−i0,134273	0,1714−i0,1377 0,171423−i0,137681

Note. Here, $\varepsilon_{n\ell} = 2n^2E_{n\ell}$, $E_{n\ell}$ is the energy of the level $\ell = n - 1$; the value $\nu_{cr} = 0.735\,758...$ corresponds to $\varepsilon^{(0)}=0$, i.e., entry into the continuum of the states with $n \to \infty$.

TABLE 2

l	$n_r=0$	$n_r=1$	$n_r=2$	$n_r=3$	$n_r=4$
1	220,2	112,7	67,89	45,19	32,17
2	91,34	58,11	40,03	29,17	22,161
3	49,831	35,3894	26,3507	20,3422	16,1565
4	31,3436	23,79911	18,64622	14,98086	12,28614
5	21,5246	17,095136	13,883520	11,485754	9,651169
6	15,69109	12,871464	10,736148	9,082952	7,778558
7	11,94453	10,039759	8,548708	7,361194	6,401072
8	9,396001	8,049286	6,967264	6,085773	6,358781
9	7,584126	6,597033	5,787098	5,114915	4,551345
10	6,250053	5,505091	4,883140	4,358925	3,913274
11	5,239411	4,663419	4,175494	3,758824	3,400377
12	4,455497	4,000992	3,611188	3,274549	2,981971
13	3,835226	3,470302	3,153976	2,878120	2,636219
14	3,336024	3,308601	2,778385	2,549519	2,347238
15	2,928314	2,682716	2,466087	2,274117	2,103259

Note. We have given the critical values of the screening parameters $\mu_{cr}(n, \ell)$ for the Yukawa potential multiplied by 10^3; $n_r = n - \ell - 1$.

$$\frac{1}{72}(x^6 + 19{,}5x^5 - 48x^4 - 102x^3 + 54x^2 + 216x + 108)\Big] e^{-2x},$$

and the following coefficients $\varepsilon^{(k)}(\nu)$ can be readily calculated on a computer if the recursion relations from Sec. 2 are used.

Note that for $x = 1$ we have $\varepsilon^{(0)}=0$ and $\nu = 2e^{-1} = 0.735\,758...$, this corresponding to a "critical" value of the parameter ν for $n \to \infty$. For $x = x_* = (1 + \sqrt{5})/2$, $\nu = \nu_* = 0.839\,962...$ there is a "collision" of the two classical solutions, after which the equilibrium point $x_0 = \mu r_0$ enters the complex plane, and $\varepsilon^{(k)}$ acquires an imaginary part. Such a solution obviously loses its meaning in classical mechanics, but in the quantum case it determines the position and width of the Breit–Wigner resonances with $\ell \sim n \gg 1$ (for $\nu > \nu_*$) (a similar phenomenon occurs for other screened potentials (2.3), for example, for the Hulthén potential [2]).

With increasing k, the coefficients in (1.1) initially decrease, but then, for $k \gtrsim 10$, begin to increase rapidly. Already five or six terms of the 1/n expansion determine the energy to accuracy 10^{-5}, although overall the series (1.1) is evidently only asymptotic (for more details, see [2]). For the results of the calculations, see Table 1, in which we give the "reduced" energy $\varepsilon_{n\ell} = 2n^2E_{n\ell}$ for several characteristic values of the screening parameter μ (Yukawa potential). The upper row for given ℓ and $\nu = n^2\mu$ corresponds to summation of the (divergent) perturbation-theory series [17], and the lower row corresponds to the 1/n expansion. The agreement between the two methods is very good.

A question of independent interest is the calculation of the critical screening parameter, at which the level energy becomes zero. By analogy with (4.8), we shall seek μ_{cr} in the form of the expansion [18]

TABLE 3

L	$F=0.25$	
	$n=1$	$n=5$
1	1,1575 + i0,1047	1.111152 + i4.548436(−2)
2	1,1724 + i0,1367	1.111958 + i4,833566(−2)
5	1,1768 + i0,1639	1,111586 + i4.917573(−2)
10	1,1745 + i0,1702	1,111534 + i4,916391(−2)
12	1,1741 + i0,1706	1,111534 + i4,916261(−2)
14	1,1738 + i0,1708	1,111534 + i4.916228(−2)
16	1.1737 + i0,1708	1,111535 + i4.916222(−2)
18	the same	the same

L	$F=1.0$	
	$n=1$	$n=5$
1	1,26141 + i1,28643	1,282988 + i7,449322(−1)
2	1,23175 + i1,28946	1,282600 + i7,449273(−1)
5	1,23502 + i1,28587	1,282607 + i7,449231(−1)
10	1,23511 + i1,28577	to the
12	1,23510 + i1,28577	» »
14	1,23510 + i1,28577	» »
16	the same	» »
18	» »	» »

Note. We have given (with sign reverse) the values of the diagonal Padé approximants [L/L] (1/n). The data relate to the levels $|0, 0, n-1\rangle$, where n is the principal quantum number.

$$\mu_{cr}(n, l) = \Lambda^{-2}\nu_{cr} = \sum_{k=0}^{\infty} \nu_{cr}^{(k)}\Lambda^{-(k+2)}. \tag{5.2}$$

From the condition $\varepsilon = \sum_{k=0}^{\infty} \varepsilon^{(k)}\Lambda^{-k} = 0$ (for $\nu = \nu_{cr}$) we find $\nu_{cr}^{(0)} = \nu_{cr}(n\to\infty) = 2e^{-1}$, and $\nu_{cr}^{(k)}$ for $k \geq 1$ can be expressed in terms of the coefficients $\nu_{cr}^{(i)}$ with $i < k$ if one solves the equation, linear in $\nu_{cr}^{(k)}$, which follows from the condition $\varepsilon^{(k)} = 0$.

We give the final formula, which includes six terms of the expansion (5.2) in the case $\Lambda = [l(l+1)]^{\frac{1}{2}}$:

$$\nu_{cr}(n, l) = 2e^{-1}\left[1 - 2^{1/6}\beta\Lambda^{-1} + \left(\frac{35}{24}\beta^2 - \frac{47}{288}\right)\Lambda^{-2} - \right.$$

$$\frac{\beta}{2^{17/2}3^3}(12\,788\beta^2 - 3\,385)\Lambda^{-3} + \frac{1}{2^{15}3^65^2}(645\,792\,720\beta^4 - 284\,523\,960\beta^2 + 17\,520\,481)\Lambda^{-4} -$$

$$\left.\frac{\beta}{2^{39/2}3^75^2}(32\,292\,401\,104\beta^4 - 21\,674\,608\,440\beta^2 + 3\,494\,487\,713)\Lambda^{-5} + \ldots\right], \tag{5.3}$$

where $\beta = n - l - \frac{1}{2}$.

Note that by differentiating (4.8) term by term with respect to the variable ν for $\nu = \nu_{cr}$ we can also expand in a series the derivative of the energy with respect to μ at $\mu = \mu_{cr}$, i.e., the slope of the level when it enters the continuum:

$$\frac{d}{d\mu}E\Big|_{\mu=\mu_{cr}} = e^{-1}(1 - 3\cdot 2^{-1/6}\beta\Lambda^{-1} + \ldots). \tag{5.4}$$

The states with $l = n - 1$ have nodeless radial functions concentrated in the neighborhood of the minimum of the effective potential. For them, the quantum corrections $\nu_{cr}^{(k)}$ take the values with the smallest modulus, and the sum of the five terms of the series (5.2) approximates $\mu_{cr}(n, l)$ for all $l > 0$ with a relative error less than 0.03%. The values of these partial sums are given in the second column of Table 2. For $n_r \geq 1$, the partial sums of the series (5.3) oscillate around the limiting value and for $l \leq n_r$ no longer give a satisfactory approximation to μ_{cr}, although the Padé approximants appreciably improve the convergence of the approximations. In the last four columns of Table 2 we give

the values of μ_{cr} obtained using the Padé approximants [5/4] and [5/5] (only their common decimal places are given; in fact for $\ell > 7$ the accuracy of the calculations is an order of magnitude higher than is indicated in Table 2). For the n and ℓ for which comparison with the previous calculations is possible the obtained values of μ_{cr} agree with the results of [19-22], and for $\ell = n - 1$ they agree with those of [17].

The "funnel" potential $V(r) = -r^{-1} + gr$ is often used to describe the spectra of multiquark systems [15,16,23]. In this case $\mu = g^{\frac{1}{2}}$, $v(x) = f(x)/x = x^{-1} - x$, and the coefficients $\varepsilon^{(k)}$ can be expressed in terms of elementary functions [2]. The results of calculation are given in [3] (the same values of the parameters as were used in [16] for four-quark states were taken). At the same time, use was made of the fact that the scaling transformation $r \to \rho = \alpha r$ in the Schrödinger equation reduces the "funnel" potential to the standard form [15]

$$\left[\frac{d^2}{d\rho^2} + \frac{\lambda}{\rho} - \rho - \frac{l(l+1)}{\rho^2} + \zeta\right]\chi = 0, \tag{5.5}$$

from which the eigenvalues $\zeta = \zeta_{n\ell}(\lambda)$, where λ is the Coulomb parameter, are determined. The calculations show that when $\ell \geq 3$ already three terms of the 1/n expansion ensure an accuracy of order 10^{-4} in the energy. At the same time, the 1/n expansion converges more rapidly the larger n and ℓ, whereas the accuracy of the numerical solution of the Schrödinger equation decreases with increasing ℓ.

As a last example, we consider the Stark effect in the hydrogen atom. Using the recursion relations of Sec. 3, we calculated the coefficients $\varepsilon^{(k)}$, after which we summed the 1/n expansion by means of Padé approximants [L/L](1/n), see [24]. This made it possible to calculate the "reduced" energy $\varepsilon_n = 2n^2(e_0 - i\Gamma/2)$ of the quasistationary states into which the states $|n_1 n_2 m\rangle$ of the discrete spectrum pass when an electric field $\mathscr{E}$ is applied. To obtain five stable figures in ε_n it was sufficient to take $L \sim 15$, i.e., about 30 terms of the 1/n expansion (3.9) (see Table 3, which illustrates the convergence of the 1/n expansion for the energy of the states $|0, 0, n-1\rangle$). Note that the 1/n expansion is particularly helpful in the region of strong fields ($F = n^4\mathscr{E} \geq 0.25$) and for Rydberg ($n \gg 1$) states (for more detail, see [25]).

For the other examples (Yukawa and "funnel" potentials) the convergence of the 1/n expansion is similar. It would be interesting to obtain theoretical estimates of the convergence (or asymptoticity) of the expansion (1.1). We hope to return to this question in the future.

6. Thus, the 1/n expansion is an effective approximate method of calculating energy eigenvalues. However, it does not work near the point of collision of classical solutions ($\nu = \nu_*$) since the coefficients $\varepsilon^{(k)}$ have there a singularity, and for $k \geq 2$ they become infinite.* For a different choice of the expansion parameter in (4.8), we shall have

$$\frac{1}{\Lambda} = \frac{1}{n} + \frac{A+1}{2n^2} + \frac{(A+1)(A+3)+4B}{8n^3} + \ldots, \tag{6.1}$$

with $\varepsilon^{(0)} \equiv \bar{\varepsilon}^{(0)}$, and $\varepsilon^{(k)}$ and $\bar{\varepsilon}^{(k)}$ with $k \geq 1$ differ. All the $\varepsilon^{(k)}$ have a singularity at $\nu = \nu_*$, while the singularity of $\bar{\varepsilon}^{(k)}$ is at the point $\bar{\nu}_* = (\Lambda/n)^2\nu_*$, which for finite n is displaced relative to ν_*. This makes it possible to sum the series (4.8) at $\nu = \nu_*$. Thus, choosing $\Lambda = [\ell(\ell+1)]^{\frac{1}{2}}$, we obtain for the Yukawa potential

$$E = \begin{cases} -0.00181, & l = 1, \\ (6.1 - i\cdot 0.3)\cdot 10^{-4}, & l = 3, \\ (5.47 - i\cdot 0.22)\cdot 10^{-4}, & l = 4, \\ (2.219 - i\cdot 0.054)\cdot 10^{-4}, & l = 9 \end{cases}$$

(here $\ell = n - 1$, $\nu = \nu_* = 0.8399\ldots$). This simple device makes it possible to use the 1/n expansion in the region $\nu \approx \nu_*$ as well.

*This follows from the recursion relations (2.9)-(2.14) if one bears in mind that in the limit $\nu \to \nu_*$ the vibration frequency $\omega \sim (\nu_* - \nu)^{\frac{1}{2}} \to 0$. In the case of the Stark effect, the collision point corresponds to a field $F = F_* = 2^{12}\cdot 3^{-9} = 0.2081$; at the same time, the frequency ω_1 remains finite while $\omega_2 \propto (F_* - F)^{1/4} \to 0$.

LITERATURE CITED

1. V. S. Popov, V. M. Vainberg, and V. D. Mur, Pis'ma Zh. Eksp. Teor. Fiz., 41, 439 (1985).
2. V. S. Popov, V. M. Vainberg, and V. D. Mur, "Classical mechanics and the 1/n expansion," Preprint No. 178 [in Russian], Institute of Theoretical and Experimental Physics, Moscow (1985); "The 1/n expansion in quantum mechanics," Preprint No. 69 [in Russian], Institute of Theoretical and Experimental Physics, Moscow (1986).
3. V. S. Popov, V. M. Vainberg, and V. D. Mur, Yad. Fiz., 44, 1103 (1986).
4. A. D. Dolgov and V. S. Popov, Phys. Lett. B, 86, 185 (1979).
5. A. D. Dolgov, V. L. Eletskii, and V. S. Popov, "The anharmonic oscillator: Perturbation theory, semiclassical treatment, the Padé method," Preprint No. 72 [in Russian], Institute of Theoretical and Experimental Physics, Moscow (1979).
6. L. D. Mlodinov and N. Papanicolaou, Ann. Phys. (N.Y.), 128, 314 (1980).
7. C. M. Bender, L. D. Mlodinov, and N. Papanicolaou, Phys. Rev. A, 25, 1305 (1982).
8. U. Sukhatme and T. Imbo, Phys. Rev. D, 28, 418 (1983).
9. L. G. Yaffe, Phys. Today, 8, 50 (1983).
10. R. F. Stebbings and F. B. Dunning (eds.), Rydberg States of Atoms and Molecules, Cambridge University Press (1983).
11. L. D. Landau and E. M. Lifshitz, Quantum Mechanics: Nonrelativistic Theory, 2nd ed., Pergamon Press, Oxford (1965).
12. A. D. Dolgov and V. S. Popov, Phys. Lett. B, 79, 403 (1978); Zh. Eksp. Teor. Fiz., 75, 2010 (1978); 79, 1704 (1980).
13. Y. Aharonov and C. K. Au, Phys. Rev. Lett., 42, 1582 (1979); Phys. Rev. A, 20, 2245 (1979).
14. A. V. Turbiner, Zh. Eksp. Teor. Fiz., 79, 1719 (1980); Usp. Fiz. Nauk, 144, 35 (1984).
15. E. Eichen, K. Gottfried, et al., Phys. Rev. D, 17, 3090 (1978).
16. A. M. Badalyan, B. L. Ioffe, and A. V. Smilga, Nucl. Phys. B, 281, 85 (1987).
17. V. M. Vainberg and V. S. Popov, "Logarithmic perturbation theory for the screened Coulomb potential," Preprint No. 171 [in Russian], Institute of Theoretical and Experimental Physics, Moscow (1980); Dokl. Akad. Nauk SSSR, 272, 335 (1983).
18. A. V. Sergeev, Methods of Atomic Calculations [in Russian], Nauka, Moscow (1983), p. 149.
19. F. J. Rogers, H. C. Graboske, and D. J. Harwood, Phys. Rev. A, 1, 1577 (1970).
20. R. N. Kesarwani and Y. P. Varshni, J. Math. Phys., 19, 819 (1978).
21. D. Singh and Y. P. Varshni, Phys. Rev. A, 29, 2895 (1984).
22. A. V. Sergeev and A. I. Sherstyuk, Zh. Eksp. Teor. Fiz., 82, 1070 (1982).
23. A. A. Bykov, I. M. Dremin, and A. V. Leonidov, Usp. Fiz. Nauk, 143, 3 (1984).
24. J. Baker and P. Graves-Morris, Padé Approximation [Russian translation], Mir, Moscow (1986).
25. V. M. Vainberg, V. D. Mur, V. S. Popov, and A. V. Sergeev, Pis'ma Zh. Eksp. Teor. Fiz., 44, 9 (1986).